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FUNCTION AND VARIABILITY OF METABOLIC NETWORKS

 $\mathbf{B}\mathbf{Y}$

KEITH DUFAULT-THOMPSON

A DISSERTATION SUBMITTED IN PARTIAL FULFILLMENT OF THE

REQUIREMENTS FOR THE DEGREE OF

DOCTOR OF PHILOSOPHY

IN

CELL AND MOLECULAR BIOLOGY

UNIVERSITY OF RHODE ISLAND

DOCTOR OF PHILOSOPHY DISSERTATION

OF

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ABSTRACT

The study of bacterial growth has highlighted the importance of metabolism in how microorganisms have evolved and how they survive in different conditions. The introduction of next-generation sequencing methods has allowed for the study of metabolism in new ways by predicting metabolic phenotypes based on gene annotations. The development of GEnome-scale models (GEMs) of metabolism from these annotations has provided another method to investigate microbial metabolism. An overview of GEM development and simulation methods is provided in Appendix I.

In Manuscript I, a GEM was developed for the psychrotolerant, piezotolerant, deep-sea bacteria *Shewanella piezotolerans* WP3. Despite the broad differences in environmental adaptations across the *Shewanella* genus, the WP3 model provided evidence of conserved energy production strategies that may contribute to these organisms' ability to survive in a broad range of environments. This model's application to study energy metabolism in WP3 demonstrated the utility of these models in the study of non-model organisms.

The mechanisms of environmental adaptation were further explored in Manuscript II, where a GEM of the psychrotolerant, deep-sea bacteria *Shewanella psychrophila* WP2, was used to investigate metabolic changes that occur during acclimation to different growth temperatures. This study combined transcriptomic analysis with an integrated modeling approach to provide a complete illustration of the changes that occur in various metabolic pathways at different temperatures. WP2 exhibited many of the common transcriptional responses to temperature seen in other psychrophiles, and simulations with the GEM illustrated how these changes resulted in changes in energy and biomass production efficiency at non-optimal temperatures.

In Manuscript III, the concept of using metabolic reconstructions to study metabolism was extended from single organisms to the prokaryotic tree of life. In this study, the metabolic pathways of all prokaryotic organisms in the Kyoto Encyclopedia of Genes and Genomes (KEGG) database were analyzed as mathematical networks. Previously used network representation methods were compared to a new type of network generated through the use of the FindPrimaryPairs algorithm. The application of this algorithm provided insights into the influence of carbon, nitrogen, and phosphorus transfers in the metabolism. Further network analyses using networks generated from published GEMs also highlighted differences in the structure of core metabolic pathways required for growth versus non-essential pathways.

In conclusion, these studies have highlighted the use of GEMs and metabolic networks in the study of metabolism. The studies revealed metabolic features that play critical roles in the adaptations of *Shewanella* to different environments and may have broader implications for other deep-sea microorganisms. The broader context of metabolism structures across prokaryotes provided through a network-based approach shows promise in advancing the understanding of how metabolic pathways are organized and evolved.

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I thank my parents Amy and Sean for all of their support and guidance throughout the years, and I couldn't be where I am now without them. For my brother Ryan, I would like to thank him for always being a happy distraction when I needed it the most. Most of all, I'd like to thank my wonderful wife, Elizabeth, for always being there for me supporting me while I pursue my dreams.

PREFACE

This dissertation has been prepared in the manuscript format following the guidelines established by the Graduate School of the University of Rhode Island. Manuscript 1, "Genome-Scale Model of Shewanella piezotolerans Simulates Mechanisms of Metabolic Diversity and Energy Conservation", was published in mSystems in 2017, and involves the development and application of a Genome-scale model of metabolism to study the energy metabolism of the bacterium Shewanella piezotolerans WP3. Manuscript 2, "Reconstruction and analysis of a thermodynamically constrained metabolic models reveal mechanisms of metabolic remodeling under temperature perturbations of a deep-sea bacterium", is formatted for and will be submitted to PLOS Computational Biology and explores the metabolic responses of the deep sea piezophile, Shewanella psychrophila WP2, during acclimation to different growth temperatures. Manuscript 3, "Investigation of the Structure of Element Transfer Networks within Metabolism", is formatted for publication and will be submitted to Nature Communications and explores different ways to represent metabolism as mathematical networks. A summary of the overall conclusions and future directions for this work is provided in the Conclusions chapter. Appendix I contains an overview of Genome-scale model development and metabolic simulation methods.

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Introduction

Metabolism is a central component of biological sciences, influencing how they grow, survive in different conditions, and interact with other organisms. In total, the metabolism of an organism is made up of metabolic pathways consisting of individual reactions which an organism can use to consume and break down nutrients from the environment and convert them into energy, cellular biomass, and other products. In this dissertation, microbial metabolism is examined using a variety of approaches and from different perspectives. These studies highlight how the use of different methods to study metabolism can allow for the study of complex metabolic processes in organisms from traditionally difficult to study environments like the deep-sea. They also demonstrate that approaching metabolism from different perspectives can lead to new views that would be missed if the picture of metabolism was limited to what has been described in the textbook examples of metabolic pathways.

Up until recently the study of microbial metabolism has been limited to model organisms and culturing-based techniques, leading to a deep understanding of metabolism in these systems, but also to a limited view of the broader metabolic landscape. Before DNA and RNA sequencing methods became available, metabolism was mostly studied through culture-based methods where the response of an organism to the addition or loss of nutrients could be closely monitored in a controlled laboratory environment. While these methods provided a wealth of physiological information and set up the foundation of how metabolism is looked at up to modern times, they were limited in scope because only certain organisms like *Escherichia coli*

and *Saccharomyces cerevisiae* could be efficiently grown and studied in the laboratory [1–4]. The advancement of DNA sequencing technology in the late 20th century has expanded the view of metabolism from the small subset of model organisms to a wide range of organisms from different environments and from across the tree of life through genome sequencing [5]. The study of these genomes through gene annotation and comparative genomic analyses has allowed for the prediction of metabolic functions based on what genes are present in different genomes. These analyses have revealed an extreme degree of variation in metabolic pathways with even core metabolic pathways like glycolysis and the citric acid cycle having many different variations across the tree of life [6–8]. Genome sequencing and analysis alone provides a way to predict the metabolic potential of an organism, but recently using genome sequences to develop Genome-Scale Models (GEMs) of metabolism has become a popular method to extend functional predictions to simulations of growth.

GEMs have become increasingly popular tools to study the metabolism of organisms from all environments. These GEMs are computational representations of the metabolic functions of an organism based on their gene content and can be used to perform simulations of how an organism would grow and what pathways and reactions it would use. Modeling of metabolism started with the development of models for well-studied organisms like *E. coli [9]*, but since then GEMs have been developed and applied to organisms from all three domains of life and from a wide range of environments [10–12]. A major benefit of using GEMs in the study of metabolism has been in their application to non-model organisms. The development of GEMs for difficult to culture organisms has allowed for the prediction of the

metabolic phenotypes of these organisms providing insights into their evolution and ecological importance [13–15]. These models have also provided a new way to look at metabolism, with simulations showing how different metabolic pathways do not function in isolation but instead are connected at a genome-scale.

In this dissertation Genome-scale modeling of metabolism is applied to look at the metabolism of microorganisms from different perspectives. In Manuscript 1, "Genome-Scale Model of Shewanella piezotolerans Simulates Mechanisms of Metabolic Diversity and Energy Conservation", a GEM of the deep-sea bacteria Shewanella piezotolerans WP3 was developed and used to simulate its growth on different substrates. Through different modeling approaches the connections between carbon and energy metabolism in S. piezotolernas WP3 were studied, demonstrating the interdependence of different pathways and the importance of the global energy balancing mechanisms in the organism. In Manuscript II, "Metabolic Variations During Acclimation to Different Temperatures-a Case Study in the Psychrophilic Bacteria, Shewanella psychrophila WP2", the genome-scale modeling methods were extended to incorporate transcriptomic and thermodynamic data during the simulation of the growth of *Shewanella psychrophila* WP2 at different temperatures. This study highlights the importance of approaching metabolism from different perspectives, demonstrating the importance of an integrated view of metabolic changes at different growth temperatures. Lastly in Manuscript III, "Investigation of the Structure of Element Transfer Networks within Metabolism", metabolism is approached from a different perspective as a mathematical network. This study highlights the implications of using different network representation methods on how metabolic networks are

understood and interpreted. The continued application of the methods presented in these studies and others like them promises to advance the study of metabolism and continue to provide new ways to look at this central component of growth and evolution.

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Manuscript I

Publication Status: Published in mSystems, 2017

Title: Genome-Scale Model of *Shewanella piezotolerans* Simulates Mechanisms of Metabolic Diversity and Energy Conservation

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ABSTRACT

Shewanella piezotolerans WP3 (WP3) belongs to the Group 1 branch of the Shewanella genus and is a piezotolerant and psychrotolerant species isolated from the deep sea. In this study, a genome-scale model was constructed for WP3 using a combination of genome annotation, ortholog mapping, and physiological verification. The metabolic reconstruction contained 806 genes, 653 metabolites, and 922 reactions, including central metabolic functions that represented non-homologous replacements between the Group 1 and Group 2 Shewanella. Metabolic simulations with the WP3 model demonstrated consistency with existing knowledge about the physiology of the organism. A comparison of model simulations with experimental measurements verified the predicted growth profiles under increasing concentration of carbon sources. The WP3 model was applied to study mechanisms of anaerobic respiration through investigating energy conservation, redox balancing, and the generation of proton motive force. Despite being an obligate respiratory organism, WP3 was predicted to use substrate-level phosphorylation as the primary source of energy conservation in anaerobic conditions, a trait previously identified in other Shewanella species. Further investigation of the ATP synthase activity revealed a positive correlation between the availability of reducing equivalents in the cell and the directionality of ATP synthase reaction flux. Comparing the WP3 model with an existing model of a Group 2 species, S. oneidensis MR-1, revealed that the WP3 model demonstrated higher flexibility in ATP production in the anaerobic conditions. Such flexibility could be advantageous to WP3 for its adaptation to fluctuating availability of organic carbon sources in the deep sea.

IMPORTANCE

The well-studied nature of the metabolic diversity of *Shewanella* makes species from this genus a promising platform for investigating the evolution of carbon metabolism and energy conservation. The *Shewanella* phylogeny is diverged into two major branches, referred to as Group 1 and Group 2. While the genotype-phenotype connections of Group 2 species have been extensively studied with metabolic modeling, a genome-scale model has been missing for the Group 1 species. The metabolic reconstruction of *Shewanella piezotolerans* WP3 represented the first model of *Shewanella* Group 1 and the first model among piezotolerant and psychrotolerant deep sea bacteria. The model brought insights into the mechanism of energy conservation in WP3 under anaerobic conditions and highlighted its metabolic flexibility under diverse carbon sources. Overall, the model opens up new opportunities for investigating energy conservation and metabolic adaptation, and it provides a prototype for systems-level modeling of other deep-sea microorganisms.

INTRODUCTION

Members of the *Shewanella* genus are present in a wide range of environments including fresh and salt waters, food products, sewage systems, and deep sea sediments (1–3). The *Shewanella* genus is known to utilize diverse carbon sources and electron acceptors, leading to its broad adaptation to various environmental conditions (3–6). A 16S rDNA based phylogenetic reconstruction has revealed two major groups in the *Shewanella* genus (7). Generally, Group 1 includes species that are capable of

producing eicosapentaenoic acid (EPA) and are piezotolerant and psychrotolerant, such as *S. benthica* and *S. violacea*, which have been isolated from the deep sea. Group 2 species are generally pressure-sensitive and mesophilic and include *S. oneidensis*, *S. baltica*, and *S. putreficans*, which have been isolated from a variety of environments including freshwater lakes and spoiled meat products.

The ability of *Shewanella* species to utilize a broad range of electron acceptors makes this genus a target for studying metabolic energy conservation and anaerobic respiration. Several recent studies have focused on identifying the relative contributions of two distinct ATP-producing mechanisms (8–10), oxidative phosphorylation and substrate-level phosphorylation. Oxidative phosphorylation is typically associated with respiration, where the reduction of terminal electron acceptors is coupled to proton motive force (PMF) generation, and the PMF subsequently contributes to ATP synthesis via ATP synthase (ATPase). Substratelevel phosphorylation is associated with the production of ATP through direct transfer of a phosphoryl group to ADP through the action of enzymes like phosphotransacetylase (Pta) and acetate kinase (AckA). In S. oneidensis MR-1, substrate-level phosphorylation is the primary source of ATP during anaerobic growth, while ATPase has either minor contributions to ATP production or acts as an ATP driven proton pump that generates PMF (8). This is surprising given that Shewanella are obligated to utilize terminal electron acceptors when growing under anaerobic conditions. An understudied aspect of these features of metabolism is how ATP production, PMF generation, and redox reactions interact and jointly contribute to the utilization of metabolic pathways and energy conservation strategies in Shewanella.

Shewanella piezotolerans WP3, hereafter referred to as WP3, has been isolated from West Pacific sediment at a depth of 1914 m. It is piezotolerant and psychrotolerant, reflecting its adaptations to the deep sea environment (11). A 16Sbased phylogeny suggests this organism belong to Group 1 of the *Shewanella* genus (12). The ability of WP3 to utilize diverse carbon sources and electron acceptors demonstrates a metabolic flexibility that is comparable with other *Shewanella* species (11, 13). The full genome of WP3 encodes diverse c-type cytochrome genes, which support anaerobic respiration using various terminal electron acceptors, such as nitrate, iron, trimethylamine N-oxide (TMAO), and dimethyl sulfoxide (DMSO) (13). WP3 is also known to produce EPA and alter its lipid content to contain more unsaturated and branched chain fatty acids in low temperature and high pressure environments (14). These features enlist WP3 as a good representative of the Group 1 *Shewanella* species.

GEnome-scale Models (GEMs) of metabolic networks have broad applications in phenotype prediction, evolutionary reconstruction, functional analysis, and metabolic engineering (15). By connecting a set of biochemical reactions with the enzymatic functions encoded in a genome, GEMs provide a framework for simulating the associations between genotypes and phenotypes (16–19). The reconstruction of genome-scale models can be challenging due to the complexity in managing diverse data sets and maintaining model consistency through iterative manual curations. These challenges have been addressed with the recent releases of tools and automated pipelines to facilitate the modeling process (20–23). GEMs are available for four Group 2 *Shewanella* species, including *S. oneidensis* MR-1, *S. denitrificans*,

Shewanella sp. MR-4, and *Shewanella* sp. W3-18-1 (24, 25), while currently no GEM is available for any Group 1 species.

This study focuses on WP3 as a prototype for metabolic modeling among Group 1 Shewanella. WP3 presents the conserved features of the Group 1 Shewanella (e.g., piezotolerance, psychrotolerance, EPA production, etc.) and is a well-studied species in this group. Previous studies have provided detailed evidence related to the function and annotation of multiple key metabolic pathways in WP3, including nitrate utilization (26), DMSO respiration (27), iron reduction and biomineralization (28–30), and fatty acid synthesis (14). In addition to functional annotations, extensive data is available on the expression of key metabolic genes, connecting individual pathways with their functional roles under changing environmental conditions (31-36). These studies provide a broad knowledgebase for constructing the WP3 GEM. Furthermore, WP3 has established protocols for genetic manipulations (37–40). The experimental accessibility of this organism would enable the verification of modeling outcomes and support future research of molecular adaptations through combined GEM simulation and experimental verification. Overall, WP3 serves as an ideal organism for modeling the metabolism of Group 1 species in the Shewanella genus.

In this study, a GEM of WP3 was constructed and applied in simulating the carbon metabolism and energy conservation under both aerobic and anaerobic conditions. The model was verified based on the known physiology of the organism and new experimental data. Evolutionary analysis of the central metabolic genes revealed non-homologous replacements between WP3 (and other Group1 species) and the Group 2 *Shewanella*. Comparing the WP3 model with the model of a Group 2

representative, *S. oneidensis* MR-1 (here referred to as MR-1), revealed similarities and differences between the two organisms in their aerobic growth and anaerobic energy conservation.

RESULTS

Phylogenetic position of Shewanella piezotolerans WP3

The phylogenetic positioning of S. piezotolerans WP3 was confirmed following a phylogenomic analysis using the protein sequences of 661 conserved single copy genes (CSCGs) in the full genomes of 24 Shewanella species and five closely related Gammaproteobacteria that served as the outgroup to the Shewanella genus (Materials and Methods). The phylogenomic reconstruction demonstrated the differentiation of the Group 1 and Group 2 Shewanella species into distinct evolutionary branches (Figure 1) and concurred with a previously published 16S rRNA gene based phylogeny (7). An exception to this concurrence was with the positioning of S. amazonensis, where the 16S rRNA gene based phylogeny located S. amazonensis in the Group 2 taxa (7) while the genome based phylogeny positioned S. amazonensis as one of the deepest branching species among all of the analyzed Shewanella. According to the genome-wide phylogeny, WP3 was located in the Group 1 branch with S. pealeana and S. halifaxensis as its closest neighbors. The four previously modeled Shewanella species were marked with blue stars to indicate their position on the phylogeny while WP3 was marked with a red star (Figure 1).

Genome-scale metabolic reconstruction of Shewanella piezotolerans WP3

The complete metabolic reconstruction of WP3, GEM-iWP3, was released in a public Git repository at <u>https://github.com/zhanglab/GEM-iWP3</u>. It contained 806 genes, 653 metabolites, and 922 metabolic reactions. The reconstruction was achieved in three steps. First, gene-protein-reaction (GPR) associations were incorporated through mapping orthologous genes to the existing *Shewanella* reconstructions (24, 25) (Materials and Methods). This identified 596 genes (619 reactions) that were conserved between WP3 and all four of the other modeled *Shewanella* species as well as 130 genes (131 reactions) that were conserved between WP3 and some (but not all) of the four previously modeled species, leading to the inclusion of 726 genes associated with 750 reactions in the WP3 reconstruction.

Next, the WP3 metabolic reconstruction was expanded through manual curation of the WP3 genome using information from published literature (12, 14, 41), protein domain conservation, and evidence from the genomic and functional context of the metabolic genes (42). This expansion led to the inclusion of another 137 reactions associated with new gene annotations and the addition of a periplasmic compartment to account for cellular localizations of nutrient transporters and electron transport reactions. For example, the carbohydrate utilization pathways were annotated based on prior study of sugar catabolism in *Shewanella* (41) and further verified based on predictions of protein localization in the cell (43–45) (Figure 2). The reduction of soluble electron acceptors, such as nitrate, nitrite, thiosulfate, and TMAO, were represented as periplasmic reactions, while the reduction of DMSO and oxidized metals, such as Fe (III), Mn (IV), uranium (VI), and chromium (VI), were represented as extracellular processes following existing knowledge of the cellular

compartmentalization of the different electron transport processes in *Shewanella* species (46–55). Putative outer membrane transporters were identified and curated to identify what genes were responsible for nutrient exchange between the extracellular space and periplasm. A number of non-specific porins were identified, including distant homologs to the *E. coli* OmpC and OmpF proteins (56), as well as a homolog to the OprF protein in *Pseudomonas* aeruginosa (57, 58). This analysis also identified functionally specific outer membrane proteins that were responsible for the uptake of carbohydrates (e.g. LamB and OprB), phosphate (OprP), cobalamin (BtuB), long-chain fatty acids (FadL), and nucleosides (Tsx) (41, 59–63).

The assembly of cell components in WP3 was represented with the addition of 8 synthesis reactions. The biomass equation was introduced to represent the composition of cell mass, including carbohydrates, proteins, RNA, DNA, lipids, vitamins, and cofactors (Table S1). The stoichiometry of biomass equation was normalized to reflect the *mmol* concentration of individual components in one gram of cell dry weight (Materials and Methods). The composition of macromolecules, such as lipids, proteins, DNA, and RNA, were represented using equations that defined the composition of basic building blocks, such as fatty acids, amino acids, and nucleotides. The stoichiometry of these biosynthesis equations was determined according to existing *Shewanella* reconstructions and experimental measurements performed on WP3. Specifically, stoichiometry of the lipid biosynthesis equation (Table S2) was calibrated based on experimentally measured concentrations of saturated, unsaturated, and branched-chain fatty acids in WP3 (14).

The WP3 metabolic reconstruction also included three reactions for the diffusion of O₂, CO₂, and urea across the cell membrane, and 24 gap filling reactions for unblocking the production of biomass components. These gap filling reactions reflected knowledge gaps in the synthesis of biomass compounds, where the metabolic mechanisms were either unknown or not yet associated with any annotated genes in the WP3 genome. These gap filling reactions included dihydroneopterin mono- and tri-phosphate dephosphorylases, which were involved in the synthesis of the cofactor tetrahydrobiopterin, as well as glycolaldehyde dehydrogenase and 5,10-methylenetetrahydrofolate reductase, which were involved in folate metabolism. Three gap filling reactions were compound sinks that allowed for the removal of metabolic side products whose metabolic pathways are currently unknown and are not involved in other reactions in the metabolic network. These included sinks for the compound S-Adenosyl-4-methylthio-2-oxobutanoate, a side product in the synthesis of biotin.

Finally, 109 exchange reactions were defined to represent the exchange of nutrients and metabolic products in the simulated environment (Table S3). These included reactions for the uptake of carbon sources, electron acceptors, trace metals, and vitamin precursors, as well as the diffusion of metabolic byproducts. These exchange reactions were set to represent the basal constraints specified in Table S3 and were subsequently modified during metabolic simulations to represent different environmental conditions (Materials and Methods).

Evolution of central metabolic genes

During manual curation of the WP3 metabolic reconstruction, non-homologous genes were identified between WP3 and the previously modeled *Shewanella* species for carrying out central metabolic functions. These included acetylornithine deacetylase (argE), which was essential for the biosynthesis of arginine, and glucosamine-6phosphate deaminase (nagB), which was essential for utilizing N-acetyl-Dglucosamine (GlcNac). Both genes were experimentally identified in MR-1 and were found to be non-homologous to the canonical genes in E. coli (64, 65). A broader comparison of the Group 1 and Group 2 Shewanella suggested that they were conserved within each group but had diverged between the two groups (Figure S1). Exceptions were found for the *argE* gene in *S. amazonensis*, *S. loihica* and *S.* frigidimarina, where the deep-branching S. amazonensis and S. loihica encoded both non-homologous copies of argE, and the Group 2 species S. frigidimarina encoded a single *argE* of the Group 1 type. The genomic contexts of *argE* and *nagB* were well conserved among the Group 1 species, while they were variable among the Group 2 species. Consistent with the observed variability of the genomic contexts, mobile element proteins were encoded in proximity to argE and nagB in MR-1, as well as an argE in S. loihica that is homologous to the Group 2 type. The Group 2 genes had a diverse origin, with the *argE* homologous to genes in *Klebsiella* and a limited subset of host-associated Enterobacteriaceae, and the nagB homologous to genes in the deep branching bacteria and archaea (65). In contrast, the Group 1 genes were conserved with evolutionarily related genera of Shewanella, such as Marinomonas, Colwellia, and Pseudoalteromonas. Taken together, the central metabolic genes argE and nagB

evolved from distinct origins among the *Shewanella* Group 1 and 2. The WP3 genome encoded the gene copies that were conserved in the Group 1 species.

Metabolic simulations match experimental growth measurements.

Simulations of biomass production with the WP3 metabolic model were consistent with the known physiology of this organism. This included utilizing glucose, lactate, maltose, and GlcNac as carbon sources, and using Fe(III), nitrate, nitrite, thiosulfate, TMAO, and DMSO as terminal electron acceptors for anaerobic respiration (13). From the metabolic simulations, 53 sole carbon sources supported biomass production of the WP3 model under aerobic conditions, including various carbohydrates, amino acids, nucleotides, and fatty acids (Figure 2 and Table S3).

To quantitatively evaluate the prediction of biomass concentrations by the WP3 metabolic model, batch cultures were set up using a minimal medium developed in this study to experimentally measure the growth of WP3 with sole carbon sources (Supplemental Text S1). The sole carbon sources examined in this study were pyruvate, glucose, maltose, and an amino sugar (GlcNac), and the experiments were carried out under aerobic conditions using oxygen as the sole terminal electron acceptor. The concentrations of carbon sources ranged between 2 mM and 40 mM in the experimental media. Cell growth was measured in three independent replicates and converted to biomass concentrations (Materials and Methods). Metabolic simulations were performed with the WP3 model to predict the biomass fluxes under the conditions defined by the experimental media. This was achieved by modifying the flux bounds of the exchange reactions in the model. The lower bound of exchange

reactions for carbon, nitrogen, sulfur, and phosphorous sources were specifically calibrated to reflect their concentrations in the minimal media (Table 1), the exchange of oxygen was unlimited to simulate aerobic respiration, and the lower and upper bounds of other exchange reactions were assigned based on default settings in the basal constraints (Table S3, Materials and Methods).

The biomass fluxes predicted by the model demonstrated overall consistency with experimentally measured biomass concentrations at the stationary phase (Figure 3). The quantitative values slightly deviated from experimental measurements at relatively low (i.e., 2 mM of pyruvate or glucose) or high carbon source concentrations. Experimental measurements showed that the biomass production stopped increasing when the concentration of sole carbon sources increased beyond 60 mM in the count of carbon elements [i.e., 20 mM, 10 mM, or 5 mM of pyruvate (3 Carbons), glucose (6 Carbons), or maltose (12 Carbons), respectively]. This trend was also seen in the WP3 model simulations. Further, under high concentrations of pyruvate, glucose, and maltose, metabolic simulations identified NH_4^+ as the limiting factor of biomass production. This was because the uptake of these carbon sources was limited by the uptake bound of the NH_4^+ exchange flux that corresponded to its concentration in the experimental media. Allowing for higher uptake of NH_4^+ by the model led to higher biomass production and higher uptake of these carbon sources. In contrast, the model was not limited by the availability of NH_4^+ when an amino sugar, GlcNac, was used as a sole carbon source. This was because each molecule of GlcNac produced one molecule of NH_4^+ during its utilization, providing additional nitrogen that could be used during growth. As a result, higher biomass was observed with

GlcNac as a carbon source, and this trend was seen in both the experimental measurements and the model simulations (Figure 3).

The aerobic growth of WP3 was also compared with MR-1 [model iMR1_799 (25)] based on simulations of growth on 28 sole carbon sources that have been experimentally confirmed to support growth in either WP3 (13) or MR-1 (24, 25) (Figure S2). The MR-1 model was able to utilize almost all the examined carbon sources except for maltose. The WP3 model, in contrast, was viable in maltose but was not able to utilize six carbon sources, including the amino acids asparagine and glutamine, the nucleic acids inosine and thymidine, and the small molecules ethanol and 2-oxoglutarate. Simulations of biomass production using the two models revealed that WP3 had slightly higher biomass yields than MR-1 with most of the growth supporting carbon sources, including carbohydrates, small carbon molecules, and amino acids, while MR-1 had slightly higher biomass yield when malate, adenosine, or deoxyadenosine were used as sole carbon sources.

Metabolic energy conservation of WP3.

The relative roles of oxidative and substrate-level phosphorylation were examined by simulating mutant models with reactions blocked from the two pathways, respectively (Figure 4, Materials and Methods). For measuring the role of oxidative phosphorylation, biomass production of the wild type (WT) model and a deletion mutant of ATP synthase (Δatp) was simulated using flux balance analysis (FBA) under both aerobic (O₂) and anaerobic (fumarate) conditions using either GlcNac or lactate as sole carbon sources. Under aerobic conditions, the Δatp mutant produced less than half of the WT biomass, indicating that oxidative phosphorylation played an important role in the aerobic growth of WP3. Under anaerobic conditions, however, the biomass production was comparable between the WT and Δatp models, demonstrating that oxidative phosphorylation had only a minor role in supporting anaerobic growth (Figure 4B).

For measuring the role of substrate-level phosphorylation, FBA was performed with the WP3 WT model and three mutant models that represent the single deletion of phosphotransacetylase (Δpta) or acetate kinase ($\Delta ackA$), or the double deletion of both genes ($\Delta pta\Delta ackA$). When lactate was used as a sole carbon source, the WT model was able to produce non-zero biomass flux, while the Δpta , $\Delta ackA$, and $\Delta pta\Delta ackA$ models had a maximum biomass flux of zero indicating that these mutants are not viable in the lactate media. When GlcNac was used as a sole carbon source, both the WT and mutant models were viable in the anaerobic media. Compared to the WT, Δpta had a slight decrease in biomass production (97% of the WT flux), and $\Delta ackA$ and $\Delta pta\Delta ackA$ resulted in a greater reduction of the biomass to less than 50% of the WT (Figure 4C). The decrease or inhibition of biomass production in the $\Delta ackA$ and $\Delta pta\Delta ackA$ mutants indicated an important role of substrate-level phosphorylation in supporting anaerobic growth of WP3.

Additional examination of the internal fluxes obtained from FBA revealed changes in ATP production, PMF generation, and redox functions in the WT and mutant models (Figure 4D). In the WT model, substrate-level phosphorylation mediated by AckA was used for ATP production, while oxidative phosphorylation via ATP synthase (ATPase) played a minor role in this process. The activity of formate

dehydrogenase (Fdh) was coupled with terminal electron acceptor reduction to generate PMF, and NADH dehydrogenase (Ndh) was used for reducing the quinone pool. In the Δpta model, reaction fluxes were redirected to xylulose-5-phosphate phosphoketolase (Xpk) from the pentose phosphate pathway so that substrate-level phosphorylation through AckA was maintained. This redirection resulted in reduced Fdh flux, potentially due to decreases in formate production, and increased Ndh flux, potentially for maintaining the redox activities in the electron transport chain. In the $\Delta ackA$ and $\Delta pta\Delta ackA$ models, a more significant shift was observed in the distribution of metabolic fluxes. The inhibition of AckA led to blockage of the upstream fluxes through Pta and Xpk, and increased flux through pyruvate kinase (Pyk) to partially compensate for the loss of AckA mediated ATP production.

Variability of the internal fluxes was further examined using flux variability analysis (FVA) with biomass production constrained to its maximum under each simulation condition (Supplemental Table S4). This revealed consistent flux values for all the above-mentioned reactions in the WT and Δpta models and for the ATPase, AckA, Pta, and Xpk reactions in the $\Delta ackA$ and $\Delta pta\Delta ackA$ models. However, the Pyk, Fdh, and Ndh reactions had variable fluxes in the $\Delta ackA$ and $\Delta pta\Delta ackA$ mutants, indicating that these mutants had alternative strategies for balancing the ATP production, PMF generation and redox activities in the cell.

ATPase activity and anaerobic growth of Shewanella

One surprising feature of the *Shewanella* anaerobic growth was the lack of oxidative phosphorylation via ATPase despite the obligate requirement for respiration through

terminal electron acceptors (8). To further investigate how the ATPase activity (i.e., in either ATP production or PMF generation directions) was related to the redox balancing of *Shewanella* during anaerobic respiration, the *NAD⁺/NADH* homeostasis was modeled with a robustness analysis to simulate the connections between redox state (as measured by the differences in *NAD⁺* and *NADH* concentrations) and the activity of ATPase in both the WP3 and MR-1 models (Materials and Methods). The simulation demonstrated a positive correlation between the availability of reducing equivalents and the flux of ATPase reaction for both WP3 and MR-1 (Figures S3, S4). This indicated that when the system was provided with more reducing equivalents, the ATPase flux would increase, and activity would be shifted towards the ATPproducing direction. In contrast, when the system had less reducing equivalents, the ATPase flux would decrease, and activity would be flipped to the proton pumping and PMF-generating direction.

The comparison of redox states in WP3 and MR-1 models when ATPase reaction flux approached zero revealed metabolic differences between these two organisms across diverse carbon sources when using fumarate as the sole electron acceptor (Figure 5). The WP3 model produced excess reducing equivalents in a wide range of carbon sources, including amino sugars, small carbon compounds, amino acids, and nucleotides (Figure 5A). Considering the positive correlation of the redox state and the ATPase flux (Figures S3, S4), the excess reducing equivalents in WP3 could potentially enable the production of additional ATP via ATPase. The MR-1 model, in contrast, produced excess reducing equivalents only when specific carbon sources were provided, such as malate, aspartate, and serine. Thus, the ATPase could

have little contribution to the ATP production but may instead be used for PMF generation in MR-1. Overall, the two representatives of Group 1 and Group 2 *Shewanella*, WP3 and MR-1, demonstrated complex interactions of ATP generation, PMF generation, and redox balancing processes under anaerobic growth. The WP3 model displayed higher capacity than MR-1 in producing excess reducing equivalents in most of the examined carbon sources. This may provide additional advantages to WP3 in its natural environment by enabling additional ATP production when using a diverse range of carbon sources.

DISCUSSION

In this study, a genome-scale model was constructed for WP3, a piezotolerant and psychrotolerant representative of the Group 1 *Shewanella* species (Figure 1). Extensive annotations of the WP3 genome were incorporated into the metabolic reconstruction, and the carbon utilization reactions were curated based on the current literature available (Figure 2). A periplasmic compartment was introduced to the WP3 reconstruction to account for the cellular localization of carbon utilization and electron transport reactions. This represented a new component not previously included by other metabolic reconstructions of *Shewanella* species.

Evolutionary analysis of central metabolic genes in WP3 revealed instances of non-homologous replacements among the Group 1 and Group 2 *Shewanella*. The *argE* and *nagB* in WP3 and other Group 1 species were conserved within bacterial species closely related to *Shewanella*. Hence, they could represent the ancestral genes conserved during early differentiation of the *Shewanella* genus. The Group 2 copies of
these genes were adjacent to mobile genetic elements, suggesting a possible acquisition of these genes through horizontal gene transfer. Further, the conservation of these acquired genes across Group 2 species and their presence in a few Group 1 species suggested they could be introduced to the genome during early differentiation of the Group 2 *Shewanella*.

The WP3 model represented known physiology of this organism, including its growth under a wide variety of carbon sources and electron acceptors. A comparison of biomass production from model simulations and experimental measurements revealed that the WP3 model represented growth trends consistent with what was observed in experimental cultures using the sole carbon sources pyruvate, glucose, GlcNac, and maltose (Figure 3). The slight deviations from the experimental results under low or excess carbon concentrations could be attributed to the differential regulation of gene expressions but was beyond the scope of this study. Additional confidence in the WP3 model was established when it was applied for the prediction of growth-limiting nutrients. The prediction of NH_4^+ as the limiting nutrient when excess carbon source was provided was corroborated by the fact that the amide molecule, GlcNac, was able to overcome this growth limit by serving as both a carbon and a nitrogen source.

A comparison of the WP3 model with an existing model of a Group 2 representative, *S. oneidensis* MR-1, revealed similarities and differences in carbon utilization and energy conservation of these two organisms. While MR-1 lacked enzymes for utilizing maltose, WP3 lacked identified transporters that are required for utilizing six carbon sources, including the amino acids asparagine and glutamine, the

nucleic acids inosine and thymidine, and the small molecules ethanol and 2oxoglutarate (Figure S2). The anaerobic energy conservation strategies of WP3 were explored by simulating the deletion of genes responsible for oxidative (Δatp) and substrate-level ($\Delta ackA$, Δpta and $\Delta pta\Delta ackA$) phosphorylation (Figure 4). Using GlcNac and lactate as sole carbon sources and fumarate as the sole electron acceptor, the biomass production and reaction flux distributions of WP3 wild type and mutant models revealed that substrate-level phosphorylation was the primary source of anaerobic energy conservation, a trait that has been noted in MR-1 (8, 10). This indicates the primary usage of substrate-level phosphorylation could be a conserved feature in the anaerobic respiration of both Group 1 and Group 2 and suggests that this feature could have evolved during the early differentiation of *Shewanella*.

Internal redox balancing has been shown to play critical roles in the ability for other organisms to utilize nutrients and is a major driver of changes in metabolic strategy (66–68). Simulation of the *NAD*⁺/*NADH* homeostasis and its connections to the ATPase activity in WP3 and MR-1 provided insights into the complex interactions of ATP production, PMF generation, and redox balancing processes in *Shewanella*. While both the WP3 and MR-1 models presented a positive correlation between the availability of reducing equivalents and the reaction flux of ATPase (Figures S3, S4), the two models demonstrated distinct redox states when different carbon sources were utilized (Figure 5). The production of excess reducing equivalents was supported by a wide range of carbon sources in WP3 but was restricted to only a few carbon sources in MR-1. This suggested a capacity for WP3 to produce additional ATP via the ATPase activity and could potentially enable the adaptation of WP3 to the fluctuating

availability of carbon sources at the deep sea by maintaining ATP production when different carbon sources became available.

Overall, the WP3 model represents the first genome-scale model of the Group 1 *Shewanella* and a first model of piezotolerant and psychrotolerant deep-sea species. It opens up new opportunities for the future studies of environmental adaptation and metabolic pathway utilization, for example, through incorporating environment specific features like the altered fatty acid compositions in different temperature and pressure (14) or the differential expression of key metabolic genes in different environmental conditions (31, 33, 36). The WP3 model also provides a framework for integrating additional parameters, such as enzyme thermostability (69) or contextspecific information (70) during the study of temperature and pressure adaptations. The experimental accessibility of WP3 would make it possible to verify extensions to the model. Finally, future studies combining molecular evolution and metabolic simulation of the Group 1 and Group 2 *Shewanella* could lead to a better understanding of bacterial adaptations to low temperature and high-pressure environments and permit the exploration of metabolic potentials at the deep sea.

MATERIALS AND METHODS

Ortholog mapping and phylogenomic reconstruction of the Shewanella genus

An updated phylogeny of the *Shewanella* genus was constructed based on conserved single-copy genes (CSCGs). A dataset of 24 *Shewanella* genomes was downloaded from the KEGG database (71). Five additional genomes were used as the outgroup for rooting the *Shewanella* phylogeny, including *Pseudoalteromonas haloplanktis*,

Colwellia psychrerythraea, Psychromonas ingrahamii, Photobacterium profundum, and Moritella viscosa. An initial ortholog mapping among these species was identified using a bi-directional best hit BLAST analysis as defined in a previous study (72). The ortholog mapping was further refined based on a consensus of additional evidence from other sources, including a published ortholog table of the *Shewanella* genus (25), the KEGG Orthology database (71), as well as automated predictions by OrthoMCL (73). From analyzing ortholog groups that were consistently defined by all the abovementioned approaches, CSCGs were identified as the orthologs that occurred once and only once in each of the analyzed genomes. Individual alignments were constructed on the protein sequences of each CSCG using MUSCLE v3.8.31 (74). The alignments were then concatenated to create a master alignment of the CSCGs in Shewanella and the outgroups. RaxML v 8.2.3 (75) was used for reconstructing a maximum likelihood protein phylogeny using the JTT substitution model with the GAMMA model of rate heterogeneity. Branch support values were estimated by performing bootstrapping with 100 replications.

Development of the genome-scale metabolic reconstruction

The WP3 metabolic reconstruction was developed using the version v0.27 of the PSAMM software package (23). The reconstruction was represented in a YAML format that is designed to represent variable model definitions and simulation conditions. Simulations with the model were performed in PSAMM using the IBM ILOG CPLEX Optimizer version 12.6.2 linear programming solver. An initial reconstruction was first developed based on ortholog mapping to the existing

metabolic reconstructions of S. oneidensis MR-1, Shewanella sp. MR-4, S. denitrificans OS217, and Shewanella sp. W3-18-1 (25). The orthologs were identified according to a global mapping of ortholog clusters among all Shewanella (described in the above paragraph). Gene-protein-reaction (GPR) associations in the initial WP3 reconstruction were mapped from conserved genes in the modeled species following logic expressions that represent the "AND" and "OR" relationships of enzyme coding genes. The "AND" logic was used to indicate multiple subunits of an enzyme complex, and the "OR" logic was used to indicate alternative enzymes. A GPR association was introduced from existing reconstructions only if orthologs were identified in the WP3 genome for all subunits of at least one alternative enzyme. The WP3 reconstruction was further expanded through manual curation by referencing existing annotations in the KEGG (71), SEED (42), and BioCyc (76) databases. Additional considerations in the manual curation process included examining genomic context using the SEED viewer tool (77), searching for conserved sequence domains (78), and reviewing current literature (12, 14, 41, 79). Finally, metabolic gaps in the production of biomass components were identified using the PSAMM gapfill function (23). A number of gap filling reactions were included to enable biomass production with experimentally confirmed carbon sources and electron acceptors (13). These gap reactions were further scrutinized through manual inspection of the biosynthetic pathways leading to the various biomass components and were reviewed with the *fluxcheck* function using the "--unrestricted" option in PSAMM to confirm their flux consistency. Stoichiometric consistency of the model was validated by using the masscheck function in PSAMM. Additional verification of the formula and charge

balance was performed with *formulacheck* and *chargecheck* functions. By default, the exchange reactions, compound sources or sinks (e.g., 4HBASink, 5DRIB_Sink, and AMOB_Sink), macromolecular synthesis equations (e.g., Core_Biomass, Growth, and PASYN_WP3_20C), and reactions involving the acyl carrier protein or its apo form (e.g., ACPS1, ACPSc, and AGPEPHOS) were excluded from formula and charge checks due to the presence of undefined R or X groups in the metabolites.

Formulating the biomass objective function

A biomass equation was formulated in the WP3 reconstruction to simulate the production of components required for cell growth. The biomass equation incorporates the cellular composition of the total cellular carbohydrates, proteins, RNA, DNA, lipids, vitamins, and cofactors (Table S1). Biomass compositions from experimental measurements of WP3 and evolutionarily related species was used as references for formulating the stoichiometry of the biomass equation. First, the composition of carbohydrates, proteins, DNA, RNA, and lipids was estimated using approximations from S. oneidensis MR-1 (24, 25). The addition of vitamins and cofactors into WP3 biomass was achieved by using an approximation of the experimental measurements from E. coli as a representation of gram-negative bacteria (80). Further calibration of the biomass composition in WP3 involved formulating the stoichiometry of the phosphatidic acid synthase reactions according to experimental measurements of branched-chain, unsaturated, and saturated fatty acids in this organism (14) (Table S2). The overall biomass equation was scaled so that the stoichiometry of biomass components corresponds to their millimole (mmol) amounts in a gram of cell dry

weight (gDW). This calibration enabled the comparison of computationally simulated biomass productions with experimental measurements.

Formulating the basal constraints of metabolic simulations

A list of basal constraints was defined for exchange reactions in the model using lower and upper bounds specified in Table S3. The basal constraints were used to set default bounds for the uptake of nutrient sources and the removal of metabolic byproducts. For trace elements, vitamin precursors, and salts, the default bounds were unlimited on both directions; for metabolic byproducts, the lower bounds were set to zero while the upper bounds were unlimited, indicating that they can be freely released from the system. The basal constraints also defined exchange reactions for 71 potential carbon sources and 13 electron acceptors in the model. Uptake of carbon sources and electron acceptors was blocked in the basal constraints and was defined during individual simulations. Unless specified, in the simulations the lower bound of the sole carbon source was set to -10 to limit its uptake to $10 \ mmol/L$, and uptake of the sole electron acceptor was unlimited.

Comparing WP3 metabolic simulations with experiments and the MR-1 model

The growth of WP3 when utilizing a variety of sole carbon sources was examined in aerobic batch cultures using 50 mL of LMO-812 minimal media (Supplemental Text S1) supplemented with alternative sole carbon sources at different concentrations (2 mM, 5 mM, 10 mM, 20 mM, or 40 mM). Cultures were grown in triplicate at 20 degrees Celsius and were continuously shaken at 200 rpm. The growth curve of WP3 was determined using turbidity measurements at 600 nm (OD₆₀₀). The growth measurements at early stationary phase were converted to gDW/L of biomass concentration using a previously determined correlation between OD₆₀₀ and dry weight in *Shewanella* species (24). To simulate the experimental growth conditions, the PSAMM *fba* function was applied to perform FBA simulations using the biomass equation as the objective function. The exchange of carbon, nitrogen, sulfur, and phosphorous nutrients were constrained based on their availability in the experimental media (Table 1), the exchange of oxygen was unlimited to simulate aerobic respiration with oxygen as the sole electron acceptor, and other exchange reactions were defined with the basal constraints. The unit of the uptake fluxes was assigned to *mmol/L*, which corresponds to the unit of nutrient concentrations in the experimental media. Since the biomass equation in WP3 was calibrated to reflect the millimole (*mmol*) amounts of biomass components in a gram of cell dry weight (*gDW*), the biomass concentrations were predicted based on the biomass fluxes (*v_B gDW/L*).

Comparisons of the WP3 with the MR-1 model were performed by simulating the aerobic growth of the organisms using 28 sole carbon sources that have been experimentally confirmed to support growth in either WP3 (13) or MR-1 (24, 25) (Figure S2). The latest metabolic reconstruction of MR-1, iMR1_799 (25) was used in all MR-1 simulations performed in this study. The simulations with both models were set up using the basal constraints with default bounds for sole carbon sources (i.e., [-10, 1000]) and the sole electron acceptor, oxygen (i.e., [-1000, 1000]). The biomass yields were calculated through dividing the biomass flux by the uptake fluxes of carbon source and the electron acceptor.

Metabolic simulation of mutant phenotypes

Mutant strains of WP3 were simulated in the metabolic model by setting a flux limit of [0, 0] for all reactions catalyzed by the gene being knocked out. A list of enzymes involved in ATP production, PMF generation, and redox activities was provided in Table 2 along with their corresponding reactions, functional roles, and gene associations in the WP3 model. Media conditions were set in the WP3 model using the basal constraints with uptake enabled for a sole carbon source (lactate or GlcNac) and a sole electron acceptor (O2 or fumarate). The carbon source was constrained to a maximum uptake of 10 mmol/L, and the electron acceptor was unlimited. For simulations with fumarate as the electron acceptor the succinate/fumarate antiporter reaction, SUCFUMtdc, was blocked as it has been noted to be able to form artificial loops with other transporters (80) and the fumarate hydrogen symporters FUMt4 and FUMt4_2 were also blocked to prevent utilization of fumarate as an additional carbon source. When GlcNac was used as the sole carbon source, the lactate dehydrogenase and glycerol-3-phosphate dehydrogenase reactions were blocked to prevent the formation of artificial loops in NADH cycling. Metabolic reaction fluxes were determined by optimizing the biomass objective function using *fba* with the *l1min* loop removal approach implemented in PSAMM (23, 81). Additional analysis of flux variability was performed on internal reactions with the *fva* function in PSAMM by fixing the biomass flux to its maximum. The reaction flux for Fdh was calculated based on the sum of fluxes through the FDH9 and FDH10 reactions, and the reaction flux for Ndh was calculated based on the sum of fluxes through the NADH4,

NADH12, and NADH14 reactions. All other fluxes were directly obtained from the FBA and FVA simulations according to the reactions listed in Table 2.

Metabolic Simulations of the NAD⁺/NADH homeostasis

The $NAD^+/NADH$ homeostasis was used as an approximation for investigating redox states in the WP3 model and the MR-1 model, iMR1 799 (25). To simulate the $NAD^+/NADH$ homeostasis, an artificial reaction, EQ1: $NAD^+ + H^+ \le NADH$, was introduced to the model to account for differences in the concentrations of NAD⁺ and *NADH*. First, a robustness analysis was performed by varying the flux value of EQ1 while optimizing the biomass production. This was performed using the robustness function in PSAMM (23), where flux values of EQ1 were probed in the range of [-10,10] at 500 steps. For each step, FBA simulation was performed with the *l1min* loop removal, and the simulated ATPase flux was plotted with the corresponding flux of EQ1 (Figures S3, S4). Next, a linear model was fit to the data using the equation: $v_{ATPase} = k \cdot v_{EQ1} + b$, where v_{ATPase} was the flux of the ATPase reaction and v_{EQ1} was the flux of the EQ1 reaction. To identify the connections between ATPase activity (i.e., ATP production or PMF generation) and the redox state of a cell, the intersection of the linear model with the EQ1-axis was used to determine the difference in NAD^+ and NADH concentrations when the ATPase reaction flux approached zero. A negative intersection of the linear model on the EQ1-axis would indicate $[NAD^+] - [NADH] < 0$, suggesting the homeostasis was pushed towards generating more NADH; A positive intersection would indicate $[NAD^+] - [NADH] >$ 0, suggesting that the homeostasis was pushed towards generating more NAD^+ . Both

the WP3 and MR-1 models were simulated using basal constraints with the addition of fumarate as the anaerobic electron acceptor paired with one of 12 sole carbon sources that are growth supporting in both models (Figures 5, S3, and S4). The exchange flux of the sole carbon source was constrained to [-10,1000], and the exchange of the electron acceptor was unlimited. The fumarate transport reactions SUCFUMtdc, FUMt4, and FUMt4_2 were blocked as mentioned above to avoid artificial loops and prevent the utilization of fumarate as an additional carbon source. The proton-pumping NADH dehydrogenase in MR-1 was blocked due to the lack of evidence of its participation in energy metabolism (8, 24, 25). All other internal reactions in WP3 and MR-1 models were constrained based on the reaction reversibility using default settings in PSAMM.

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Tables and Figures Manuscript I

Table 1. Exchange reaction constraints representing the concentrations of carbon, nitrogen, sulfur, and phosphorous sources in the minimal media of WP3 batch cultures. All other exchange reactions in the WP3 model were defined with settings in the basal constraints. The compounds pyruvate, glucose, maltose, and GlcNac, were used as sole carbon sources. The LB and UB columns indicated the lower and upper bounds of exchange reaction fluxes, where the negative values indicated that uptake of the nutrient was permitted. Concentrations of the sole carbon sources varied from 2 mM to 40 mM; the concentration of the sulfur, phosphorus, and nitrogen sources were set according to their concentration in the experimental media.

Nutrient Source	Compound Name	Media Concentraton	LB	UB
Carbon Sources	Glucose/Maltose/GlcNac/Pyruvate	2mM	-2.00	1000.00
		5mM	-5.00	1000.00
		10mM	-10.00	1000.00
		20mM	-20.00	1000.00
		40mM	-40.00	1000.00
Sulfur Source	SO4	9.8mM	-9.80	1000.00
Phophorus	POI	0.7mM	-0.70	1000.00
Source	F 04	0.7111111		
Nitrogen Source	NH4	5.6mM	-5.60	1000.00

Table 2. Metabolic enzymes involved in ATP production and PMF generation (Figure 4) with their corresponding reactions, functional roles, and gene associations in the WP3 model.

Enzyme	Reactions	Function	Gene association
Pta	PTAr	Phosphotransacetylase	swp_1948
AckA	ACKr	Acetate kinase	swp_1949
ATPase	ATPS4r	ATP synthase	swp_5155 AND swp_5156 AND swp_5157 AND swp_5158 AND swp_5159 AND swp_5160 AND swp_5161
Pyk	РҮК	Pyruvate kinase	swp_2388
Pfl	PFL	Formate C- acetyltransferase	swp_1952
Xpk	ХРК	Xylulose-5-phosphate phosphoketolase	swp_3738
Ndh	NADH4, NADH12, NADH14	NADH dehydrogenase	swp_1298 OR swp_2117 OR swp_4014
Fdh	FDH9, FDH10	Formate dehydrogenase	(swp_5024 AND swp_5025 AND swp_5023) OR (swp_5027 AND swp_5028 AND swp_5029)



Figure 1. Phylogenetic reconstruction of the *Shewanella* genus based on the concatenated sequences of 661 conserved single copy genes identified in the full genomes of *Shewanella* and five outgroup species. Support values based on 100 iterations of bootstrapping were indicated as labels of the internal nodes. Only support values above 80 were shown. The four *Shewanella* species with available GEMs were marked with blue stars and WP3 was marked with a red star.







Figure 3. Comparison of experimentally measured and computationally simulated biomass production. Error bars represented the standard deviation of the experimentally measured biomass concentrations (gDW/L) from three independent replicates.



model and the mutant models *JackA*, *Apta*, and *AptaJackA* using GlcNac or lactate as a sole carbon source and fumarate as Comparison of biomass fluxes in the wild type and the *datp* mutant models of WP3 with GlcNac or lactate as a sole carbon GlcNac as a sole carbon source. Abbreviations: MK-Menaquinone; CymA-Tetraheme c-type cytochrome; ATPase-ATP synthase; Fdh-Formate dehydrogenase; Ndh-NADH dehydrogenase; AckA-Acetate kinase; Pra-Phosphotransacetylase; source in aerobic and anaerobic conditions. C) Biomass fluxes from anaerobic growth simulations of the WP3 wild type a sole electron acceptor. D) Internal reaction fluxes of the WP3 and mutant models from the simulations in C) using Figure 4. A) A schematic representation of key reactions involved in the production of ATP and PMF in WP3. B) Pvk–Pvruvate kinase: Xnk–Xvlulose-5-nhosnhate nhosnhoketolase.





Supplemental Material Manuscript I:

Supplemental Text S1: Components of the LMO-812 minimal media used for culture-based experiments done with *Shewanella piezotolerans* WP3. Media components are adapted from a previously described defined marine media. Widdel, Friedrich. 2005. 8.1.1. Media for sulphate-reducing bacteria, p 102-104. In HERMES, Handbook of Methods for Microbial Ecology, Sept 2005 Edition.

LMO-812: Full Media	
(Adjust final pH to 7.0 with Na ₂ CO ₃ so	olution)
Component	Amount
Full Marine Salt Solution	950 mL
Trace Element Mixture	1 mL
Vitamin Mixture	1 mL
Thiamine Solution	1 mL
Vitamin B12 Solution	1 mL
NaHCO ₃ Solution	20 mL
Full Marine Salt Solution	
Component	Amount
Distilled Water	950 mL
NaCl	26.0 g
$MgCl_2 \cdot 6 H_2O$	5 g
$CaCl_2 \cdot 2 H_2O$	1.4 g
Na_2SO_4	4.0 g
NH ₄ Cl	0.3 g
KH ₂ PO ₄	0.1 g
KCl	0.5 g
Trace Element Mixture	
(Adjust final pH of solution to 6.0 with	NaOH solution)
Component	Amount
Distilled Water	1000 mL
EDTA	5.2 g
H ₃ BO ₃	10 mg
$MnCl_2 \cdot 4 H_2O$	5 mg
$FeSO_4 \cdot 7 H_2O$	2100 mg
$CoCl_2 \cdot 6 H_2O$	190 mg
$NiCl_2 \cdot 6 H_2O$	24 mg
$CuCl_2 \cdot 2 H_2O$	10 mg
$ZnSO_4 \cdot 7 H_2O$	144 mg
$Na_2MoO_4 \cdot 2 H_2O$	36 mg
Vitamin Mixture	
Component	Amount
Sodium Phosphate, 10 mM, pH 7.1	100 mL

4-Aminobenzoic acid D(+)-Biotin Nicotinic Acid D(+)-Pantothenic Acid, Calcium Salt Pyridoxine dihydrochloride	4 mg 1 mg 10 mg 5 mg 15 mg	
Thiamine Solution Component Sodium Phosphate, 10 mM, pH 3.4 Thiamine chloride dihydrochloride	Amount 100 mL 10 mg	
Vitamin B12 Solution Component Distilled Water Cyanocobalamin	Amount 100 mL 5 mg	
Bicarbonate Solution Component Distilled Water NaHCO ₃	Amount 1000 mL 84 g	



Supplemental Figure S1. Phylogenetic trees of ArgE and NagB proteins encoded in the genomes of Group 1 (A and C) and Group 2 (B and D) *Shewanella* species. Support values based on 100 iterations of bootstrapping were indicated as labels on the internal nodes. Only support values above 80 were shown. The Group 1 and Group 2 copies of the corresponding proteins had no detectable homology, indicating non-homologous replacements of the ArgE and NagB function in the two groups of *Shewanella*.



Supplemental Figure S2. Biomass yields for WP3 and MR-1 simulated across 28 carbon sources in aerobic conditions.



Supplemental Figure S3. Linear models for the prediction of $NAD^+/NADH$ homeostasis in the WP3 model (Materials and Methods). Fluxes of the ATPase reaction (black dots) were plotted based on a robustness simulation across varied fluxes of the EQ1 reaction. Linear models (red lines) were fitted to the observed correlations between EQ1 and ATPase fluxes and was used to calculate the differences in NAD^+ and NADH concentrations where the ATPase flux approached zero.



Supplemental Figure S4. Linear models for the prediction of $NAD^+/NADH$ homeostasis in the MR-1 model (Materials and Methods). Fluxes of the ATPase reaction (black dots) were plotted based on a robustness simulation across varied fluxes of the EQ1 reaction. Linear models (red lines) were fitted to the observed correlations between EQ1 and ATPase fluxes and was used to calculate the differences in NAD^+ and NADH concentrations where the ATPase flux approached zero.

Manuscript II

Publication Status: Formatted for submission to PLOS Computational Biology Title: Reconstruction and analysis of a thermodynamically constrained metabolic models reveal mechanisms of metabolic remodeling under temperature perturbations of a deep-sea bacterium

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<u>Abstract</u>

Microbial acclimation to different environmental conditions can involve broad changes in gene expression and shifts in the utilization of metabolic pathways, but a systems-level view of these metabolic responses, however, is currently missing. In this study, an integrated metabolic modeling approach that combined transcriptomic and thermodynamic constraints was used to investigate the metabolic changes that occur during temperature acclimation to suboptimal (4 °C), optimal (15 °C), and supraoptimal (20 °C) temperatures in the deep-sea psychrophilic bacteria Shewanella psychrophila WP2. A comparison of the predicted growth at each temperature showed the 4 °C model to have a lower ability to produce both cellular biomass and energy, while the 20 °C model was able to produce energy at similar rates to the 15 °C model but was not able to efficiently use that energy to produce biomass. At 4 °C, thermodynamic changes were predicted to prevent the utilization of the payoff phase reactions of glycolysis, resulting in the utilization of less efficient pathways to produce both energy and metabolic precursors. At 20 °C, the model was predicted to use similar pathways to produce energy as the 15 °C model but was predicted to have higher flux through these pathways, resulting in less of the carbon source being used to produce biomass and more of it being secreted as acetate. The analysis of the differential expression of genes between the temperatures provided indications of stress at both 4 °C and 20 °C providing further context to the metabolic changes seen in the models. This study highlights how metabolic flexibility can allow organisms to remodel their growth to broad ranges of conditions and demonstrates the utility of modeling approaches that integrate multiple methods and sources of data.

Author Summary

Metabolic changes are a central component of any organism's ability to survive and adapt to changes in environmental conditions. This study combines modeling approaches that account for the effects of gene expression changes and reaction thermodynamics on metabolic pathways. Using this integrated modeling approach, growth of *Shewanella psychrophila* WP2 at non-optimal temperatures was simulated predicting global changes in pathway utilization and metabolic efficiency between the conditions. The changes in efficiency were contextualized by predicted differences in reaction thermodynamics, changes in pathway utilization, and observed differences in gene expression. Taken together the combination of modeling and gene expression analysis helps to build a systems level view of the metabolism of WP2 at different temperatures. Overall, this study highlights how diverse metabolic changes can be within an organism when exposed to different conditions and highlights the utility of modeling approaches that integrate multiple data sources in expanding and contextualizing these changes.

Introduction

Temperature is a major driving force in microbial growth and physiology, causing physical changes in cellular structures that cells respond and acclimate to. Physical changes in the cell include altered enzyme stability [1–3], differences in reaction kinetics [1], and altered membrane fluidity [4]. When experiencing changes in temperature, microbial cells adjust their physiology through the production of heat

shock and cold shock proteins [5], altered gene expression patterns [6–8], and the production of different kinds of membrane lipids [4,9]. Responses to temperature do not happen in isolation within the microbial cell and can often involve broader changes in metabolism as the organism shifts its growth strategies to acclimate to the new condition. Some microorganisms respond to temperature changes through the induction of specific stress responses, which allow for short-term survival in changing environments [5,10].

The metabolic changes that occur during growth at non-optimal temperatures in mesophilic microorganisms have been studied extensively, but the adaptations of psychrophilic organisms are less understood. Cold shock responses to low temperatures are not always seen in psychrophiles, with many strains showing constitutive expression of proteins typically associated with a cold shock response in mesophiles [11,12]. The metabolic changes that occur in psychrophiles in response to low-temperature conditions generally include a decreased utilization of central carbon and energy production pathways and increased utilization of branched-chain amino acid and unsaturated fatty acid metabolism [9,13–16], while the regulation of other metabolic pathways like amino acid, nucleotide biosynthesis, and vitamin metabolism is highly variable between strains [15]. While the response of psychrophiles to higher temperatures is much less understood, there has been evidence of a temperatureinduced production of heat shock proteins [17] and broad changes in energy metabolism during high-temperature growth [18].

In addition to changes in specific metabolic pathways, global changes in the metabolic efficiency at different temperatures have been observed in many microbial
communities. Carbon Use Efficiency (CUE) is a measure of how much of a carbon growth substrate is used for growth versus how much of it is secreted as metabolic byproducts like carbon dioxide or acetate. Studies that have measured or estimated CUE in different microbes have shown that it varies broadly between microbial species [19] and that it can be altered by environmental factors like temperature [20– 22], pH [23], and the availability of other nutrients [24]. While CUE has been extensively studied in many soil microbial communities, little is known about it in psychrophilic bacteria. Changes in temperature have also been shown to lead to altered ATP concentrations in the cell in psychrophilic bacteria with some strains showing a decrease in cellular ATP concentrations at low temperatures [18] and others showing increases in ATP concentration [25]. These broader measures in efficiency can provide important context to specific changes in metabolic pathway utilization, allowing for a broader perspective on the effects of temperature on physiology.

Bacteria from the Shewanella genus have long been studied because of their broad environmental adaptations and diverse metabolic capabilities [26–29]. Bacteria in this genus have been broadly classified into two clades, one with mostly psychrophilic deep-sea strains referred to as Group 1, and one clade with adaptations to a broader range of environments referred to as Group 2 [29]. Recent studies have rapidly expanded this genus introducing new strains from both groups from a variety of new environments [30–32]. While Group 2 *Shewanella* have been extensively studied for their uses in bioengineering [33–35], Group 1 *Shewanella* have recently become a focus of studies related to their environmental adaptations to low temperature and high pressure [7,36–40]. The Group 1 *Shewanella* strain *Shewanella*

psychrophila WP2 exhibits the hallmark metabolic versatility that is seen in many *Shewanella* and is a psychrophile, but its growth in different conditions has not been investigated [26]. WP2 was isolated from benthic sediment in the South China Sea where the ambient environmental temperature was approximately 4 °C [41]. Its optimal growth temperature has been determined to be between 10 °C and 15 °C with an overall growth supporting temperature range between 0 °C and 20 °C [26,41]. Understanding how this organism grows at different temperatures can provide insights into the adaptations found in the *Shewanella* genus and more broadly within psychrophiles.

Genome-scale metabolic modeling has become a common technique to investigate bacterial metabolism and advancements in the development of Genome-Scale Models (GEMs) of metabolism and methods to simulate growth have allowed for GEMs to be applied to increasingly complex questions. Traditional simulation methods utilize reaction stoichiometry during the maximization of growth [42,43]. These stoichiometry-based approaches, however, often result in large solution spaces due to the lack of specific constraints across metabolic pathways. Newer methods have extended this framework to incorporate additional constraints as a way to approach new biological problems. An increasingly popular approach has involved the introduction of transcriptomic constraints into GEMs allowing for the effects of complex environmental factors like temperature to be accounted for based on the gene expression changes that occur in the organism. These methods typically involve the introduction of new constraints into a GEM that relate the utilization of metabolic reactions to their gene expression. One type of approach applied in algorithms like E-

Flux [44] and iMTBGO [45] involves directly limiting metabolic fluxes proportionally to the expression of their associated genes. The other major type of approach involves utilizing the gene expression data to generate context-specific models based on the identification of highly and lowly expressed genes in the transcriptomes. This type of approach is applied in algorithms like GIMME [46], INIT [47]and StanDep [48] and they typically start with a full GEM and then attempt to remove reactions from the GEM if they are associated with lowly expressed genes. These methods used for the integration of transcriptional data into GEMs have the benefit of being able to account for the broad changes that can be captured in a transcriptomes of an organism growing at two temperatures, but they can only account for the factor of temperature indirectly through the gene expression changes.

Modeling methods have looked to address the effects of temperature directly through the incorporation of additional constraints into the model, rather than indirectly through data like gene expression. Because temperature can have such broad effects on an organism's physiology, the simulation methods that account for temperature have addressed a variety of different factors including enzyme stability and folding at different temperatures [49] and reaction thermodynamics [50,51] but these methods have not been broadly applied to look at changes in metabolism that occur between different growth temperatures and their application is often hampered by the availability of thermodynamic or kinetic data for reactions. One of these approaches, Thermodynamics-Based Metabolic flux Analysis (TMFA) involves the incorporation of metabolite concentrations, thermodynamic constraints, and temperature to simulate metabolism while accounting for the feasibility of metabolic

reactions in a GEM and has been applied to simulate growth in model organisms like *Eschericia coli* [50,51]. The use of computational methods to predict standard Gibbs Free Energy of Reaction values like the Group Contribution [52] and Component Contribution [53,54] methods has allowed for methods like TMFA to account for mode thermodynamic constraints in GEMs, even when experimental measurements of these values are not available. In this study the effects of temperature are addressed using a combination of TMFA to simulate specific changes in reaction thermodynamics at different temperature and Gene Inactivity Moderated by Metabolism and Expression (GIMME) to address the broader changes in gene expression between different temperatures and to fill in some gaps in pathway where thermodynamic data is missing. The combination of these methods allows for the development of temperature-dependent versions of an overall GEM, which can be used to simulate the effects of temperature on metabolism.

In this study, the metabolic response of the psychrophilic *Shewanella* strain *S*. *psychrophila* WP2 was examined by combining transcriptomics and thermodynamicsbased genome-scale metabolic modeling. Transcriptomic profiles of the response of WP2 to growth at optimal, sub-optimal, and supraoptimal conditions revealed broad shifts in amino acid and nucleotide metabolism during non-optimal growth. Optimal growth was characterized by the high expression of genes in pathways typically associated with active growth. A modeling approach that combined transcriptomic and thermodynamic constraints into the WP2 GEM was used to simulate the growth of WP2 at optimal and non-optimal growth temperatures. These simulations revealed differences in metabolic pathway utilization at different temperatures, which explain

differences in the model's efficiency in converting the growth substrates to biomass and cellular energy. The simulations were further compared to the differential expression of genes in WP2 during growth at the three temperatures, providing a broader picture of how this organism's metabolism is remodeled during acclimation to different conditions.

<u>Results</u>

Temperature-dependent, thermodynamically constrained genome-scale models of WP2

The construction of temperature-dependent, thermodynamically constrained models was performed by integrating experimental growth measurements, thermodynamic properties of reactions, and gene expression profiles from optimal (15°C), supraoptimal (20°C), and suboptimal (4°C) temperatures (**Fig 1**). A GEM representing the complete metabolic potentials of WP2 was first developed, which contained 929 reactions, 789 genes, and 685 metabolites. The model represented the growth/no-growth phenotypes for all experimentally confirmed carbon sources (e.g., glucose, galactose, cellobiose, etc.) and electron acceptors (e.g., nitrate, TMAO, Fe³⁺, etc.), with the exception of acetate and fumarate, where growth was not observed in a prior experiment but genes for the metabolism of acetate and fumarate were identified in the WP2 genome (**Table A in Data S1**).

The WP2 GEM served as the basis for predicting thermodynamic constraints and establishing the temperature-dependent models. The standard Gibbs free energy change of reactions ($\Delta_r G'^\circ$) was assigned to over 93% (868 reactions) of the 929

reactions included in the WP2 GEM using the group contribution approach [52]. Three temperature-dependent models were subset from the overall WP2 GEM based on the identification of actively expressed genes from the late exponential phase transcriptomes and by applying growth constraints based on the experimentally measured growth rates under the three temperatures (Materials and Methods). A total of 87 reactions were associated with lowly expressed genes across all three temperature conditions and were subsequently not included in any the temperaturedependent models. These included functions in cofactor biosynthesis, nucleotide salvage pathways, compound transport and alternative carbon metabolism, with their low expression levels likely driven by the experimental media rather than the temperature conditions. In addition, 27 reactions, while showing a low expression level of their genes in all three conditions, were included in the temperature-dependent models due to their essential roles in cell envelope biosynthesis, cofactor biosynthesis, and nucleotide metabolism. Of the three temperature-dependent models, the 15°C model was more streamlined and contained the lowest number of reactions based on gene expression data, while the 4°C model had the highest number of reactions, including functions that were absent in the 15°C and 20°C models, such as purine degradation, aromatic and branched-chain amino acid metabolism, alternative carbon metabolism, phosphate and sodium transporters, and two peroxidases (Table B in Data S1).

The integration of thermodynamic constraints with the temperature-dependent models was achieved through the application of the TMFA approach [50,51,55], which resulted in the prediction of reaction fluxes, metabolite concentrations, and the

Gibbs free energy change of reactions ($\Delta_r G'$). The concentration of 62 intracellular metabolites were predicted to be constrained across all three temperature-dependent models (**Table A in Data S2**). For example, the concentration of ATP was constrained towards the upper bounds and the concentrations of ADP, AMP, and phosphate were constrained towards the lower bounds of intracellular metabolite concentrations across all temperatures, indicating the potential importance of ATP production in WP2. The concentrations of central carbon metabolites, including glyceraldehyde-3-phosphate (G3P), phosphoenolpyruvate (PEP), malate, and 2oxoglutarate (AKG), were differentially constrained in the different temperatures, highlighting potential temperature-dependent variations in the central metabolism of WP2 (**S1 Fig**).

Of the 671 thermodynamically constrained reactions that were in all three temperature-dependent models, 171 reactions were thermodynamically feasible in both directions (i.e., $\Delta_r G'$ spanning a range from negative to positive values), 462 reactions were constrained as monodirectional, but the directionality was consistent across all three temperatures, and the remaining 38 reactions showed differences in thermodynamic feasibility among different temperatures (**Table B in Data S2**). The central metabolic reactions, glyceraldehyde-3-phosphate dehydrogenase (GAPD), fumarase (FUM), and phosphate acetyltransferase (PTAr), were thermodynamically constrained to different directions among the different temperatures. While the GAPD reaction was constrained to the 1,3-bisphosphoglycerate (1,3 BPG) producing direction under 15 °C and 20 °C, it was constrained to the opposite direction under 4 °C (**S2 Fig**). Similarly, the phosphate acetyltransferase reaction (PTAr) was

constrained to the production of acetyl-phosphate (AcP) under 15 °C and 20 °C but was constrained to the production of acetyl-CoA (AcCoA) under 4 °C, leading to the utilization of distinct pathways in energy generation and production of precursor metabolites (Fig **2**). The fumarase (FUM) reaction, in contrast, had similar constraints under 4 °C and 15 °C permitting the production of malate from fumarate, while it was constrained to the opposite direction under 20 °C (**S3 Fig**). Other reactions were constrained to one direction under certain temperatures while being unconstrained at the others. For example, the glycolysis reactions, phosphoglycerate kinase (PGK), phosphoglycerate mutase (PGM), enolase (ENO), and pyruvate kinase (PYK), were thermodynamically constrained under 15 °C and 20 °C to the final production of pyruvate (PYR) from the pathway, while these reactions were thermodynamically unconstrained under 4 °C (**S2 Fig**).

Variability in metabolic fluxes between temperatures

A quantitative comparison of all metabolic fluxes in the 4 °C, 15 °C, and 20 °C simulations was performed with the flux values normalized by the biomass yield in each corresponding condition (**Table C in Data S2**). To assess the overall variability of the metabolic fluxes, flux ranges were measured by calculating the differences between the maximum and minimum feasible fluxes of each reaction under each simulation condition (**Materials and Methods**). The analyses revealed 88 reactions that were present in all three temperature-dependent models and carried variable fluxes in at least one of the three simulations. Interestingly, the 4 °C model had significantly higher flux variability than the 15 °C or 20 °C model based on a pairwise Wilcoxon

Rank Sum test, indicating potentially higher metabolic flexibility of WP2 under the 4 °C condition. In contrast, a low variability of metabolic fluxes was observed in the 15 °C and 20 °C models, and the flux ranges showed no significant difference between the two temperatures (**S4 Fig**). Another 93 reactions that had invariable fluxes in all three temperatures and had non-zero fluxes in at least one temperature, showed differences in the value of normalized metabolic fluxes among different temperatures. The N-Acetyl-D-Glucosamine (GlcNac) catabolism, PPP, and ACKr had higher biomass normalized fluxes in the 4 °C and 20 °C models than the 15 °C model. The citrate synthase (CS) and aconitase (ACONT) reactions of the TCA cycle carried higher normalized fluxes in the 4 °C and 15 °C models than the 20 °C model. A precursor reaction of the ED pathway, glucose-6-phosphate isomerase (PGI), had a higher normalized flux in the 4 °C model than either 15 °C or 20 °C models (**Table C in Data S2**).

As was documented for other known *Shewanella* species, WP2 lacks a complete Embden-Meyerhof-Parnas glycolytic pathway because an essential gene, encoding the 6-phosphofructokinase function, is missing in its genome [28]. The payoff phase of glycolysis and the gluconeogenesis pathway, however, are encoded in the WP2 genome. Hence, WP2 carries the metabolic potential of converting G3P to PEP via the GAPD, PGK, PGM, and ENO reactions, as well as the potential of producing fructose-6-phosphate (F6P) from G3P via the fructose-bisphosphate aldolase (FBA) and the fructose bisphosphatase (FBP) reactions. Additionally, the Entner-Doudoroff (ED) pathway and the pentose phosphate pathway (PPP) are also

encoded in the WP2 genome and could be used as alternative paths of carbon utilization.

The comparison of metabolic fluxes in the carbon metabolism pathways of WP2 revealed a remodeling of central metabolic processes in the acclimation to different temperatures (**Fig 2**). Specifically, the ED pathway was exclusively used in the 4 °C condition but carried no flux in the 15°C and 20°C conditions. In contrast, the payoff phase of glycolysis was active under 15°C and 20°C but was inactivated in the 4 °C model due to thermodynamic infeasibility of the GAPD reaction. This resulted in the dependency of the 4 °C model on phosphoenolpyruvate synthase (PPS), an ATP-consuming reaction required for the production of PEP, an essential compound and a precursor of downstream reactions. Next, the non-oxidative PPP was used in all three temperatures in a direction opposite to the canonical PPP, carrying higher fluxes at 4 °C and 20 °C and lower fluxes at 15 °C. Finally, the FBA and FBP reactions of gluconeogenesis carried twice the flux in the 4 °C than the 20 °C simulation, while they were not used in the 15 °C simulation (**Fig 2 and S3 Fig**).

Additional variations of metabolic fluxes were observed in substrate-level phosphorylation reactions. While the acetate kinase reaction (ACKr) was identified as an important mechanism of ATP production in WP2 under all three temperature conditions, its upstream reaction, PTAr, was utilized differently in the different temperatures (**Fig 2**). Under 4 °C, PTAr contributed to the conversion of AcP, which was generated from the non-oxidative PPP, to AcCoA, a precursor of the TCA cycle. Under 15 °C and 20 °C, PTAr was utilized in the opposite direction, converting the

AcCoA produced from the payoff phase of glycolysis into AcP and subsequently driving substrate-level phosphorylation via ACKr.

The utilization of the tricarboxylic acid (TCA) cycle reactions was also different among the three temperatures (**Fig 2 and S3 Fig**). Under 4 °C and 15 °C, the glyoxylate shunt was utilized by activating the isocitrate lyase (ICL) reaction that converts isocitrate to succinate. The succinate was subsequently converted to succinyl-CoA (SucCoA), an important metabolic precursor, and to fumarate and malate, leading back to the production of PYR via the malic enzyme (ME2) reaction. The glyoxylate shunt was not utilized in the 20 °C model. Instead, metabolic flux was directed from oxaloacetate (Oaa) to the production of succinate. Like many other *Shewanella* species, WP2 was characterized by the utilization of a partial TCA cycle. Despite variations in the mechanism of succinate production, the production of alpha-ketoglutarate (AKG) recruited the same pathway in all three temperatures, where Oaa and AcCoA acted as precursors for the production of AKG (**Fig 2**).

Temperature-dependent changes in carbon use efficiency and energy costs of biosynthesis

The remodeling of metabolic fluxes was further reflected in the calculation of global parameters that measure the carbon and energy efficiency of WP2 metabolism under different temperature conditions (**Materials and Methods**). Specifically, an over two times higher carbon use efficiency (CUE) was observed in the 15 °C model than the 4 °C or 20 °C models (**Figure 3A**). Such differences in CUE were largely attributed to the high efficiency of the 15 °C model in coupling ATP generation and the production

of biosynthesis precursors through the payoff phase of glycolysis. Although the 20 °C model similarly used the glycolysis pathway for ATP and biosynthesis precursor production, it had a higher ATP demand resulting in higher flux through the ACKr reaction, leading to potential carbon loss through the increased production of acetate. In contrast, the payoff phase of glycolysis was blocked in the 4 °C model due to thermodynamic infeasibility of the GAPD reaction. As a result, the process of ATP generation relied primarily on having higher flux through the ACKr reaction and higher acetate production (**Table C in Data S2**).

In line with the CUE measurements, the energy efficiency of WP2 was evaluated based on the combined measurements of ATP production and ATP consumption fluxes (**Materials and Methods**). The 20 °C model demonstrated a similar ATP production efficiency to the 15 °C model (**Figure 3B**), reflecting the shared capacity of utilizing the payoff phase of glycolysis, an efficient energy production and precursor biosynthesis pathway, under both temperature conditions. The ATP cost of biomass production, however, was higher in the 20 °C model than in the 15 °C model (**Figure 3C**), reflecting a higher ATP demand and the potential carbon loss via the increased production of acetate in 20 °C. The 4 °C model, in contrast, had lower ATP production efficiency (**Figure 3B**) and higher ATP cost in biomass production (**Figure 3C**) than the 15 °C model.

Overall, a global remodeling of metabolic fluxes in WP2 was revealed through the simulation of thermodynamically constrained models under supraoptimal (20°C) and suboptimal (4°C) temperatures as compared to the optimal (15°C) temperature. While the optimal temperature demonstrated the highest efficiency in CUE, ATP

production, and biomass production, the acclimation to suboptimal and supraoptimal temperatures resulted in varied remodeling of metabolic fluxes, with the former driven by changes in thermodynamic feasibility in the central metabolism and the later driven by the increased demand of ATP in biomass production.

Differential gene expression of WP2 across different temperatures and growth phases

A comparison of the gene expression profiles across the early exponential, late exponential, and stationary phases of WP3 growth further elucidated the different metabolic responses of the organism under the supraoptimal and suboptimal temperatures (Data S3). When WP2 was acclimated to the suboptimal temperature (4 $^{\circ}$ C) as compared to the optimal temperature (15 $^{\circ}$ C), genes encoding the ATP synthase (ATPS4r), pyruvate dehydrogenase (PDH), pyruvate formate lyase (PFL), and cytochrome c oxidase (CYOO2) reactions were significantly downregulated in the early and/or late exponential phases, genes encoding the NADH dehydrogenase reaction (NADH11/NADH13) were significantly downregulated in the stationary phase, while genes encoding the CS, ICL, malate synthase (MALS), and the purine allantoinase (ALLTN), and OHCU decarboxylase (5HPUDICDCs) reactions were significantly upregulated during the late exponential phase (Fig 4, Tables A, B, and C in Data S3). In contrast, the acclimation to the supraoptimal temperature (20 °C) was characterized by the upregulation of NADH dehydrogenase and the downregulation of genes encoding the XPK, PFL, and PYK reactions during late exponential phase (Fig 4, Table E in Data S3). These regulatory changes were largely consistent with the

simulation of metabolic fluxes. The PFL reaction carried higher fluxes under 15 °C than the suboptimal or supraoptimal temperature, and had a higher flux in the upstream glycolytic pathway relative to the 4 °C. In parallel, the ATP synthase reaction carried flux in the ATP-driven proton pumping direction at 15 °C but was inactive in either of the other two temperatures, indicating the potential abundance in ATP production at the optimal temperature. The TCA cycle reactions, CS and ICL, carried higher biomass normalized fluxes under 4 °C compared to 15 °C, indicating a higher reliance on these reactions during suboptimal conditions. Finally, the NADH dehydrogenase reaction carried a higher flux under 20 °C, indicating a potentially higher cost in redox balancing than either of the other temperatures.

In addition to the differential expression of metabolic genes, the comparison of transcriptomes highlighted regulatory variations in environmental responses, secretion systems, and motility (**Fig 4**). Signs of stress were observed at both the suboptimal and supraoptimal temperatures during early exponential phase, as the cultures were going through the initial period of acclimation to the different temperatures. At 4 °C, a possible stress response was observed through the significant upregulation of a putative cold shock protein, transposes and integrases), and TonB receptor functions in early exponential phase (**Fig 4, Tables A and H in Data S3**). At 20 °C, a possible heat shock response was indicated through the upregulation of a putative heat shock protein relative to 15 °C (**Figure 4, Table F in Data S3**), the upregulation of GroES chaperone genes, DNA damage repair genes, and redox stress-related genes relative to 4 °C (**Table G in Data S3**) and the upregulation of group II intron reverse transcriptases was observed during late exponential phase relative to both other

temperatures (**Figure 4, Tables E and H in Data S3**). Multiple genes related to the secretion systems were also differentially regulated. Specifically, a putative type III secretion system was significantly downregulated at 4 °C during late exponential phase, while a type VI secretion system was significantly downregulated at 20 °C throughout all growth phases (**Figure 4, Tables A, B, C, G, H, and I in Data S3**). Multiple flagellar proteins and the sigma factor *fliA*, a transcriptional regulator of the flagellar complex, were upregulated in the 4 °C condition during early exponential phase but downregulated in contrast to the 15 °C and 20 °C conditions during stationary phase (**Figure 5, Table A, G, and I in Data S3**). Overall, the changes in expression of both the metabolic and non-metabolic genes between the temperatures further highlighted the different responses of WP2 to different conditions and provided a broader context to the metabolic remodeling seen in the temperature-dependent models.

Discussion

Genome-scale metabolic modeling has been applied to a variety of different biological problems, but the incorporation of complex environmental factors like pH, pressure, or temperature into GEMs remains challenging. In this study, a thermodynamically and transcriptomically constrained GEM of *Shewanella psychrophila* WP2 was developed and used to simulate growth in optimal and non-optimal temperatures. The *Shewanella* genus has been studied through a variety of experimental and computational approaches because of their environmental and metabolic diversity. Multiple genome-scale models have been developed and applied to study metabolism in the *Shewanella*

genus including four models of strains from the broadly adapted Group 2 clade of the Shewanella [27,56] and two models from the deep-sea, low-temperature adapted Group 1[36,57] (Fig 5). The WP2 GEM represents a previously unmodeled clade within the Group 1 Shewanella and provides a platform to further investigate the complex adaptations to low-temperature that are present in the Group 1 Shewanella. An integrated modeling approach that combined transcriptomic and thermodynamic constraints was used to investigate temperature acclimation in WP2, resulting in predictions of metabolic phenotypes that broadly agreed with what was observed in transcriptomic analysis and provided context to the metabolic changes that occurred during growth at different temperatures. Growth at the optimal growth temperature of WP2, 15 °C, was characterized by a streamlined metabolism geared toward the efficient utilization of nutrients to produce energy and biomass. WP2's growth at the supraoptimal temperature of 20 °C showed a metabolic network that used similar pathways as the optimal condition but was less efficient at using cellular energy to produce biomass. Lastly, growth at the suboptimal, but environmentally relevant temperature of 4 °C was characterized by the lower efficiency production of energy and biomass caused by the rerouting of metabolic fluxes to overcome changes in the thermodynamic feasibility of central metabolic pathways.

The application of the integrated modeling approach to simulate WP2 growth at suboptimal, optimal, and supraoptimal temperatures predicted broad differences in metabolic pathway utilization between different temperatures. Due to the lack of the 6phosphofructokinase enzyme, the Embden-Meyerhof-Parnas (EMP) glycolytic pathway is incomplete in *S. psychrophila* WP2 and other *Shewanella* strains leaving

the Entner-Doudoroff (ED) and Pentose phosphate pathway as the only routes available for sugar catabolism [28]. These two pathways were utilized in different ways between the three temperatures. The 4 °C model was predicted to use a combination of the ED pathway and Pentose phosphate pathway to catabolize Nacetyl-D-Glucosamine to glyceraldehyde 3-phosphate, acetyl-phosphate, and pyruvate. In contrast the 15 °C and 20 °C models predicted that just the pentose phosphate pathway would be utilized to produce glyceraldehyde 3-phosphate and acetyl phosphate from N-acetyl-D-glucosamine. The result of these pathway utilization differences is changes in the production of glyceraldehyde 3-phosphate and acetylphosphate that can then be used to generate energy through substrate level phosphorylation reactions.

Changes in the reaction thermodynamics between the three temperatures result in a broad remodeling of metabolic fluxes, which alters how energy and biosynthetic precursors are produced in each temperature. In the 20 °C and 15 °C models' energy in the form of ATP is produced through the reactions of the payoff phase of glycolysis and through the production of acetate. The utilization of the payoff phase reactions of glycolysis also allows the models for these two temperatures to produce phosphoenolpyruvate, an essential biosynthetic precursor, through the same set of reactions. Because of the lower temperature, the glyceraldehyde 3-phosphate dehydrogenase reaction (GAPD) was predicted to become thermodynamically unfavorable compared to the 15 °C and 20 °C conditions. This resulted in the 4 °C model not utilizing these payoff phase reactions, and instead rerouting fluxes and relying primarily on the acetate production pathway for its production of ATP. The

lower efficiency of this metabolic strategy is seen in the decrease in the amount of ATP produced per unit of GlcNac in the 4 °C model compared to the other two temperatures. Coupled with the lowered capacity to efficiently produce ATP at 4 °C is a corresponding shift toward the utilization of energy consuming reactions to produce phosphoenolpyruvate. To overcome the lack of production of phosphoenolpyruvate from the payoff phase reactions of glycolysis, the 4 °C model utilized the phosphoenolpyruvate synthase (PPS) reaction to produce phosphoenolpyruvate from pyruvate, which consumes ATP and contributes to the lower ATP consumed per biomass efficiency of the 4 °C model. The downregulation of genes involved in the payoff phase of glycolysis has been observed in multiple strains of psychrophilic bacteria including *Pseudoalteromonas haloplanktis* TAC125 [14], *Psychrobacter sp.* PAMC 21119 [58], and *Sphingopyxis alaskensis* [13][59][13]can lead to psychrophilic organisms having to maintain high concentrations of ATP in order to keep certain reactions favorable [25]

The 4 °C model had a much higher reliance on the acetate production pathway than the other two temperatures. This was a result of the model not being able to produce energy through the glycolytic substrate-level phosphorylation reactions, and instead needing to produce nearly all of its ATP through acetate production. This increase in flux through the acetate production pathway has been linked in *Shewanella oneidensis* MR-1 to an increased reliance on substrate-level phosphorylation during both aerobic and anaerobic growth [60–62], indicating that this feature may be a central part of *Shewanella* metabolism. These changes in the production of acetate coupled with the lack of energy being produced from the substrate level

phosphorylation reactions of the glycolytic pathways, contributes to the changes in efficiency seen in at the suboptimal temperature. At 4 °C the reliance on acetate production as the only route of ATP production is reflected in the lower ATP production efficiency and lower CUE relative to the 15 °C model. Unlike the 4 °C model, the 20 °C model is not predicted to have a lower ATP production efficiency than the 15 °C model and uses many of the same pathways to produce energy as the 15 °C model. Despite this similar ability to produce ATP to the 15 °C model, the CUE is lowest in the 20 °C model and the ATP cost to produce biomass is the highest among the three temperatures. Where the differences in these efficiency metrics at 4 °C can be explained by shifts in pathway utilization, the differences in 20 °C are instead based on the higher maintenance cost that is estimated at the supraoptimal temperature. This higher maintenance requirement requires the 20 °C model to divert more carbon through the acetate production pathway to produce more ATP, as can be seen through the higher normalized flux through the acetate kinase reaction at 20 °C. This extra ATP that is produced does not get used in the 20 °C model in biomass producing pathways, but instead just goes toward the non-growth associated maintenance. In total the differences between the temperatures are a result of multiple factors that end up resulting in changes in efficiency and pathway utilization in the models.

In addition to the broad changes observed in metabolic efficiency between temperatures, altered utilization of the TCA cycle was also observed between temperatures. Shewanella strains have been previously observed to utilize partial TCA cycles in both aerobic and anaerobic conditions, primarily relying on this pathway for the production of metabolic precursors [60,62–64], and this feature was observed in

the WP2 model and transcriptomes as well. All three temperature-dependent models predicted a partial utilization of the TCA cycle, and the genes for citrate synthase, isocitrate lyase, and malate synthase were all upregulated at 4 °C compared to the other two temperatures. Psychrophilic bacteria have had displayed a variety of changes in this pathway in response to low temperatures, with many strains showing a general decrease in the expression of TCA cycle genes [13,14,58], and some marine strains showing increased expression of portions of the TCA cycle, especially in the reactions that convert citrate to alpha-ketoglutarate [13,14,65] and the reactions that make up the glyoxylate shunt [59]. The utilization of a partial TCA cycle, similar to other *Shewanella* combined with the differential expression of genes in this pathway, highlight the importance of the TCA cycle within *Shewanella* metabolism and hint at broader roles that this pathway may have during acclimation to different conditions.

A comparison of gene expression between the three temperatures provided additional insights into the responses of WP2 at each temperature and helped contextualize the model predictions. The downregulation of genes related to energy metabolism like the subunits of NADH dehydrogenase and cytochrome oxidase at 4 °C is a common feature of other psychrophiles during low temperature growth [9,15,66,67], and are often indications of a transition toward a metabolic strategy that is geared toward maintaining slower growth [13–15,58,66]. These broad changes in metabolic gene expression were coupled with signs of a possible stress response including the expression of cold shock proteins, phage shock proteins, and mobile genetic elements. Taken together with the model predictions, this indicates that WP2 likely goes through a stress response during low-temperature acclimation but is able to

remodel how its metabolic pathways are used to overcome thermodynamic changes and shift its growth strategy. The 20 °C model primarily predicts a lower efficiency metabolic strategy due to the diversion of energy away from growth and toward maintenance costs. This model prediction is accompanied by various signs of stress in the 20 °C transcriptomes especially when compared to the low temperature condition. The induction of a stress response to the high temperature growth helps explain the predicted changes in efficiency seen at 20 °C and is likely reflective of the inability of WP2 to efficiently survive near the upper limit of its growth supporting temperature range.

Overall the metabolic response of WP2 to low-temperature growth showed some consistent trends with other psychrophiles, including the downregulation of portions of the central carbon metabolism [13,14,58] and the upregulation of specific amino acid metabolic pathways [9,15,66,67]. The WP2 metabolic pathways also showed hallmark characteristics of *Shewanella* metabolism that are not always consistent with other psychrophilic bacteria, including a heavy reliance on acetate production for the generation of ATP [60–62], the utilization of an incomplete TCA cycle for the production of metabolic precursors [60,62,63], and low reliance on oxidative phosphorylation during growth [60,61]. The integrated view of WP2 metabolism provided by the model predictions and transcriptomic analysis in these different temperatures demonstrates the diversity in metabolic changes that occur during acclimation to different conditions. The changes in WP2 demonstrated that the small shifts in pathway utilization observed between the temperatures can lead to large impacts on WP2's growth efficiency, providing additional context to these

observations. These kinds of approaches highlight the benefits of accounting for more than just stoichiometric constraints in a GEM and promise to allow for the simulation of increasingly complex metabolic phenotypes.

MATERIALS AND METHODS

WP2 Growth Experiments

Inoculation of three biological replicates for each growth temperature (4°C, 15°C, and 20°C) were performed in 150 mL of fresh LMO-812 media [36] with 1mL of inoculum obtained from exponential growth culture at the optimal temperature (15°C) in the 2216 Marine Medium (Difco). The cultures were grown with 5 mM GlcNac as the sole carbon source under aerobic conditions at different temperatures with shaking, and an initial OD600 of 0.002 was measured for each inoculation. Turbidity was monitored throughout the growth phases of the cultures, and the OD600 values were converted to gram dry weight values for each culture using a previously established relationship between OD and dry weight biomass in *Shewanella [56]*. Growth rates were calculated based on the periods of exponential growth for each temperature condition (**S5 Fig**).

Transcriptome sampling and Differential Expression Analysis

Samples for transcriptome sequencing were taken from the early exponential, late exponential, and stationary phases for each replicate in the 4°C, 15°C, and 20°C cultures (**S5 Fig**). Two biological replicates were prepared from each of the targeted growth phases for each temperature, where 2 mL of samples were taken from each

replicate, centrifuged at 12000 times gravity for 2 minutes, and the cell pellet was used for the application of RNA extraction and sequencing using services provided by the Sangon Biotech in Shanghai, China. Total RNA was extracted from the cell pellets and cleaned using the Ribo-off rRNA depletion kit. cDNA libraries were prepared using the VAHTS Stranded mRNA-seq V2 Library Prep kit for Illumina. Paired-end sequencing was performed on the HiSeq X Ten system generating 2 x 150 bp reads.

Raw transcriptome reads were quality filtered using Trimmomatic version 0.33 [68] to remove (1) any leading or lagging bases with quality scores less than 20, (2) any Illumina adapters, with a 5 bp sliding window filtering and a quality score of 20 or higher, and (3) any sequences shorter than 50 bp. The trimmed reads, both paired and unpaired, were then mapped to the WP2 genome using BBMap version 38.81 [68], with all default settings except for requiring a minimum identity for mapping of 90%. The mapped reads were then used to generate count tables of the number of transcripts that map to each gene using the featureCounts program version 1.6.3 [69] with default settings. Differential expression of genes among different growth phases and across different temperature conditions was identified using Deseq2 version 1.22.2 [70]. Genes were considered to be differentially expressed if the log fold change between conditions was greater than 2 or less than -2 and if the adjusted p-value for the differential expression of the gene was less than 1×10^{-3} . Temperature-dependent models were constructed based on the transcripts per million (TPM) values using the equation: $TPM = 10^6 * \frac{reads mapped to gene / gene length}{\sum_{all genes}} (reads mapped to gene / gene length)} [71,72].$

Genome-scale Metabolic Reconstruction

A genome-scale model was constructed for WP2 based on ortholog mapping and manual curations (**Table C in Data S1**). A draft model was first created using the *psammotate* function provided in the PSAMM software package version 1.1 [73]. Five template models were used for the application of the *psammotate* approach, including models of *Shewanella piezotolerans* WP3 [36], *Shewanella oneidensis* MR1 [56], *Shewanella* sp. MR4, *Shewanella sp.* W3-18-1, and *Shewanella denitrificans* OS217 [27]. Following the initial reconstruction, manual curations were performed by combining literature information, reference databases, and identification of functional domains. A biomass objective function for WP2 was constructed following standard procedures [43] combining experimentally measured composition of macromolecular components [26,41,74] and inferred values from other *Shewanella* strains [27,36,56] (**Table D in Data S1**). The complete WP2 GEM was validated through comparison to previously reported growth phenotypes for WP2 on the utilization of carbon sources and electron acceptors (**Table C in Data S1**).

Identification of Thermodynamic Constraints

Standard Gibbs free energy change of reaction $(\Delta_r G'^\circ)$ were calculated for reactions in the WP2 model under the standard conditions of 25°C and a pH 7 using The Group Contribution python package [52] (**Table E in Data S1**). In order to run the Group Contribution approach on individual reactions in the WP2 model, all metabolites participating in a reaction were represented in one of two forms: (1) identifiers in the Thermodynamics of Enzyme-Catalyzed Reactions Database (TECRdb)[75], which provides thermodynamic data for a collection of enzyme-catalyzed reactions; (2)

metabolite structure represented as Simplified Molecular-Input Line-Entry System (SMILES) strings (**Table C in Data S1**), which can be used to derive information related to metabolite properties for the $\Delta_r G'^\circ$ calculation. Metabolites in the WP2 model were first mapped to the TECRdb based on their names and formulas, and when a mapping is not available, metabolite structural information was collected from the Pubchem Database [76] in the form of the canonical SMILES strings. When SMILES strings were not available in the Pubchem database, for example, for chitin, eicosapentaenoic acid (EPA), 3-hydroxy-11-methyldodecanoic acid, 11-octadecenoic acid, and the fatty-acyl ACP compounds, metabolites structures were manually drawn using the MarvinSketch application version 19.11 (ChemAxon, https://www.chemaxon.com) and exported using the SMILES export function. The biomass objective function, macromolecular biosynthesis reactions, and several reactions in the cell wall biosynthesis pathway were not mapped with $\Delta_r G^\circ$ calculations due to the complexity of the metabolites involved.

Reconstruction of Temperature-dependent Models

Temperature-dependent models were reconstructed from the WP2 model using the PSAMM implementation of the GIMME algorithm, which creates context-specific metabolic networks based on gene expression data [46]. The transcriptome of each replicate from the 4°C, 15°C, and 20°C conditions was used as input data for running the PSAMM *gimme* (version 1.1), along with the complete genome-scale metabolic reconstruction of WP2. A gene expression threshold of no less than 35 TPM was applied, and the biomass objective constraints were set based on the experimentally

measured growth rate in each temperature (S5 Fig). The temperature-dependent models were then constructed based on a union of the metabolic functions that were either actively expressed or required for biomass productions in the replicate models. The resulting metabolic reactions in each temperature-dependent model were classified into two categories: Expressed, indicating reactions catalyzed by genes with higher expressions than the TPM threshold applied in PSAMM *gimme* in either replicate of a temperature; Used_Below, indicating reactions essential for the production of biomass but associated with gene subunits of relatively low expression (i.e., below the TPM threshold) in both replicates. Reactions associated with genes with low expressions and were not essential for biomass generation in a given temperature condition were not included in the model of that specific temperature (Table B in Data S1).

Metabolic simulations with temperature-dependent, thermodynamically constrained models

Using the temperature-dependent models, thermodynamics-based metabolic flux analysis [50,51] was performed using the *tmfa* function implemented in PSAMM (version 1.1). The PSAMM *tmfa* implementation takes as input a configuration file that references the $\Delta_r G'^{\circ}$ estimations as described in a prior section (**Table E in Data S1**), a list of reactions excluded from the $\Delta_r G'^{\circ}$ calculation due to the high complexity of the involved metabolite's structures (**Table F in Data S1**), a list of transport reactions mapped to parameters (i.e., net charge and net protons transported from outside to inside of the cell) that can be used to calculate energy associated with

electrochemical potential and pH gradient across the cell membrane (Table G in Data S1), and definitions of metabolite concentrations and exchange constraints (Tables H and I in Data S1). By default, all metabolites were constrained to be within a range of 1e-5 to 0.02 mol/L following prior studies [50,77]. All compounds present in the LMO-812 media were constrained by setting the upper bound of their concentrations according to the media composition. If the concentration of a compound was lower than the default lower bound (1e-5 mol/L) in the media, then the lower bound of its concentration was set to two orders of magnitude lower than its upper bound to allow for the potential fluctuation of compound concentrations. Following prior conventions [50], the concentrations of two metabolites, n-carbamoyl-L-aspartate and (S)dihydroorotate, were expanded with a range from 1e-6 to 0.05 mol/L, to enable thermodynamic feasibility in an essential dihydroorotase (DHORTS) reaction (Table H in Data S1). The exchange flux constraints for the TMFA simulation were formulated based on the experimental media and to allow the diffusion of metabolic products. The exchange constraints of small molecules and metal ions in the media were set as the default upper and lower bounds of the model, and the uptake bound of oxygen was set according to the solubility of oxygen in liquid media under different temperatures (**Table I in Data S1**). An ATP maintenance equation, representing an ATP-consuming non-growth-related maintenance cost to the cell, was introduced to each temperature-dependent model and was constrained for each temperature condition by specifically fitting the computationally predicted biomass production rates to the experimentally measured growth rates (S5 Fig). The ATP maintenance constraint was determined for each temperature via a robustness analysis, where the

ATP maintenance fluxes were constrained to successively increasing values while the biomass yields were profiled. An intersection between the experimentally measured and the computationally simulated biomass was identified for each temperature condition, and the ATP maintenance constraints were pinpointed based on a linear fitting over data points immediately surrounding the experimentally measured biomass (S6 Fig).

To probe for the utilization of metabolic pathways under different temperature, ranges of feasible values were predicted for the Gibbs free energy of reactions $(\Delta_r G')$, metabolite concentrations, and metabolic fluxes while constraining the temperaturespecific parameters. For example, the biomass production was constrained based on the experimentally measured growth rate in each temperature, the temperature parameter in the $\Delta_r G'$ estimation was based on the different temperatures in Kelvin, and the oxygen exchange flux was constrained based on the solubility of oxygen at a given temperature. For the direct comparison of pathway utilizations across the different temperatures, individual reaction fluxes were normalized by the biomass flux of each simulation (Table C in Data S2). An overview of the flux variability was achieved by calculating the range between maximum and minimum fluxes of each reaction, and subsequently comparing the overall distribution of temperature variability among the temperature-dependent models. Statistical significance was estimated based on a pairwise Wilcoxon rank sum test using the 'pairwise.wilcox.test' function in R with a significance threshold of p-value less than 0.05. The carbon use efficiency (CUE) was calculated for each simulation using the equation CUE =(Carbon atoms consumed – Carbon atoms secreted) following an existing approach[19], Carbon atoms consumed

where all the carbon-containing exchange compounds were grouped into lists of consumed or produced metabolites based on the direction of their exchange fluxes in a simulation, their corresponding fluxes were scaled based on the number of carbon atoms in each compound, and sums of the scaled fluxes were taken for the list of consumed and produced metabolites, respectively, to obtain the carbon atoms consumed and the carbon atoms secreted parameters in the CUE equation. To calculate the total amount of ATP produced or consumed in a model simulation, the metabolic flux of each reaction that involved ATP was multiplied by the stoichiometry of ATP in that reaction, resulting in normalized fluxes where positive values indicated the production of ATP and negative values indicated the consumption of ATP. The ATP production per unit of carbon source was calculated through dividing the sum of all normalized ATP-producing fluxes by the exchange flux of the carbon source (i.e., GlcNac). The ATP consumed per biomass gram dry weight (gDW) was calculated through dividing the sum of all normalized ATP-consuming fluxes by the biomass flux, excluding the ATP maintenance flux.

Phylogenetic Positioning of WP2

Orthologs were identified among WP2, and 44 additional complete genomes of the *Shewanella* genus based on the identification of bidirectional best BLAST hits, as documented in prior studies [36,78]. Five *Gammaproteobacteria* were included as outgroups for the phylogenomic reconstruction (*Pseudoalteromonas haloplanktis*, *Colwellia psychrerythraea*, *Psychromonas ingrahamii*, *Photobacterium profundum*, and *Moritella viscosa*). Conserved single-copy genes (CSCGs) were identified based

on the ortholog mapping. A multiple sequence alignment was built for the encoded protein sequences of each CSCG using MUSCLE version 3.8.31 [79]. The individual alignments were then concatenated as the input for phylogenetic reconstruction using RAxML version 8.2.3 [80] with the JTT substitution model and GAMMA model of rate heterogeneity. Support values were estimated by running 100 bootstrapping replicates. The phylogenomic reconstruction was visualized using iTOL [81], where clades containing multiple strains of the same species were shown in a collapsed view.

Data and Software Availability

Modeling approaches implemented in this study are accessible through the open source PSAMM software, release v1.1 and are freely available in a git repository: <u>https://github.com/zhanglab/psamm</u>. The WP2 GEM along with all input data for the TMFA simulations are available on GitHub at the following address:

https://github.com/zhanglab/GEM-iWP2.

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Figures for Manuscript II



Fig 1: Modeling development and simulation pipeline showing the steps involved in generating the integrated temperature-dependent models and performing simulations for growth at each temperature.



Fig 2: Pathway diagram showing the direction of fluxes through metabolic reactions in the different temperature simulations. Solid lines indicate that the flux of the reaction is always in the same direction, while dashed lines indicate that the reaction flux is variable and can be zero. Black lines represent all three temperatures, blue represents 4 °C, yellow represents 15 °C, and red represents 20 °C. Pathways are indicated by shaded boxes around groups of reactions.



Fig 3: A) Carbon utilization efficiency for the 4, 15, and 20 °C simulations. B) Maximum ATP produced per mmol of carbon source utilized. C) ATP cost (mmol) required to produce 1 gDW of biomass.



Fig 4: Heatmap showing selected significantly differentially expressed genes between temperatures. Comparisons are shown for the 4 °C and 20 °C conditions relative to the 15 °C condition, with red indicating that the gene was more highly expressed in that temperature relative to 15 °C and blue indicating that the gene was lowly expressed relative to the 15 °C condition. Comparisons are shown between the temperatures for the early exponential phase, late exponential phase, and stationary phase transcriptomes. Comparisons that were significant are highlighted with a black outline in the heatmap.



Tree scale: 0.1

Fig 5: Phylogenetic tree of the Shewanella genus. Clades with multiple strains of the same species are collapsed into shaded triangles. Bootstrapping values greater than 70 are shown on the tree. Blue stars indicate strains with previously published GEMs. The red star marks S. psychrophila WP2.

Supplemental Figures for Manuscript II



S1 Fig: Plots of feasible ranges the concentrations of selected metabolites involved in central metabolic processes. Ranges based on the 4 °C temperature-dependent model are shown in blue, the ranges from the 15 °C model are shown in yellow, and the ranges from the 20 °C model are shown in red.



S2 Fig: Plots of feasible ranges for the $\Delta rG'$ of reactions in the central carbon metabolism pathways based on TMFA simulations for the temperature dependent models. Ranges based on the 4 °C temperature-dependent model are shown in blue, the ranges from the 15 °C model are shown in yellow, and the ranges from the 20 °C model are shown in red. N-acetyl-D-glucosamine metabolism reactions are shown with a blue background, glycolytic and gluconeogenic reactions with orange, Entner-Doudoroff reactions with purple, pentose phosphate reactions with red, acetate production reactions with green, and TCA cycle reactions with yellow.



S3 Fig: Plots of feasible ranges the fluxes of reactions involved in central carbon metabolism pathways based on TMFA simulations for the temperature dependent models. Ranges based on the 4 °C temperature-dependent model are shown in blue, the ranges from the 15 °C model are shown in yellow, and the ranges from the 20 °C model are shown in red. N-acetyl-D-glucosamine metabolism reactions are shown with a blue background, glycolytic and gluconeogenic reactions with orange, Entner-Doudoroff reactions with purple, pentose phosphate reactions with red, acetate production reactions with green, and TCA cycle reactions with yellow.



S4 Fig: Boxplots showing the distribution of normalized flux ranges from the 4 °C, 15 °C, and 20 °C model simulations for 88 reactions that were present in all three temperature-dependent models and had a variable flux in at least one simulation. Significant differences in the distributions of flux ranges based on a pairwise Wilcoxon Rank Sum test are indicated by the asterisks and bars above the plots.



S5 Fig: Growth curves for WP2 growth experiments at 4 (blue), 15 (yellow), and 20 (red) °C. Asterisks indicate timepoints where RNA-Seq samples were taken. The solid lines indicate the region of the exponential growth over the growth curve.



S6 Fig: Scatter plots showing the ATP maintenance reaction flux vs the biomass flux for each of the three temperature subset models. The x-axis shows the flux through the ATP maintenance reaction, with higher values increased hydrolysis of ATP. The target biomass flux is indicated by a horizontal blue line and the required ATP maintenance flux to achieve this biomass is shown as a vertical blue line. The linear region used to identify the required ATP maintenance to reach the target biomass flux is indicated by a red solid line.

Manuscript III

Publication Status: Formatted for submission to Nature Communications Title: Investigation of the Structure of Element Transfer Networks within Metabolism

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ABSTRACT

Previous analyses of metabolic networks have provided insights into the organization and robustness of metabolism, but these analyses have been affected by the methods used to represent the networks. In this study, metabolic networks were generated based on the annotations of prokaryotic genomes in the KEGG database using previously established methods and a new application of the FindPrimaryPairs algorithm. A comparison of the different network representations revealed significant differences in network structure and scale-free properties, depending on the representation. Elementbased subsetting of the FindPrimaryPairs networks demonstrated the separate influence of carbon, nitrogen, and phosphorus metabolism within the overall network and highlighted the scale-free properties of the phosphorus metabolism. These properties were further investigated through reaction deletions in three published genome-scale model-based networks, revealing that while the core functions required for growth do not have a scale-free organization, the overall networks do. This study highlights the utility of the FindPrimaryPairs function in representing metabolic networks and demonstrates the need for further network analyses utilizing this type of network representation.

INTRODUCTION

Metabolism dictates how organisms respond to their environment, interact with other organisms, and adapt to new conditions. The study of the metabolism of microorganisms has provided a wealth of information about metabolic pathways and the physiology of growth. While metabolism has classically been studied through *in*

vivo culturing-based methods, the advancement of genome sequencing technology has led to an increase in the availability of genetic information, even for organisms that are not isolated in pure cultures. This genomic information has allowed for the prediction of what metabolic functions could be present in an organism based on its gene content. The widespread availability of genomic data and the rapid increase in the number of available genomes has led to the development of extensive metabolic databases like KEGG and MetaCyc, which include metabolic predictions for thousands of organisms from all three domains of life ^{1,2}. The availability of these metabolic predictions allowed metabolism to be studied in many novel ways such as through the development of *in silico* representations of an organism's metabolism called Genome-Scale Models (GEMs) ^{3–6} and the analysis of metabolism as a mathematical network ^{7–} ⁹. In particular, the application of graph theory to study metabolism as a mathematical network has led to many new insights related to the evolution and flexibility of metabolism ^{7–9}.

Graph theory has proven to be a valuable method for the analysis of a variety of natural and artificial systems ^{10–14}, but its application to metabolism remains challenging. The field of Graph theory involves the study of graphs, or networks, which represent connections (edges) between nodes (objects). In the application of graph theory to metabolism, these networks typically consist of a set of metabolites, which are the nodes, connected by metabolic reactions, which are the edges ^{15–17}. These connections are typically based on the stoichiometry of the metabolites in each reaction, where all substrates will be connected through edges to all products in a reaction. While the analysis of these metabolic networks has provided some insights

into network structure and organization ^{7–9,18}, the application of these methods has often been hampered by the ability to represent the metabolism in an accurate and meaningful way. Multiple studies have identified that metabolic networks tend to be highly centralized, have very short distances between metabolites, and to be dominated by highly connected metabolites like protons, water, ATP, and NADH¹⁸⁻²¹. These metabolites tend to be involved in many reactions as byproducts or as currency metabolites, where they participate only as cofactors related to the transfer of electrons or protons ²⁰. The outsized influence of these currency metabolites and small molecules has made it difficult to examine many properties of metabolic networks and many studies have started to handle them through filtering and removal of these types of nodes from the network entirely ^{9,22}. The removal of these nodes has resulted in much less densely connected networks with highly modular structures revealing network topologies that had previously been missed when currency metabolites were present in the networks ^{18,23,24}. The differences seen in network topology when using these different network representations highlights the importance of not only what metabolic pathways and reactions are included in a network, but also how they are represented.

An alternative to stoichiometry based metabolic network representations is to represent connections between metabolites based on the conserved chemical structures that are shared between substrates and products in reactions. In this kind of network representation, connections are only formed between a substrate and product if they share elements, meaning that the resulting network is representative of the actual biochemical transformations that occur in metabolic pathways ²¹. This approach has

resulted in dramatically different network representations compared to the stoichiometry-based approaches, where the metabolic networks had longer path lengths and were less clustered around currency metabolites, but the application of these methods relied on the availability of detailed metabolite structural information which has limited their broader application ^{21,25}. The recent development of the MapMaker ²⁶ and FindPrimaryPairs ²⁷ algorithms has allowed for the efficient prediction of the shared structures between substrates and products in metabolic reactions through the use of reaction stoichiometry and metabolite formulas, but these algorithms have not been extensively applied in the study of metabolic networks. Furthermore, a thorough comparison of metabolic networks generated using stoichiometry-based approaches to networks based on reactant/product pair predictions is lacking and is needed to fully understand the benefits and drawbacks of different network representation methods.

A major implication of the differences between network representation methods is the effects that they could have on the analysis of global network organization and structure. Two major structural properties that have been analyzed in metabolic networks have been scale-free and small-world properties. Small-world networks are characterized by having clusters of tightly connected nodes with links between the clusters ^{28,29}. This structure leads to the small world networks having a short mean path length, meaning that the distance between any two nodes is relatively small, and leads to these kinds of networks being robust to deletions of nodes or edges ^{7,30,31}. Metabolic networks have been described as generally having small-world

metabolic pathways ^{7,8,32,33}. In addition to having small-world properties, metabolic networks have also been described as having scale-free properties though these claims have varied across studied ^{8,32,34,35}. Scale-free networks are characterized by having degree distributions that follow a power-law distribution where a few nodes have many connections, while most of the nodes have only a few connections ^{34,36,37}. While some analyses of metabolic networks have found scale-free properties ^{34,36,37}, others have claimed that these properties are artifacts that arise due to the presence of currency metabolites and small molecules in the metabolic network representations ^{38,39}. Small-world and scale-free properties have been suggested to have biological meaning related to the evolution of metabolic pathways ^{32,40}, the robustness of organisms to mutation ^{41,42}, and the adaptability of organisms to different environments ⁴³. The differences between network representation methods make it difficult to fully understand these network properties and draw biologically meaningful conclusions from them.

In this study the effects of different network representation methods on metabolic network structure were analyzed, revealing the large effect that network construction approaches can have on network properties. Three network representation methods were used to generate metabolic networks based on the KEGG and MetaCyc databases, with two of the representations being based on previously used methods that rely on reaction stoichiometry, and one newly developed representation based on reactant/product pair predictions using the recently developed FindPrimaryPairs algorithm. The comparison of network descriptive statistics between different network representations demonstrated the large influence of small molecules and currency

metabolites on network structure corroborating what had been observed in previous studies. An analysis of small-world properties revealed that these properties were almost always present regardless of network representation method. In contrast the analysis of scale-free properties in metabolism suggested that the scale-free properties seen in metabolic networks largely come from the transfer of phosphorus groups in substrate level phosphorylation reactions. Lastly the robustness of the small-world and scale-free properties of metabolic networks were examined through random deletion experiments done with published GEMs. These simulations demonstrated that the maintenance of essential functions required for growth had a heavy influence on the scale-free properties of metabolism. Overall, this analysis highlights the importance of network representation methods on the structure and analysis of metabolic networks. The application of the FindPrimary pairs algorithm allows for the efficient generation of element transfer-based networks, which allows for the examination of underlying metabolic structures that is not possible with stoichiometry-based networkrepresentations. The further investigation of these networks and their properties promises to expand our understanding of the evolution and function of metabolism in different organisms.

RESULTS

Network Representations

Metabolic networks representing organisms in the domains Bacteria and Archaea were generated based on genome annotations from the KEGG database using three network representation methods, with two methods replicating previous studies and one based

on the application of a recently developed algorithm (Fig. 1). First, an All-Pairs (AP) network representation was developed to replicate a common type of network representation used in prior studies ^{8,15,44}, where each metabolite was included as a node and edges were used to connect all substrates to all products in each reaction (Fig. 1A). Second, an All-Pairs Filtered (AP-filtered) network representation was developed to replicate another commonly used network representation ^{9,18,44,45}, where the network was made by removing nodes representing 'currency metabolites' (Supplemental Table S1), which are metabolites of high turnover and are involved in diverse metabolic processes ^{18,24}, and their associated edges from the corresponding AP network (Fig. 1B). Lastly, a new, FindPrimaryPairs (FPP) network representation, was developed based on the application of the recently developed FPP algorithm that identifies element-transferring reactant-product pairs from genome-scale metabolic reconstructions ²⁷. In the FPP network, an edge was introduced for a substrate-product pair only if transferring of elements was predicted in the pair based on the FPP algorithm (Fig. 1C). Additional modifications of the network representations involved the subsetting of metabolic networks based on the composition of elements in the metabolites. For example, carbon-based networks were constructed from the AP, APfiltered, and FPP networks by keeping only the carbon-containing metabolites and their associated edges (Fig. 1D-F). Other element-based networks were constructed similarly for the nitrogen- or phosphorus-containing metabolites. A total of 3799 bacterial and 240 archaeal metabolic networks were built based on genome annotations in the Kyoto Encyclopedia of Genes and Genomes (KEGG) database¹. The network representations were derived for each organism based on the AP, AP-

filtered, and FPP definitions and the carbon, nitrogen-, and phosphorus-based networks corresponding to each definition (**Materials and Methods**).

Effects of Network Representations on Network Topology

An overview of the distribution of node degrees revealed potential variations in network topology (Fig. 2). The AP-filtered network is the most distinct among the three all-element representations due to the removal of currency metabolites in the network. The FPP network showed a similar profile to the AP network in the node distributions, with a slightly higher fraction of nodes ranked as the 10% least connected due to the removal of edges that do not contribute to element transfer. Highly connected nodes with degrees ranked in the top 5% of each network were identified, and the most frequently occurring high degree nodes were summarized for each representation (Supplemental Table S2). As expected, the AP networks were characterized by the high connectivity of common cofactors and small molecules known as the currency metabolites. For example, water, protons, phosphate, ATP, and adenosine diphosphate (ADP) were among the top 5% nodes of highest degrees for over 99% of the AP networks analyzed. The FPP networks similarly ranked many currency metabolites as the most highly connected nodes, as seen in the AP networks, but the average degree of the top connected nodes was scaled down due to the requirement of element-transferring edges. In contrast, the AP-filtered networks ranked some of the common precursor metabolites (e.g., glutamate, adenosine monophosphate (AMP), pyruvate) as the highest connected nodes, reflecting the removal of currency metabolites seen in the AP networks (Supplemental Table S2).

Descriptive statistics summarizing the network structure and organization were calculated for each of the element-based varieties of the FPP, AP, and AP-filtered networks (**Supplemental Text S1**). The median values of the descriptive statistics across the KEGG networks were compared between the FPP, AP, and AP-filtered allelements networks (**Supplemental Table S3**). The median number of nodes was similar between the FPP and AP networks, 713 nodes, and 714 nodes, respectively, but due to the filtering that was applied, the AP-filtered networks tended to be smaller (median of 608 nodes). The median number of edges was very different between the three network representations with the AP networks having the most edges (2102), the FPP networks having less (1489), and the AP-filtered networks having the fewest edges (1024), but it is notable that the number of edges was highly variable for each of the network representations. The average path length and diameter for the AP-filtered networks both tended to be higher than in the FPP and AP networks, which were similar to each other.

In addition to the all-elements networks, the descriptive statistics were also compared between the carbon, nitrogen, and sulfur networks (**Supplemental Table S4-6**). The trends between these different element-filtered networks were consistent between the three network representations. The carbon networks tended to be the largest in terms of the median number of nodes and edges, with the nitrogen networks being in the middle, and the phosphorus networks having the fewest nodes and edges. The average path lengths were generally shortest for the phosphorus networks and longest in the carbon networks. The networks' density followed the opposite trend where the density was highest for the phosphorus networks and lowest for the carbon

networks. Notably, when compared to the all-elements networks, the element subset FPP networks tended to have much larger diameters, while the AP and AP-filtered networks had similar diameters between the all-elements and element subset networks. The analysis of the descriptive statistics between the network types and elements highlighted the broad differences in these networks, but to assess differences in the overall organization of the networks, additional analysis of the small-world and scalefree properties of the networks was performed.

Influence of network representation, database, and taxonomy on network metrics With the availability of sequenced genomes, multiple databases centered around annotation of metabolic pathways have been developed. Each database has its own conventions and may represent similar pathways in different ways which could lead to differences in the metabolic networks that are derived from them. To address possible biases introduced from using the KEGG database as the source of data for the analysis of the network types, an additional set of metabolic networks was generated using the MetaCyc database. Networks were generated for an overlapping set of 2931 organisms that were present in both the KEGG and MetaCyc databases and the influence of the databases (KEGG or MetaCyc), taxonomic rank at the phylum level (32 different phyla), and network representation were assessed (FPP, AP, or AP-filtered) was assessed using through a multi-way ANOVA (Supplemental Table S7). The effect sizes, representing the amount of variance explained by a factor, of each of these factors were calculated (Materials and Methods) for each of the analyzed network metrics, showing vastly different trends for each factor (Supplemental Table S8). The

network representation explained greater than 79% of the variance for the average degree, degree assortativity, closeness centrality, diameter, and average path length, while the other two factors both explained only small fractions of the variance. For 3 of the metrics, density, transitivity, and betweenness centrality, the network's phylum explained a plurality of the variance. In contrast to network representation, which tended to explain a very high fraction of the variance, phylum tended to explain a lower percent of the variance (between 25.4% and 49.3%), and the three statistics that were driven by phylum had high fractions of unexplained variance. The differences between phyla were further examined for the all-elements FPP network representations, highlighting that the differences between phyla were only present for a few of the metrics, while many metrics were largely consistent across all of the phyla (Supplemental Figure S1). In contrast to the other two factors, the database had very little influence on the network statistics, only explaining at most 7.3% of the variance for the betweenness centrality of the networks. Overall, the comparison of database, taxonomy, and network representation, highlights that the network representations are a dominant factor in driving differences between many of the network metrics analyzed.

In addition to the broad comparison between the KEGG and MetaCyc databases, a set of 13 organisms which also had well-curated GEMs were chosen to compare between the databases and the GEM derived networks (**Supplemental Table S9**). For 12 of the organisms, only one model was used in the comparison, but for *E. coli* K-12 MG1655 three versions of the GEM that are commonly used in other analyses were included (iJR904⁴⁶, iAF1260⁴⁷, iJ01366⁴⁸). The summary statistics were

calculated and compared between the models revealing that while there were some differences present between networks generated from each of the three sources, the broader trends appeared to be largely consistent regardless of network sources (**Supplemental Figure S2**). In particular, the size of the networks generated from the GEMs and databases were fairly similar, except for in the cases of some of the more extensively studied organisms (*E. coli* K-12 MG1655 and *S. typhimurium* LT2). The differences in the reaction content between the database derived networks and GEM derived networks were examined in more depth for the iJO1366 *E. coli* model. This comparison revealed that 82% of the reactions that were present in the iJO1366 GEM but not in the KEGG based network were involved in pathways related to lipid metabolism, cell wall metabolism, and transport across membranes. These pathways tend to be less curated and are represented as generic processes in many reaction databases leading to their lack of inclusion in the database derived networks.

Small-worldness and scale-free measures of metabolic networks

To look at differences in the overall organization of the networks, the small-worldness of the networks was compared between the different network representations and elements, revealing the prevalence of small-world properties in all of the network types. The small-worldness of networks was determined through the comparison of the average path lengths between nodes and clustering coefficient of a network to random networks of the same size, following a previously established protocol ²⁸. An analysis of the all-elements networks revealed that greater than 95% of the networks in all three network representations had small world properties (**Supplemental Table S10**).

Similarly, almost all of the carbon, nitrogen, and phosphorus networks were observed to have small-world properties (**Supplemental Table S10**). The ubiquity of these properties across all network representations and elements, suggests that this property could be a universal feature of metabolism.

The scale-free properties of the different network representations and element subsets were assessed by categorizing the networks into different groups based on how strong the evidence was that they had scale-free properties, with networks being classified into the following categories in order of increasing evidence that their degree distributions followed a power law: not scale free, weakest, weak, strong, strongest (Materials and Methods). For the AP networks between 28.8% and 52.7% of the networks from the four different element-based networks had strong evidence of scale-free properties (Fig. 3A). The AP-filtered networks had a higher percentage of networks with strong evidence of scale-free properties ranging between 42.5% and 69.2% across the different network representations (Fig. 3B). The FPP networks had the largest differences between the four element networks, with the all-element transfers showing 48.5% of the network with scale-free properties, both the nitrogen and carbon networks with only 7.0% and 16.9% with evidence of scale-free properties, and the phosphorus network having 87.4% of the networks showing scale-free properties (Fig. 3C).

Robustness of metabolic networks to random and non-random reaction deletions The robustness of the small world and scale-free properties of carbon, nitrogen, and phosphorus transfer networks were examined through a set of deletion simulations done on GEMs of *E. coli* K-12 MG1655 (iJR904)⁴⁶, *T. maritima* MSB8 (iTZ479)⁴⁹, and *S. piezotolerans* WP3 (GEM-iWP3)⁵⁰. The three-element networks consistently showed small-world properties for all three models for the starting GEM based networks (**Fig. 4A**). The networks maintained these properties through the reaction deletion simulations when the models were required to maintain biomass production and when no biomass constraint was applied. In contrast to the GEM based networks, while a majority of the analogous random networks and rewired networks started off having small-world properties, the small world properties were not maintained when edges were deleted from these networks for either the carbon or nitrogen networks. The exception to this was the phosphorus graphs, which tended to maintain some small-world properties for a majority of the random and rewired networks.

The scale-free properties of the networks were also examined over the course of the deletion simulations (**Fig. 4B**). The starting GEM based networks had similar trends to the previously analyzed KEGG networks, where the Carbon and nitrogen networks for all three models did not have scale-free properties, while the phosphorus networks had strong-scale free properties. The trends for the carbon and phosphorus networks were consistent between all three GEM networks, with none of the starting models having any scale-free properties and the final models after deletions of reactions or edges only having a small percent of the networks having scale-free properties. The phosphorus networks all started out as scale-free, but this property's robustness was variable among the different deletion simulations. When reactions were randomly deleted from the GEM networks without requiring the models to produce biomass flux, the models kept their scale-free properties in a majority of the

final networks. This was not the case when reactions were deleted while requiring that biomass production was maintained. In these deletion simulations, only 1.5% of the final GEM-iWP3 networks, 4.8% of the iJR904 networks, and 3.6% of the final iTZ479 networks had strong evidence of scale-free properties. The rewired phosphorus networks all started off being scale-free and did maintain these properties throughout the edge deletions, while the random networks were not scale-free for the starting networks or final networks.

DISCUSSION

Metabolism has been investigated through many different lenses, including both experimental and theoretical approaches. Advances in genomics have led to the widespread ability to sequence the genomes of almost any organism from any environment, providing a wealth of data to analyze and help in the prediction of what these organisms might be doing in their environments. The annotation of these genomes and the collection of metabolic data databases and highlight curated GEMs has provided yet another opportunity to analyze metabolism from a different perspective, as a mathematical network. The application of graph theory to different problems has provided insights into the structure and function of manmade and natural systems, including metabolic networks ^{29,34,35}. But these analyses have been hampered by the methods that have been used to represent metabolism as a network.

An analysis of metabolic networks, consisting of a set of metabolites (nodes) connected by edges (reactions partial reactions), highlighted how large of an effect different network representation methods can have on the networks' structure and how

they are interpreted. Two previously used network representations were used as a comparison for a new type of network representation, applying a recently developed reactant-product pair prediction algorithm, FindPrimaryPairs. The AP network representation was generated by connecting all substrates in a reaction to all products of that reaction, resulting in very densely connected networks dominated by extremely high degree currency metabolites and small molecules. These currency metabolites and small molecules are present as cofactors in many reactions across the metabolism, meaning that the connections formed by them link together very distant and sometimes unrelated portions of the metabolism. Even from a visual inspection of these networks, the influence of these heavily connected hub metabolites can be seen (Supplemental Figure S3). The AP-Filtered network representation seeks to remove these hub metabolites' influence by arbitrarily filtering out certain compounds. While this representation does result in less densely connected networks with longer linear pathways, the impact of those currency metabolites is completely lost in these networks (Supplemental Figure S3). While these hub metabolites are mostly involved in the reactions where they play roles as cofactors, they do all have roles as the primary parts of reactions in some subsystems. For example, ATP, while primarily acting as a phosphorus donor in many reactions, can also be involved as a metabolite in nucleotide biosynthesis and salvage⁵¹.

The FPP algorithm was applied to generate a new kind of network representation that naturally dealt with currency metabolites' influence without having to apply arbitrary filtering to remove them. The metabolite networks that were generated using the FPP network representation tended to have longer path lengths and

larger diameters than the AP networks, and while they still contained currency metabolites as relatively high degree nodes, these metabolites did not have the same centralizing influence on the network structure (**Supplemental Figure S3**). The use of the FPP network representation also allows for the separation of different element networks within the metabolism that show the flows of important elements like carbon, nitrogen, and phosphorus. Element-based filtering can be applied to the metabolites in AP or AP-Filtered networks, resulting in slight differences between the subset networks. But even with this filtering, because the edges in the networks can't be filtered in the same way, it is difficult to disentangle the influence of different elements on the overall structure of the metabolism. In the FPP networks, all of the edges represent connections between substrates and products through shared elements. This lets the filtering be applied to both the edges and the nodes in the networks, leading to distinctly different element subset networks where the influence of different processes can be analyzed in more detail.

Almost all of the KEGG networks analyzed had small-world properties regardless of the representation or element subset. While the threshold used to test for small-world properties was relatively generous, the fact that almost all of the networks had these properties and that the properties were robust to random deletions in the GEMs indicates that small-worldness is likely an inherent feature of metabolism. On the other hand, the scale-freeness of the networks was highly variable between network representation and element subsets. The AP and AP-Filtered networks only had small variations between the element subsets, indicating that the application of an element-based metabolite filtering was not sufficient to differentiate the influence of

different elements in these networks. In contrast, the filtering by element for the FPP networks resulted in vastly different networks for the carbon, nitrogen, and phosphorus metabolism, with the phosphorus networks being almost all scale-free across the KEGG database, while the carbon and nitrogen had very few scale-free networks. The phosphorus networks were scale-free due to the presence of very high degree nodes like phosphate, ATP, and ADP forming central hubs that connected to relatively linear pathways extending out from these hubs (Supplemental Figure S3). Unlike the smallworldness of the networks, the scale-free structure of the metabolism was not maintained in the GEM networks during the deletion simulations while maintaining growth. The final networks produced from the GEMs in the growth maintaining deletion simulations can be thought of as only containing the core metabolic functions that are required for growth. The loss of the scale-free properties in these core metabolic networks shows that while the core functions needed for growth might not be organized in a scale-free manner, these properties may arise from the addition of alternative metabolic pathways that utilize common cofactors like ATP.

These analyses taken together demonstrate the major influence that different network representations can have on the structure of the metabolic network. A comparison between the KEGG networks used in this study and networks derived from GEMs and the MetaCyc database shows that network representation has a disproportionate effect on the network structure compared to the source database, highlighting the dramatic effects that these representation choices can have. Interestingly, it was found that some of the network metrics analyzed were heavily influenced by the taxonomy of the organism that they were based on. While these

phyla driven differences are difficult to analyze in the context of multiple network representations, they do warrant further study with a focus on the application of FPP and the association of additional taxonomic and ecological information about the organisms. Given the large impact of network representation on model statistics and the benefits of FPP in mitigating the impact of currency metabolism while keeping them in the network, applying the FPP algorithm to metabolic analysis could provide novel and valuable insights into the evolution and organization of metabolism. The further study of these networks using the FPP algorithm promises to provide a new way to view and interpret metabolic pathways and understand the flow of essential elements like carbon, nitrogen, and phosphorus within a broader metabolic context.

METHODS

Generating Organism Specific Reaction Databases from KEGG and MetaCyc The entire KEGG database ¹ was downloaded and converted to a YAML formatted reaction database (downloaded on 2017-07-03). The database was first filtered to remove any compounds that had undefined or variable formulas, including metabolites that represent generic electron acceptors and donors and metabolites with undefined formula like variable fatty acids of undefined length, resulting in the removal of 2,514 compounds out of the total of 18,048 compounds in the initial database. The reactions in the database were then filtered to remove any reactions that had either undefined stoichiometry or compounds of undefined or variable formula, resulting in the removal of 2,643 reactions out of a total of 10,584 reactions in the initial database. This filtered KEGG reaction database was then subset to make organism-specific reaction sets

based on the KEGG orthology annotations for each organism. These annotations consist of a mapping of genes to KEGG orthology numbers. These KEGG orthology numbers were then mapped to KEGG reaction IDs to generate the association between genes and reactions for each organism. This mapping was done for the entire set of 4190 complete prokaryotic genomes included in the 2017-07-03 version of the KEGG database.

The preparation of the MetaCyc database ² followed a similar procedure as the KEGG database. First, the entire MetaCyc database was downloaded (downloaded on 2016-07-13), and the SBML formatted reaction database was converted to the YAML format. The compounds in this database were then filtered to remove any compounds that had undefined or variable formulas resulting in the removal of 1,946 compounds out of the original 13,018 compounds. The reaction database was then filtered to remove any reactions that included these compounds or had variable stoichiometries resulting in the removal of 3,035 reactions out of the original 15,924 reactions. Organism specific mappings were obtained by extracting the gene to reaction associations for the 7,597 organisms included in the database from the organism-specific Systems Biology Markup Language (SBML) reaction databases provided in MetaCyc.

Generating AP, AP-filtered, and FPP networks

The organism-specific databases of metabolites and reactions were represented in YAML format and used for the construction of networks following definitions of the AP, AP-filtered, and FPP representations. The AP networks were produced by enumerating all reactants and products and creating edges between each reactantproduct pair in each metabolic reaction. The AP-filtered networks were created by removing all the previously identified currency metabolites (**Supplemental Table S1**) and their associated edges from the corresponding AP networks. The FPP networks were created by including all metabolites in the AP network, while trimming the edges to only keep a set of predicted element-transferring reactant-product pairs using the 'fpp' algorithm implemented in the 'primarypairs' function of the PSAMM software $(version 1.0)^{27}$. By default, the all-element networks were created following each representation, where all metabolites were included regardless of the elementcomposition of the metabolites. To create carbon-, nitrogen-, and phosphorus-specific networks, the AP and AP-filtered networks were trimmed by removing any metabolites and their associated edges if the metabolites do not include the element of interest. Besides filtering metabolites based on their element compositions, the FPP networks were further trimmed to remove any edges that were not predicted to involve the transfer of the target element.

Three sets of AP, AP-filtered, and FPP networks were constructed based on different sources of genome annotations: (1) KEGG, (2) MetaCyc, (3) expert-curated GEMs in literature (**Supplemental Table S9**). Graph operations and visualizations of each network were created with the igraph python package⁵². Parallel edges that connect the same pair of nodes were combined to a single edge in the final graph. The largest connected component (LCC) was identified for each network by identifying the subgraph that contained the largest number of nodes using the 'decompose' function in igraph and this LCC was used for all downstream analyses of network properties. All-

element networks obtained from KEGG and MetaCyc annotations sources were filtered based on the percentage of nodes incorporated in the LCC, and the threshold was selected based on the overall distribution of the percentage of nodes in LCC, as seen among all networks reconstructed from KEGG or MetaCyc, respectively.

Network descriptors statistics

Network descriptors were calculated using the 'python-igraph' package version 0.8.2 and the 'poweRlaw' R package version 0.70.6 (**Supplemental Text S1**). The organism-specific reconstructions were first mapped between the KEGG and MetaCyc databases based on the strain level NCBI taxonomy identifiers, followed by a filtering step that removed networks in phyla that had less than four species in the dataset. This resulted in a set of 2,931 organisms from 32 distinct phyla that were independently annotated by both the KEGG and the MetaCyc databases. The relative effect sizes of network representation (e.g. AP, AP-filtered, or FPP), annotation database (e.g. KEGG or MetaCyc), and taxonomic classification on the different network descriptors were assessed by calculating the eta-squared statistics, which estimates the fraction of total variance explained by each factor in the analysis⁵³, following a multi-way ANOVA. Logarithmic transformations were applied to any models demonstrating heteroscedasticity (**Supplemental Table S7**).

Comparisons of network representations and databases using ANOVA

The effects of network, database, and taxonomic distribution were assessed through a multi-way ANOVA for the KEGG and MetaCyc database. First the overlapping set of

organisms between KEGG and MetaCyc were filtered to only include phyla that had at least four species in them, resulting in a set of 2931 organisms from 32 different phyla. The effects of phylum and network representations (FPP, AP, AP-filtered), and source database on the network descriptive statistics were analyzed using a multi-way ANOVA. Logarithmic transformations were applied to any models demonstrating heteroscedasticity (**Supplemental Table S7**). Due to the large number of organisms in the analysis, all of the comparisons were seen to be significant. To provide context to what was driving these differences, the relative effect sizes of phyla and network representations were analyzed by calculating the eta-squared statistics, which estimates the fraction of total variance explained by each factor in the analysis⁵³.

Power law fitting and calculation of small world properties

The network degree distributions for the carbon, nitrogen, and phosphorus KEGG networks were fit to a power-law distribution using the poweRlaw package (version 0.70.6) in R⁵⁴. The distribution parameters including the exponent of the power law curve and a data cutoff value to determine which nodes were in the tail of the distribution ("x_{min}") were estimated using the "estimate_pars" function, and a goodness of fit test was done performing 1000 bootstrapping simulations using the "bootstrap_p" function to assess the likelihood that the distribution followed a power-law. The quality of the fitting of the data to a power-law distribution was then compared to the fitting of the data with log-normal, exponential, and Poisson distributions using the "compare_distributions" function within the poweRlaw package. Networks were assessed to be scale-free or not based on previously

established thresholds related to the power-law fitting parameters and comparisons to other distribution fittings⁵⁵. Networks were classified as weakest scale-free if they the power-law fitting was not rejected during a goodness of fit test, weak scale-free if they also had greater than or equal to 50 nodes in the tail of the distribution, strong if they had exponent values between 2 and 3, and strongest if they met the qualifications of all the other categories and the power-law fitting was the best fit of the four distributions that were tested, following the previously established criteria⁵⁵.

The small-world properties of the networks were quantified by calculating the network small-worldness, S, based on a previously established method²⁸. First, 1000 Erdős-Rényi random networks with the same number of nodes and edges as the original network were generated using the "erdos_renyi_game" function in the iGraph python package⁵². The average clustering coefficient and average mean shortest path lengths from these 1000 random graphs were calculated and compared to the clustering coefficient and mean path length of the original network using the formula:

 $S = \frac{(Clustering Coef Original / Avg Clustering Coef Random)}{(mean path length Original / Avg mean path length Random)}.$ Networks were

considered to have small world properties if their value of S was greater than 1 and to not have small world properties if S was less than 1.

GEM reaction deletion simulations

Three GEMs were used to assess the effects of reaction deletions on the structure and properties of their metabolic networks. The three models analyzed were of the organisms *E. coli* K-12 MG1655 (iJR904)⁴⁶, *T. maritima* MSB8 (iTZ479)⁴⁹, and *S. piezotolerans* WP3 (GEM-iWP3)⁵⁰. First new exchange constraints were set up for all
three models that allowed for the free uptake of all carbohydrates, vitamins, and small molecules, but prevented the uptake of amino acids, nucleotides, and their derivatives (**Supplemental Tables S11-13**). Using these exchange constraints, random reaction deletion simulations were performed for each of the three models using the 'randomsparse' command as implemented in PSAMM. Using this function, 1000 random minimal reaction networks were generated while requiring that the biomass flux for the model be maintained as greater than or equal to 20% of the maximum biomass flux for that model. A second set of 1000 simulations were done for each model where reactions were randomly deleted from the GEM without applying any biomass constraint. The number of reactions deleted from each model was based on the median number of reactions deleted in the previous 'randomsparse' simulation done while maintaining the biomass at greater than 20% of the maximum value.

Two additional sets of deletions were also done on artificial networks to serve as comparisons to the GEM based deletions. One thousand random networks with the same number of edges and nodes as the GEM networks were generated using the Erdős-Rényi game function in the igraph python package for each of the three models. The median number of edges deleted in the 20% biomass 'randomsparse' simulations was calculated for each model, and the same number of edges were deleted from the generated random graphs. The second set of artificial networks were generated by taking the original GEM networks and rewiring the edges in the network 10,000 times. The rewired networks maintain the same degree distribution as the original networks but end up having a different set of edges. One thousand deletion simulations were done on these networks for each GEM, where the number of edges deleted from the

network was the same as the median number of edges deleted in the 20% 'randomsparse' simulations. All four of these deletion simulations were done for the carbon, nitrogen, and phosphorus FPP networks for each of the three GEMs. The calculation of the small-worldness and fitting of the degree distributions to a powerlaw was done for all of the starting and final networks from the deletion simulations.

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AUTHOR CONTRIBUTIONS

K.D.T and Y.Z planned the research, interpreted the results, and wrote the manuscript. K.D.T performed the analyses. C.P. and K.D.T carried out the statistical analyses.

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Figures for Manuscript III



Fig. 1: Graphical representation of different network representations. All-element networks are shown for the AP (A), AP-filtered (B), and FPP (C) network representations. Carbon-based networks are shown for the AP (D), AP-filtered (E), and FPP (F) network representations. A classic 'textbook' network representation with the reaction equations used to make the networks are shown in panel G.



Fig. 2: Summarized degree distributions for all KEGG derived all-elements networks. The black line shows the median across all organisms, while the blue shaded regions indicate the 25th to 75th percentiles.



evidence for the all-elements, carbon, nitrogen, and phosphorus filtered versions of the FPP (A), Fig. 3: Bar plots showing the fractions of KEGG networks having each category of scale-free AP (B), and AP-Filtered (C).



Fig. 4: A) Bar plots showing the number of networks with small-world properties before deletions (light blue) and after deletions have finished (dark blue). B) Bar plots showing the number of networks with strong or strongest evidence of scale-free properties before (light blue) and after (dark blue) deletions.

Supplemental Text for Manuscript III

Supplemental Text S1: Description of network descriptors and analysis process

All network statistics were calculated using the 'python-igraph'¹ package version 0.8.2 and 'poweRlaw'² R package version 0.70.6. Networks were read into the program as edge lists and converted into iGraph graph objects. These networks were then simplified to remove any multi-edges that were present in the graphs. The graphs were then subset to only keep the nodes that were present in the largest connected component of the network. All subsequent analysis was performed using this largest connected component. Various igraph functions were then used to calculate the network metrics for each network. These metrics and how they were calculated are described in the following sections.

Number of Nodes and Edges:

The number of nodes and edges in the networks were counted based on the largest connected component of each network by using the 'len' function in python to find the number of nodes and edges contained in the 'igraph.graph' object.

Average Degree:

The average degree was calculated by summing all of the degrees of all nodes in the network and dividing that value by the total number of nodes. The degrees of the nodes in each network were found using the 'graph.degree' function in igraph.

Density:

The density of the network is a measure of how many edges are present in the network compared to the total number of edges that would be present if all nodes were connected to all other nodes. Higher values indicate that more edges are present in the network, while lower values indicate that the network is more sparsely connected. The density of the networks was calculated using the 'graph.density' function in igraph.

Transitivity:

Transitivity is a measure of the likelihood that two nodes that have a mutual connection to a third node also share a connection with each other, forming a triangle. Higher values mean that more triangles exist in the network. This metric was calculated using the 'graph.transitivty_undirected' function in igraph.

Degree Assortativity:

Assortativity is a measure that quantifies how connected nodes with similar properties are in the network. In the case of degree assortativity, this measure is related to how likely nodes of similar degrees are to be connected to each other. Low values mean that the network is disassortative, indicating that many nodes of high degree are connected to low degree nodes. Higher values indicate that nodes of similar degrees are connected to each other. This was calculated using the 'graph.assortativity_degree' function in igraph.

Average Betweenness Centrality:

The betweenness centrality of a node is a measure of how many shortest paths in the network pass through the node. The average betweenness centrality of the graph was calculated by averaging the betweenness centrality of all nodes across the network. This betweenness of each node was calculated using the 'graph.betweenness' function in igraph.

Average Closeness Centrality:

The closeness centrality of a node is a measure of how close each node is to the other nodes in the network. Lower values indicate that the nodes are more distant from each other, while higher values indicate that the nodes are all less distant from each other. The average value was calculated by taking the average of the closeness of all the nodes. The closeness of each node was calculated using the 'graph.closeness' function in igraph.

Diameter:

The diameter of a network is the length of the longest shortest path between any two nodes in the network. The diameter of the networks was calculated using the 'graph.diameter' function in igraph.

Average Shortest Path Length:

The average shortest path length is a measure of the average length of all the shortest paths in the network. This measure was calculated using the

'graph.average_path_length' function in igraph.

Small Worldness:

The small worldness of each network was quantified following the methods detailed in Humphries and Gurney 2008 ³. First the transitivity and mean shortest path lengths of the network were calculated using the 'graph.transitivty_undirected' and 'graph.average_path_length' length functions in igraph. Then 1000 random networks with the same number of nodes and edges as the original network were generated using the 'igraph.GraphBase.Erdos_Renyi' function in igrah.

Power Law Fitting:

Power law fitting was done on the network degree distributions using the 'poweRlaw' R package ². The degree distributions were fit to a power law distribution using the 'displ' and 'estimate_xmin' function and the strength of the fitting was assessed using the 'bootstrap_p' function. Fitting to a log normal distribution was done using the 'dislnorm' and 'estimate_xmin' functions. Fitting to an exponential distribution was done using the 'disexp' and 'estimate_xmin' functions. Fitting to a poisson distribution was done using the 'dispois' and estimate_xmin' functions. Comparisons of the fittings to different types of distributions was done using the 'compare_distributions' function to assess if the power law fitting was better than the other distributions.

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Supplemental Figure S2: Bar plots showing differences in network metrics between networks generated from KEGG, MetaCyc, and published GEMs of 13 organisms.





Supplemental Figure S3: Visualizations of the *Buchnera aphidicola* APS metabolic network from KEGG. Visualizations were done for each of the 3 network representations (FPP, AP, AP-Filtered) and 4 element subsets (all-elements, carbon, nitrogen, and phosphorus). Nodes representing common currency metabolites and small molecules are colored cyan in the FPP and AP networks.

Conclusions

Metabolism is central to life, dictating organisms' ability to grow, compete with other organisms, and survive in different environments. The increasing availability of genomic data has led to advancements in new ways to study metabolism, even in organisms that were previously difficult to work with. This dissertation highlights the application of metabolic modeling to investigate metabolism in non-model organisms and the further use of these methods to study the structure of metabolism across the prokaryotic tree of life.

The development of a Genome-scale model (GEM) of metabolism for *Shewanella piezotolerans* WP3 provided the first model of a *Shewanella* strain from the deep-sea clade of this genus. This model provided a platform to study energy conservation mechanisms within this traditionally challenging study of deep-sea bacteria. The WP3 GEM was used to simulate energy metabolism in WP3, showing a reliance on substrate-level phosphorylation, combined with utilization of external electron acceptors during anaerobic growth. This feature was shared with other wellstudied *Shewanella*, indicating that these mechanisms may be a conserved growth strategy in the genus. Further simulations highlighted the ability of ATP synthase to act as a proton balancing mechanism depending on the availability of reducing equivalents within the model. The metabolic flexibility demonstrated with this GEM shows the importance of metabolic flexibility as a part of WP3's adaptation to the variable conditions of the deep-sea.

The study of deep-sea metabolism was continued through the development of a GEM for another deep-sea *Shewanella* strain, *Shewanella* psychrophila WP2. Unlike

WP3, which is psychrotolerant, WP2 is a psychrophilic strain. This low-temperature adaptation in WP2 was investigated through a combination of transcriptomics and the application of transcriptome and thermodynamic data into the GEM. Broad metabolic changes characterized the growth of WP2 at sub-optimal, optimal, and supra-optimal growth temperatures. The differential expression of genes within central carbon pathways in WP2 was contextualized by the use of thermodynamics-based metabolic flux analysis. These simulations revealed that changes in the flux through central metabolic pathways led to global changes in WP2's efficiency in producing biomass and energy. The metabolic shifts and utilization of lower efficiency growth strategies in WP2 were similar to previously reported growth trends in other psychrophiles. The investigations of the metabolism of WP2 and WP3 through a combination of experimental and modeling methods led to a broader understanding of metabolism in the Shewanella genus. These studies highlight the importance of metabolic flexibility within the Shewanella genus and demonstrate the critical roles that conserved metabolic strategies play in these organisms' ability to survive in extreme environments.

Both the WP2 and WP3 models demonstrated the utility of GEMs for investigating specific metabolic mechanisms and features within single organisms. The analysis of metabolism was then extended to look at common metabolic functions across all prokaryotes. This analysis utilized the mathematical field of graph theory to examine the structure and organization of metabolism when it is represented as a mathematical network. This analysis focused on the methods used to represent metabolic networks and highlighted the application of the FindPrimaryPairs algorithm

to generate a new kind type of metabolic network. This new type of network had the benefit of not requiring arbitrary filtering and allowing for the filtering of the network to show different element transfer networks. The further analyses of these network structures revealed distinct differences in the organization of carbon, nitrogen, and phosphorus metabolism and can contribute to the broader understanding of how these networks have evolved.

The work described in this dissertation highlights the complexity of metabolism. The application of multiple methods in studying metabolic processes will be critical to future research in this field. The future integration of techniques like genomes scale modeling and network analysis combined with sequencing and growth experiments will allow for the exploration of increasingly complex systems. While any one of these methods will not provide a full context on its own, each of these methods can enhance each other and lead to new and exciting conclusions.

Appendix I: GEM Reconstruction and Simulation Methods

INTRODUCTION

GEnome-scale Models of Metabolism have been increasing in popularity and utility since the start of their development. Modern models are made for a variety of organisms and can be used to simulate many aspects of metabolism and growth, but early models were much more limited in what they represented and could be used for. The comprehensive GEMs currently being developed have their origins in the modeling and reconstruction of specific pathways or cells with simple metabolic functions [1-3]. These early pathway reconstructions proved to be useful in predicting metabolic phenotypes, and eventually, they were expanded to become representations of the full metabolism of organisms. The first true GEM that represented metabolism at a whole-genome scale was published in 2000 and was based on Escherichia coli K-12 [4]. This early E. coli model, iJE660, only included functions encoded by 660 of the 4391 protein-coding genes in the *E. coli* K-12 genome. However, even with its relatively small size, this model was still used to predict gene deletion phenotypes and broad metabolic growth phenotypes [4]. Over the two following decades, GEMs have been more broadly developed to include more metabolic pathways and to represent organisms from all three domains of life [5,6]. The creation of new GEMs has corresponded with an expansion of simulation methods that can be used with the models. These methods range from the fundamental Flux Balance Analysis, where the flow of metabolites through a network is simulated based on stoichiometric constraints [7], to more complex simulations that account for thermodynamics [8] and growth over time [9]. The increased availability of genome data and the improvements that are

being made in gene annotation pipelines have made GEMs a more useful and available tool that can contribute to a wide range of different research projects.

COMPONENTS OF A GEM

GEMs are representations of the metabolism of an organism based on that organism's annotated genome. As representations of metabolism, these models primarily contain data related to metabolites and metabolic reactions, but they also include additional information related to the setting up simulations like artificial reactions, reaction flux limits, and exchange conditions representing growth media [10].

Reactions

The reactions in a GEM consists of metabolic reaction equations and the associated metadata for that reaction. The reaction equation is similar to what would be seen in a textbook representation of a metabolic function, consisting of a series of metabolite IDs with some form of an equal's sign representing the separation of the products and reactants (Figure 1A). These equations represent metabolic processes that occur in a cell either catalyzed by enzymes or occurring through spontaneous processes. GEMs for many organisms will represent different cellular locations like the extracellular space, cytosol, periplasm, and for eukaryotes different organelles. To specify where reactions occur in the modeled cell, the reaction equations will often contain some specified reaction ID alongside the metabolites to designate where the metabolic reaction occurs. Reactions are often associated with additional data that allows the GEM to be used as an annotation reference as well as a simulation tool. The

other data can include reaction names, enzyme commission numbers, gene associations, and literature references.

Metabolites

The metabolites in GEMs are what make the reaction equations are made up from. Each metabolite in the model is often involved in multiple reactions. Similar to the reactions, metabolites in GEMs are typically associated with additional information (Figure 1B). Metabolites can be associated with biochemical data like formulas, ionic charges, and molecular masses. The metabolites' properties can be used to ensure that the reaction equations in the GEM are balanced in terms of conserving charge and mass in the reaction equations. GEMs often include additional metadata like metabolite names and database IDs and the metabolites' biochemical properties.

Artificial Reactions

The reactions and metabolites in a GEM are mostly based on biochemical data and the current understanding of enzymatic processes in a cell. Still, there are some processes related to growth that have to be represented through artificial reactions. These reactions often represent larger-scale processes related to growth, like DNA synthesis and protein synthesis, that can't necessarily be represented by single enzyme associated reactions. To overcome the challenge of representing these parts of growth in a model, the overall processes are often condensed down into summary reactions (Figure 2A). For example, DNA synthesis involves multiple steps catalyzed by different enzymes and is an iterative process, where bases get added to a growing

DNA strand successively. In the context of a GEM, this process, along with all of its energy requirements, is summarized into a condensed reaction representing the cost of DNA synthesis in terms of the amount of each base and the amount of energy in the form of ATP. These artificial growth reactions are typically normalized to represent the synthesis of 1 gDW of the product. This normalization is then used when the products of these reactions are combined into an overall biomass reaction equation (Figure 2B). This biomass reaction is formulated based on measured or estimated compositions of the dry weight of an organism. For example, if the protein made up 50% of the cells' dry weight, then the biomass reaction would reflect this by having the synthesized protein be 50% of the reaction. The final formulation of the biomass reaction represents the production of 1 gDW of biomass, which allows for easier comparisons of model simulation results to experimental results [11,12].

Simulation Settings

In addition to the biology-related GEM features like reactions and metabolites, some additional features are included in GEMs related to setting up simulations with the GEM. The first of these features is limits on reaction fluxes. These limits can be set up to force reactions to be used in the model or force them only to be used in specific ways. Flux limits like this are typically simulation specific and can be used to constrain the model better to replicate experimental conditions. A prevalent example of reaction limits in the model involves forcing flux through an artificial ATP maintenance reaction. This type of maintenance reaction is used to represent the non-growth associated maintenance energy in a cell, and reaction limits are used to force a certain amount of ATP to be hydrolyzed in the model to replicate this cost [12–14].

The other part of GEMs related to simulation settings is the exchange settings. These exchange settings are analogous to a growth media, and they are used to define what nutrients are available and can be produced in the simulation. Like the limits, these exchange settings are typically conditioned specific and can be changed depending on the type of experiment replicated with the model.

Overall, GEMs are a collection of information related to setting up metabolic simulations and the annotations of metabolic functions in an organism. With the development of more GEMs from diverse groups of organisms, they have started to shift from being primarily used to perform simulations of growth to now being useful annotation resources that can be used to bring together genomic, biochemical, and physiological data [6,15,16].

GETTING FROM A GENOME TO A GEM

Early GEMs were based mainly on experimental data. They leveraged the extensive research history of model organisms, which is why they were mostly based around well-known pathways and well-studied microorganisms like *E. coli* [4,17]. This process involved manual curation of metabolic functions and the gradual expansion of the models from one pathway to another based on experimental verification of the functions. Unfortunately, this process is impossible for many organisms due to the limited experimental history of many non-model organisms. This challenge has been highlighted by the growth in environmental sequencing methods, where it is now possible to obtain nearly complete genomes of organisms from environmental samples, even when it is not possible to isolate them in pure cultures

[18,19]. To overcome these limitations, there have been concurrent advancements in gene annotation methods [20–22] and the development of extensive gene orthology and metabolic pathway databases [23–26]. These tools have made it possible to develop GEMs for almost any organism that has an available genome.

Gene-Protein-Reaction Associations

The central concept in the development of a GEM is the gene-protein-reaction (GPR) association. This GPR concept is made from the idea that a gene present in an organism can be predicted, then translated to a protein sequence, analyzed, and then, based on the putative function, assigned a metabolic function [27,28]. The process of developing a GEM consists of generating these GPR associations for as many genes as possible in an organism's genome. This overall process is often aided by the use of automated tools and databases, followed by extensive manual curation.

Gene and Protein Analysis

The starting point for a new GEM is a genome sequence. The first step to generate the GPR associations for a new GEM involves predicted the open reading frames from the genomes and translating those ORFs to putative protein sequences. Various tools have been developed to do this task that can account for alternative codon usage in different phyla and utilize previously annotated genomes as templates, including GeneMark and Prodigal [29,30]. The bulk of the analysis is then done on the protein sequence associated with a gene. This sequence can be analyzed using a variety of tools that contribute different pieces of evidence about a gene's potential functions. Sequence homology searches are a typical first step with protein sequence

analysis. Tools like BLAST can be used to search for similar sequences in online databases or in other organisms' genomes [20]. These similar sequences may provide evidence of the functions of the new genes through their annotation or through published studies. In addition to these broad sequence similarity searches, more specific gene orthology predictions can be performed to try to group the new sequence into groups of potentially related orthologs using databases like COG, EggNOG, or KEGG [23,26,31]. The next steps typically consist of performing protein domain analysis on the predicted protein sequence. Tools like Pfam, ScanProsite, and TMHMM can be used to predict protein structural domains and compare them to wellannotated reference proteins [21,22,32]. The presence of certain domains in a protein can be strong indications of what types of substrates that protein might bind to or what enzymatic activity that protein might have (protein domain analysis to function annotation). Additional evidence can also be brought into the gene annotation process from previous studies and from direct experimental evidence of gene function, but these two pieces of evidence are only available for certain organisms. All of the evidence from these different processes are used together to make a determination of what type of enzyme this gene might encode for.

Reaction Association

Once a prediction about what enzyme the gene encodes is made, the next step is to associate that enzyme with a metabolic reaction to complete the GPR association. This process relies on two major sources of information, previously published GEMs and metabolic pathway databases. Previously published GEMs are often used as a starting point for new models either as a reference or if the organisms are closely

related as a template for generating a draft set of reactions for a new GEM [33–35]. No GEM is going to be a perfect match for a new organism through, and there will likely be holes that need to be filled in with new reactions. This process is done through referencing metabolic pathway databases like KEGG and MetaCyc and other resources that include enzyme functional data like BRENDA [23,24,36]. These reactions can be collected into an overall set of metabolic reactions for the GEM and assembled into a complete GEM in one of the various formats used by the different modeling software such as the YAML format [5,10], SBML format [37], or JSON format [25].

SIMULATION METHODS

The purpose of developing GEMs is to use them to perform simulations of the growth of the organism. The fundamental method for doing this is to translate the model into a set of linear constraints and use a type of mathematics called linear programming to maximize the flux through the biomass reaction. This method is called Flux Balance Analysis (FBA) and forms the basis for almost all other modeling methods developed [7,38].

The Stoichiometric Matrix

Reactions in a GEM are typically stored as text, where reaction equations are written out using metabolite IDs and stoichiometry. Before any simulations are done with the GEM, these reactions are converted to a matrix called the stoichiometric matrix. In this matrix, the rows represent metabolites, the columns represent reactions, and the values represent the stoichiometry of a given metabolite in a reaction [38]. As most metabolic reactions only contain a small number of unique metabolites, the

stoichiometric matrix is typically sparse. This matrix forms the basic structure of most constraint-based simulation methods.

Fluxes

Reaction fluxes are what is solved for in most modeling methods. These fluxes obtained from metabolic simulations represent the activity of each reaction in the GEM and can be related to measurable flux values that can be obtained through experimental methods through the scaling of the uptake and production rates in the model[11,38,39]. These fluxes are represented as a vector where each value in the vector corresponds to the flux through a single reaction. The result of an FBA simulation is a flux vector that has been solved for, where one value in the flux vector has been maximized.

Steady State Assumption

The steady-state assumption is the last fundamental component of setting up a stoichiometric modeling problem. This assumption means that in the modeling problem, the amount of any metabolite that is produced must be equal to the amount of that metabolite that is consumed. This means that there cannot be any accumulation of metabolites in the model or any consumption of non-produced metabolites.

Maximization of an Objective Function Flux through Linear Programming

The final step in stoichiometric modeling is the conversion of the stoichiometric matrix along with other model constraints to a linear programming problem. This process involves converting the stoichiometric matrix and flux vector into a series of linear equations based on the values in the stoichiometric matrix. The steady-state assumption allows for the formulation of linear constraints in the problem, where each linear constraint represents the overall consumption and production of metabolites through multiple reactions. In addition to the linear constraints based on the stoichiometric matrix, many models also include additional constraints that are added to the model to limit flux ranges to reasonable values, establish which nutrients are available or can be produced, or to force certain reactions to carry specific fluxes [7].

FBA Variations and Other Simulation Methods

Many additional modeling methods have been developed using the basic FBA framework and expanding it. Some of these methods, like Flux Variability Analysis (FVA), have been developed to explore the inherent variability that results from solving large linear programming problems [7,40]. Other methods like Thermodynamics-based metabolic flux analysis [8] and Metabolic Adjustment by Differential Expression [41] focus on expanding the basic FBA framework through the incorporation of thermodynamic and transcriptomic data respectively. Regardless of the type of simulation, most of the constraint-based analysis approaches utilize the same basic formulation of the stoichiometric constraints as FBA does.

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Appendix I Figures

A)	В)
Reactions:	Compounds:
- id: PYK	- id: PYR
equation: ATP[c] + PYR[c] <=> ADP[c] + PEP[c]	name: Pyruvate
name: Pyruvate Kinase	formula: C3H4O3
ec: 2.7.1.40	CAS: 127-17-3
- id: PYRt	- id: PEP
equation: PYR[e] + H[e] <=> PYR[c] + H[c]	name: Phosphoenolpyruvate
name: Pyruvate transport via proton symport	molecular_mass: 168.042
tc: 2.A.1.13.6	pubchem: 1005

Figure 1: Example representations of metabolic reactions (A) and metabolites (B) in a GEM.


Figure 2: Schematic representation of a macromolecule synthesis reaction (A) and the overall biomass reaction of a GEM (B).

Appendix II: Supplemental Tables for Manuscript I

Supplemental Table S1. Stoichiometry of the biomass compounds involved in the biomass synthesis equation of the WP3 GEM.

Compound_ ID	Stoichiometry	Compound_ Name	Molecular Weight (g/mol)	Weight (g/gDW)
cpd_12dag3p	0.000078	1,2-Diacyl-sn- glycerol 3- phosphate	645.2608	5.033034E-05
cpd_12dgr	0.139174	1,2- Diacylglycero 1	567.2988	7.895324E-02
cpd_5mthf	0.050000	5- Methyltetrahy drofolate	458.4620	2.292310E-02
cpd_accoa	0.000050	Acetyl-CoA	805.5480	4.027740E-05
cpd_amp	0.001000	AMP	345.2160	3.452160E-04
cpd_coa	0.000006	CoenzymeA	763.5120	4.581072E-06
cpd_dna	0.001819	DNA	30792.5160	5.601159E-02
cpd_fad	0.000050	FAD	783.5480	3.917740E-05
cpd_lps_Cor e	0.011270	LPS	3052.1980	3.439675E-02
cpd_nad	0.002150	NAD	662.4280	1.424220E-03
cpd_nadh	0.000050	NADH	663.4360	3.317180E-05
cpd_nadp	0.000130	NADP	740.3900	9.625070E-05
cpd_nadph	0.000400	NADPH	741.3980	2.965592E-04
cpd_pe	0.078517	Phosphatidyle thanolamine	690.3468	5.420396E-02
cpd_peptx	0.031434	Peptidoglycan subunit crosslinked	899.8900	2.828714E-02
cpd_pgly	0.022716	Phosphatidylg lycerol	720.3468	1.636340E-02
cpd_protein	0.000551	Protein	1083383.934 0	5.969445E-01
cpd_rna	0.000003	RNA	32013.8140	9.604144E-05
cpd_succoa	0.000003	Succinyl-CoA	862.5760	2.587728E-06
cpd_udpg	0.003000	UDP-Glucose	564.2860	1.692858E-03

cpd_glycoge n	0.472431	Glycogen	162.1400	7.659996E-02
cpd_ptrc	0.035000	Putrescine	90.1720	3.156020E-03
cpd_spmd	0.007000	Spermidine	148.2760	1.037932E-03
cpd_k	0.169185	K+	38.9637	6.592084E-03
cpd_nh4	0.011279	NH4	18.0390	2.034622E-04
cpd_mg2	0.007519	Mg2+	23.9850	1.803515E-04
cpd_ca2	0.004512	Ca2+	39.9626	1.802956E-04
cpd_fe2	0.006767	Fe2+	55.9349	3.785345E-04
cpd_cu2	0.012698	Cu2+	63.5460	8.069333E-04
cpd_mn2	0.012698	Mn2+	54.9380	6.976254E-04
cpd_mobd	0.012698	Molybdate	159.9400	2.030984E-03
cpd_cobalt2	0.012698	Co2+	58.9332	7.483581E-04
cpd_cl	0.019048	Chloride	34.9689	6.660743E-04
cpd_so4	0.015873	SO4	96.0620	1.524794E-03
cpd_pydx5p	0.000223	Pyridoxal 5'- phosphate	245.1270	5.474503E-05
cpd_pheme	0.000223	Protoheme	690.6269	1.542400E-04
cpd_udcpdp	0.000055	Undecaprenyl diphosphate	924.2580	5.116008E-05
cpd_chor	0.000223	Chorismate	224.1680	5.006419E-05
cpd_amet	0.000223	S-Adenosyl- L-methionine	399.4520	8.921095E-05
cpd_ribflv	0.000223	Riboflavin	376.3690	8.405574E-05
cpd_sheme	0.000223	Siroheme	908.6969	2.026394E-04
cpd_ubq8h2	0.000223	Ubiquinol-8	729.1430	1.625989E-04
cpd_mqn7	0.000223	Menaquinone 7	719.1510	1.603707E-04
cpd_cobamc oa	0.000223	Cobamide coenzyme	1579.5818	3.522467E-04
cpd_thmpp	0.000223	Thiamine diphosphate	422.2950	9.417179E-05
cpd_btn	0.000002	Biotin	244.3100	4.886200E-07

Supplemental Table S2. Stoichiometry of the fatty acid components in the lipid biosynthesis equation of the WP3 GEM. The stoichiometry of unsaturated, saturated, and branch-chain fatty acids were calibrated based on experimental measurements of the WP3 fatty acid composition at 20°C and 0.1 MPa (Wang et al., 2009).

Compound_ID	Туре	Stoichiometry
fallACP	Iso-C17:0	0.2210
fa13ACP	Iso-C13:0	0.0649
falACP	Iso-C14:0	0.2040
fa3ACP	iso-C15:0	0.0759
fa6ACP	Iso-C16:0	0.2550
hdeACP	n-C16:1	0.1346
hpdACP	n-C17:0	0.0510
hpdeACP	C17:1	0.4250
ocdACP	n-C18:0	0.0340
octeACP	n-C18:1	0.0434
palmACP	n-C16:0A	0.2210
pdACP	n-C15:0	0.0340
pdeACP	C15:1	0.2040
ера	20:5	0.0321

Supplemental Table S3. Basal constraints for metabolic simulations performed in the WP3 and MR-1 models (Materials and Methods). Compound ID/Name: the identifiers/names of extracellular compounds with defined exchange reactions, which were used to simulate the availability of nutrients and the removal of metabolic byproducts. The compound identifiers were shown for both the WP3 and MR-1 models. Lower/Upper Bound: basal constraints for the lower and upper bounds of exchange reaction fluxes. Negative lower bounds would indicate compounds provided as nutrient sources to the model, and a lower bound of zero would indicate a compound that could only be released as a metabolic byproduct but not acquired from the environment. Type: classification of the exchange compounds. Growth supporting in WP3: the growth supporting carbon sources and terminal electron acceptors were marked as TRUE in this column.

Compound ID	Compound Name	Lower Bound	Upper Bound	Туре	Growth Supporting
cpd_h[e]	H+	-1000	1000	Basal media	-
cpd_h2o[e]	H2O	-1000	1000	Basal media	-
cpd_na1[e]	Sodium	0	1000	Basal media	-
cpd_ca2[e]	Calcium	-1000	1000	Basal salt media	-
cpd_cl[e]	Chloride	-1000	1000	Basal salt media	-
cpd_k[e]	K+	-1000	1000	Basal salt media	-
cpd_mg2[e]	Mg	-1000	1000	Basal salt media	-
cpd_nh4[e]	Ammonium	-1000	1000	Basal salt media	-
cpd_pi[e]	Phosphate	-1000	1000	Basal salt media	-
cpd_so4[e]	Sulfate	-1000	1000	Basal salt media	-
cpd_ac[e]	Acetate	0	1000	Carbon source	TRUE
cpd_acgam[e]	N-Acetyl-D- glucosamine	0	1000	Carbon source	TRUE
cpd_adn[e]	Adenosine	0	1000	Carbon source	TRUE
cpd_ala-D[e]	D-Alanine	0	1000	Carbon source	TRUE
cpd_ala-L[e]	L-Alanine	0	1000	Carbon source	TRUE
cpd_asp-L[e]	L-Aspartate	0	1000	Carbon source	TRUE
cpd_bgl[e]	Cellobiose	0	1000	Carbon source	TRUE
cpd_chitin[e]	Chitin	0	1000	Carbon source	TRUE
cpd_cytd[e]	Cytidine	0	1000	Carbon source	TRUE
cpd_dad-2[e]	Deoxyadenosi ne	0	1000	Carbon source	TRUE
cpd_damp[e]	dAMP	0	1000	Carbon source	TRUE
cpd_dcmp[e]	dCMP	0	1000	Carbon source	TRUE
cpd_dcyt[e]	Deoxycytidine	0	1000	Carbon source	TRUE
cpd_dna[e]	DNA	0	1000	Carbon source	TRUE
cpd_dodca[e]	Dodecanoic acid	0	1000	Carbon source	TRUE

cpd_duri[e]	Deoxyuridine	0	1000	Carbon source	TRUE
cpd_for[e]	Formate	0	1000	Carbon source	TRUE
cpd_fum[e]	Fumarate	0	1000	Carbon source	TRUE
cpd_gal[e]	D-Galactose	0	1000	Carbon source	TRUE
cpd_galactan[e]	Galactan	0	1000	Carbon Source	TRUE
cpd_glc-D[e]	D-Glucose	0	1000	Carbon source	TRUE
cpd_glu-L[e]	L-Glutamate	0	1000	Carbon source	TRUE
cpd_gly-asp- L[e]	Glycyl-L- aspartic acid	0	1000	Carbon source	TRUE
cpd_gly-glu- L[e]	Glycyl-L- glutamic acid	0	1000	Carbon source	TRUE
cpd_gly[e]	Glycine	0	1000	Carbon source	TRUE
cpd_glyc-R[e]	(R)-Glycerate	0	1000	Carbon source	TRUE
cpd_glyc[e]	Glycerol	0	1000	Carbon source	TRUE
cpd_hdca[e]	hexadecanoate (n-C16:0)	0	1000	Carbon source	TRUE
cpd_ile-L[e]	L-Isoleucine	0	1000	Carbon source	TRUE
cpd_lac-D[e]	D-Lactate	0	1000	Carbon source	TRUE
cpd_lac-L[e]	L-Lactate	0	1000	Carbon source	TRUE
cpd_lami[e]	laminarin	0	1000	Carbon source	TRUE
cpd_leu-L[e]	L-Leucine	0	1000	Carbon source	TRUE
cpd_mal-L[e]	L-Malate	0	1000	Carbon source	TRUE
cpd_malt[e]	Maltose	0	1000	Carbon source	TRUE
cpd_malthp[e]	Maltoheptaose	0	1000	Carbon source	TRUE
cpd_malthx[e]	Maltohexaose	0	1000	Carbon source	TRUE
cpd_maltpt[e]	Maltopentaose	0	1000	Carbon source	TRUE
cpd_malttr[e]	Maltotriose	0	1000	Carbon source	TRUE
cpd_maltttr[e]	Maltotetraose	0	1000	Carbon source	TRUE
cpd_ocdca[e]	Octadecanoate (n-C18:0)	0	1000	Carbon source	TRUE
cpd_panose[e]	Panose	0	1000	Carbon Source	TRUE
cpd_ppa[e]	Propionate	0	1000	Carbon source	TRUE
cpd_pro-L[e]	L-Proline	0	1000	Carbon source	TRUE
cpd_ptrc[e]	Putrescine	0	1000	Carbon source	TRUE
cpd_pyr[e]	Pyruvate	0	1000	Carbon source	TRUE
cpd_ser-L[e]	L-Serine	0	1000	Carbon source	TRUE
cpd_succ[e]	Succinate	0	1000	Carbon source	TRUE
cpd_thr-L[e]	L-Threonine	0	1000	Carbon source	TRUE
cpd_ttdca[e]	tetradecanoate (C14:0)	0	1000	Carbon source	TRUE
cpd_tyr-L[e]	L-Tyrosine	0	1000	Carbon source	TRUE

cpd_uri[e]	Uridine	0	1000	Carbon source	TRUE
cpd_val-L[e]	L-Valine	0	1000	Carbon source	TRUE
cpd_dgmp[e]	dGMP	0	1000	Carbon source	FALSE
cpd_dgsn[e]	Deoxyguanosi ne	0	1000	Carbon source	FALSE
cpd_dtmp[e]	dTMP	0	1000	Carbon source	FALSE
cpd_glyclt[e]	Glycolate	0	1000	Carbon source	FALSE
cpd_indole[e]	Indole	0	1000	Carbon source	FALSE
cpd_lys-L[e]	L-Lysine	0	1000	Carbon source	FALSE
cpd_met-L[e]	L-Methionine	0	1000	Carbon source	FALSE
cpd_thymd[e]	Thymidine	0	1000	Carbon source	FALSE
cpd_trp-L[e]	L-Tryptophan	0	1000	Carbon source	FALSE
cpd_ura[e]	Uracil	0	1000	Carbon source	FALSE
cpd_xan[e]	Xanthine	0	1000	Carbon source	FALSE
cpd_cro4[e]	chromate	0	1000	Electron acceptor	TRUE
cpd_dmso[e]	Dimethyl sulfoxide	0	1000	Electron acceptor	TRUE
cpd_fe3[e]	Fe3+	0	1000	Electron acceptor	TRUE
cpd_h2o2[e]	Hydrogen peroxide	0	1000	Electron acceptor	TRUE
cpd_mn4o[e]	Manganese(I V) oxide	0	1000	Electron acceptor	TRUE
cpd_no2[e]	Nitrite	0	1000	Electron acceptor	TRUE
cpd_no3[e]	Nitrate	0	1000	Electron acceptor	TRUE
cpd_o2[e]	O2	0	1000	Electron acceptor	TRUE
cpd_tmao[e]	Trimethylami ne N-oxide	0	1000	Electron acceptor	TRUE
cpd_tsul[e]	Thiosulfate	0	1000	Electron acceptor	TRUE
cpd_tttnt[e]	tetrathionate	0	1000	Electron acceptor	TRUE
cpd_urnyl[e]	Uranyl	0	1000	Electron acceptor	TRUE
cpd_cobalt3[e]	Co3+	0	1000	Electron acceptor	FALSE
cpd_co2[e]	CO2	0	1000	Metabolic byproduct	-
cpd_CrOH3[e]	Cr(OH)3	0	1000	Metabolic byproduct	-
cpd_dms[e]	Dimethyl sulfide	0	1000	Metabolic byproduct	-
cpd_h2s[e]	Hydrogen sulfide	0	1000	Metabolic byproduct	-
cpd_so3[e]	Sulfite	0	1000	Metabolic byproduct	-
cpd_tma[e]	Trimethylami ne	0	1000	Metabolic byproduct	-
cpd_urdio[e]	Uranium dioxide	0	1000	Metabolic byproduct	_

cpd_urea[e]	Urea	0	1000	Metabolic byproduct	-
cpd_cobalt2[e]	Co2+	-1000	1000	Trace element	-
cpd_cu2[e]	Cu2+	-1000	1000	Trace element	-
cpd_fe2[e]	Fe2+	-1000	1000	Trace element	-
cpd_mn2[e]	Mn2+	-1000	1000	Trace element	-
cpd_mobd[e]	Molybdate	-1000	1000	Trace element	-
cpd_pmcoa[e]	Pimeloyl-CoA	-1000	1000	Vitamin precursor	-
cpd_cbl1[e]	Cob(I)alamin	-1000	1000	Vitamin solution	-

Supplemental Table S4. Maximum and minimum flux values obtained from flux variability analysis (FVA) corresponding to the simulation condition in Figure 4D. FVA was performed in the WP3 wild type model and the Δpta , $\Delta ackA$, and $\Delta pta\Delta ackA$ mutant models with biomass production set to its maximum (Materials and Methods). Numbers in this table indicated raw values of the minimum and maximum fluxes before they were normalized by the biomass flux.

REACTION ID	W	Τ/T	DP	ТА	DA	АСК	DPTA/DACK	
	Lower	Upper	Lower	Upper	Lower	Upper	Lower	Upper
ATPS4R	1.723547	1.723547	0.462743	0.586943	0.201432	0.201432	0.201432	0.201432
FDH	10.046548	10.046548	6.302506	6.488806	2.662379	18.064684	2.662379	18.064684
NDH	7.109320	7.109320	9.918376	9.918376	2.526106	75.846249	2.526106	75.846249
PTAR	6.353348	6.353348	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
ACKR	12.445169	12.445169	12.972714	13.034814	0.000000	0.000000	0.000000	0.000000
РҮК	6.257749	6.257749	6.184985	6.309184	3.286322	8.420424	3.286322	8.420424
ХРК	6.091821	6.091821	12.972714	13.034814	0.000000	0.000000	0.000000	0.000000
CORE_BIO MASS	0.537444	0.537444	0.521138	0.521138	0.226851	0.226851	0.226851	0.226851

Appendix III: Data S1 for Manuscript II

Data S1 Table A: Comparison of overall WP2 GEM grow/no-growth predictions to experimentally confirmed growth supporting nutrients.

Table A: Comparison of overall			
WP2 GEM grow/no-growth			
confirmed growth supporting			
nutrients.			
Nutrient Condition	Experimentally Confirmed	Model Predicted	Literature Support (PMID)
A orobic	Conditions	Growth	
A cetate ± 02	NG	G	17220442
Cellobiose + O2	NG	NG	17220442
Citrate + O2	G	G	17220442
D-Galactose + O2	NG	NG	17220442
D-Glucose + O2	NG	NG	17220442
Maltose + O2	NG	NG	17220442
N-acetyl-D-Glucosamine + O2	G	G	17220442
Sucrose + O2	G	G	17220442
D-Trehalose + O2	G	G	17220442
Anaerobic	Conditions		
Lactate + Irone 3+	NG	NG	17220442
Lactate + TMAO	G	G	17220442
Lactate + DMSO	G	G	17220442
Lactate + Fumarate	NG	G	17220442
Lactate + Nitrate	G	G	17220442
Lactate + Nitrite	NG	NG	17220442

Data S1 Table B: Table showing differences between 4, 15 and 20 temperaturedependent models. The reactions are marked as being Expressed, if they were included in the model and all associated genes were above the expression threshold. Used below if they were kept in the final model so that biomass could be produced but were associated with genes that fell below the expression threshold. Below if they were associated with genes below the expression threshold and were not kept in the final model.

		in 4C	in 15C	in 20C	Reaction	
Reaction	Subsystem	Model	Model	Model	Name	Genes
	Alanine					
	and					
	Aspartate				L-alanine	
	Metabolis				dehydroge	sps_RS053
ALAD_L	m	Expressed	Expressed	Expressed	nase	00
	Alanine					
	and				Alanine-	
	Aspartate				glyoxylate	
ALAGLY	Metabolis	- 1	- 1	- 1	transamına	sps_RS154
X	m	Expressed	Expressed	Expressed	se	05
	Alanıne					
	and					
	Aspartate	Used Dala	Used Dala		-1i	
	Metabolis	Used_Belo	Used_Belo	Evenessed	alanine	sps_K5254
ALAK	111 A lawing	W	W	Expressed	racemase	33
	and					
	Aspartate				I -alanine	
	Metabolis				transamina	sps_RS038
ALATA L	m	Expressed	Expressed	Expressed	se	05
	Alanine					
	and					
	Aspartate				Alanyl-	
	Metabolis				tRNÅ	sps RS201
ALATRS	m	Expressed	Expressed	Expressed	synthetase	90
	Alanine				N-	
	and				acetylmura	
	Aspartate				moyl-L-	
	Metabolis				alanine	sps_RS250
AMAA	m	Expressed	Expressed	Expressed	amidase	25
	Alanine					
	and					sps_RS062
	Aspartate				L-	80 or
	Metabolis				asparagina	sps_RS039
ASNN	m	Expressed	Below	Expressed	se	35

	Alanine				asparagine synthase	
	and				(glutamine	
	Aspartate				-	DC022
ASNS1	m	Expressed	Expressed	Expressed	a)	sps_KS025 60
	Alanine	Lapressea	Expressed	Lapressea	5)	
	and					
	Aspartate				Asparagin	
	Metabolis	F 1	F 1	F 1	yl-tRNA	sps_RS036
ASNTRS	m A lawing	Expressed	Expressed	Expressed	synthetase	90
	Alanine				aspartate	
	Aspartate				1-	
	Metabolis				decarboxyl	
ASP1DC	m	Expressed	Expressed	Expressed	ase	Gap
	Alanine					Desti
	and				agrantata	sps_RS044
	Aspariale				transamina	90 or
ASPTA1	m	Expressed	Expressed	Expressed	se	90
	Alanine					
	and					
	Aspartate				Aspartyl-	
	Metabolis	F 1	F 1	F 1	tRNA	sps_RS057
ASPIRS	M Altomata	Expressed	Expressed	Expressed	synthetase	60
	Carbon				arabinose-	
	Metabolis	Used Belo	Used Belo	Used Belo	phosphate	sps RS256
A5PISO	m	W	w	W	isomerase	00
	Alternate				acetate-	sps_RS102
	Carbon				CoA ligase	10 and
	Metabolis	Used_Belo	D -1	D - 1	(ADP-	sps_RS025
ACCOAL	M Altomata	W	Below	Below	Iorming)	/0
	Carbon				acetyloluc	
	Metabolis				osamine	sps RS116
ACGAMK	m	Expressed	Expressed	Expressed	kinase	15
					2-	
					aminoethyl	
	Altomata				phosphona	
	Carbon				nuruvate	
	Metabolis				transamina	sps RS203
AEPPAT	m	Below	Below	Below	se	60

					N-	
					acetylgluc	
	Alternate				osamine-6-	
	Carbon				phosphate	
	Metabolis				deacetylas	sps_RS116
AGDC	m	Expressed	Expressed	Expressed	e	10
					alcohol	
	Alternate				dehydroge	
	Carbon				nase	
	Metabolis			_	(ethanol:	sps_RS037
ALCD2x	m	Expressed	Expressed	Expressed	NAD)	65
	A 1.				aldehyde	
	Alternate				dehydroge	
	Carbon				nase	D C01(
	Metabolis	F 1	F 1	D - 1	(acetalden	sps_RS016
ALDD2X	m A ltana ata	Expressed	Expressed	Below	yde, NAD)	10
	Alternate				Amylomali	
	Matabalia				ase (maltatriag	and DS112
ΔΜΔΙΤΙ	m	Everaged	Evprogod	Everaged		sps_K5115
AWALTI	111 Altornata	Expressed	Expressed	Expressed	c) A mylomalt	55
	Carbon				Alliyioillan	
	Metabolis				(maltotetra	sns RS113
AMALT2	m	Expressed	Expressed	Expressed	(manotetra	55 ST
	Alternate	Lipressea	Lipressea	Linpressea	Amvlomalt	
	Carbon				ase	
	Metabolis				(maltopent	sps RS113
AMALT3	m	Expressed	Expressed	Expressed	aose)	55
	Alternate	· ·		1	Amylomalt	
	Carbon				ase	
	Metabolis				(maltohexa	sps_RS113
AMALT4	m	Expressed	Expressed	Expressed	ose)	55
	Alternate				Succinyl-	sps_RS102
	Carbon				CoA:butyr	60 and
BUTSUC	Metabolis				ate-CoA	sps_RS102
CCOA	m	Expressed	Expressed	Expressed	transferase	65
	Alternate					
	Carbon					D.010(
	Metabolis	D 1	D 1	D 1	1	sps_RS126
CHITINS	m	Below	Below	Below	chitinase	90 DC140
	Alternate					sps_KS140
	Carbon					30 or
DNA_CU	ivietabolis	Dalarr	Dalarr	Dalarr	DNA Uvdaalaas	sps_KSU/5
1	M Alternet:	Below	Below	Below	Dearwrit	13 ma D0125
עססס	Alternate	Errancesse	Evenesse 1	Exercise 1	Deoxyr1bo	sps_KS135
DKRK	Carbon	Expressed	Expressed	Expressed	kinase	30

	Metabolis					
	m					
	Alternate				deoxyribos	
	Carbon				e-	
	Metabolis				phosphate	sps_RS208
DRPA	m	Expressed	Expressed	Expressed	aldolase	80
						(sps_RS06
						355 and
						sps_RS058
						93 and
						sps_K3002 95 and
						sps RS003
						00) or
					Fatty acid	(sps RS05
					oxidation	895 and
					(dodecano	sps_RS239
					ate:ubiquin	35 and
	Alternate				one) and	sps_RS002
	Carbon				swp_0034	95 and
	Metabolis	- 1	- 1	_ 1	and	sps_RS003
FAO4	m	Expressed	Expressed	Expressed	swp_0035)	00)
						(sps_RS06
						355 and $\mathbf{PS}058$
						sps_K3038 95 and
						sps RS002
						95 and
						sps RS003
						100 or
					Fatty acid	(sps_RS05
					oxidation	895 and
					(tetradecan	sps_RS239
					oate:ubiqui	35 and
	Alternate				none) and	sps_RS002
	Carbon				swp_0034	95 and
EAO5	Metabolis	Evenessed	Evenessed	Evenegad	and (0025)	sps_KS003
гаоз	111	Expressed	Expressed	Expressed	Swp_0033) Fatty acid	(cng RSA6
					oxidation	(sps_1500 355 and
					(hexadecan	sps RS058
					oate:ubiqui	95 and
	Alternate				none) and	sps RS002
	Carbon				swp_0034	95 and
	Metabolis				and	sps_RS003
FAO6	m	Expressed	Expressed	Expressed	swp_0035)	00) or

						(sps_RS05
						sps RS239
						35 and
						sps_RS002
						95 and
						sps_RS003 00)
						(sps_RS06 355 and
						sps_RS058 95 and
						sps_RS002 95 and
						sps_RS003 00) or
					Fatty acid	(sps_RS05
					oxidation	895 and
					oate:ubiqui	35 and
	Alternate				none) and	sps_RS002
	Carbon				swp_0034	95 and
FA07	Metabolis	F 1	F 1	F 1	and	sps_RS003
FAO/	M Alternate	Expressed	Expressed	Expressed	swp_0035)	00)
	Carbon				dimethylbe	
FMNRDD	Metabolis				nzimidazol	sps_RS013
MBZ	m	Below	Below	Below	e synthase	25
	A 1/				glycerol-3-	
	Alternate				phosphate	
	Metabolis				nase	sps_RS276
G3PD2	m	Expressed	Expressed	Expressed	(NADP)	70
	Alternate				glucosami	
	Carbon				ne-6-	DC241
GADDA	Metabolis	Evpressed	Evpressed	Expressed	phosphate	sps_RS241
UUI DA	111	Expressed	Expressed	Expressed	galactose-	30
	Alternate				1-	
	Carbon				phosphate	
GAL1PUR	Metabolis				uridylyltra	sps_RS035
1	m	Below	Below	Expressed	nsferase	10
	Alternate				Reta_	
	Metabolis				galactosida	sps RS143
GALACN	m	Below	Below	Below	se	90

	Alternate					
	Metabolis				galactokin	sps_RS144
GALKr	m	Expressed	Expressed	Expressed	ase	00
GALU	Alternate Carbon Metabolis m	Expressed	Expressed	Expressed	UTP- glucose-1- phosphate uridylyltra nsferase	sps_RS180 75
GBEZ	Alternate Carbon Metabolis m	Expressed	Expressed	Expressed	1,4-alpha- glucan branching enzyme	sps_RS113 50
GLCGSD	Alternate Carbon Metabolis m	Expressed	Below	Below	glucan 1,4- alpha- glucosidas e	sps_RS034 90
CLVCVb	Alternate Carbon Metabolis	Palaw	Palaw	Palaw	glycerate	sps_RS094
GLICKD	m A ltannata	Below	Below	Below	kinase	90
GLYK	Carbon Metabolis m	Expressed	Expressed	Expressed	glycerol kinase	sps_RS161 90
HMGDy	Alternate Carbon Metabolis	Evpressed	Evpressed	Evpressed	S- (hydroxym ethyl)gluta thione dehydroge	sps_RS211 45
	Alternate Carbon Metabolis	LAPICSSCU	LAPICSSCU	LApressed	S- (hydroxym ethyl)gluta thione	sps_RS247 90 or sps_RS073
HMGSs	m	Expressed	Below	Expressed	synthase	40
ΗΟΧΡΡν	Alternate Carbon Metabolis m	Fypressed	Below	Below	2-hydroxy- 3- oxopropio nate reductase (NAD)	sps_RS066 90
	Alternate Carbon Metabolis	Expressed		Delow	Hydroxypy ruvate	sps_RS228
HPYKRX	m	Expressed	Expressed	Expressed	reductase	25

	Alternate				TT 1	
	Carbon Metabolis				Hydroxypy	one RS228
HPYRRv	m	Expressed	Expressed	Expressed	reductase	25 sps_R3220
	Alternate Carbon Metabolis	Liprobed	Liprobed	Liprobod	Hexosamin	sps_RS116 20 or sps_RS081
HXAD	m	Expressed	Expressed	Expressed	idase	20
MCITD	Alternate Carbon Metabolis m	Expressed	Below	Expressed	2- methylcitra te dehydratas e	sps_RS099 50
	Alternate	1		1		
MCITS	Carbon Metabolis m	Expressed	Expressed	Expressed	2- methylcitra te synthase	sps_RS099 55
	Alternate	1		1		sps_RS104
MEAMP1 _GLU- ASP	Carbon Metabolis m	Expressed	Expressed	Expressed	Dipeptide hydrolase	85 or sps_RS095 00
MEAMP1 _GLY-	Alternate Carbon Metabolis	Evenerad	Evenegad	Evenessed	methionyl aminopepti	sps_RS104 85 or sps_RS095
ASP	M Alternate	Expressed	Expressed	Expressed	dase	$\frac{00}{\text{spc}} \mathbf{PS} 104$
MEAMP1 _GLY-	Carbon Metabolis				methionyl aminopepti	85 or sps_RS095
GLU	m	Expressed	Expressed	Expressed	dase	00
	Alternate Carbon Metabolis				2- methylisoc itrate	sps_RS264
MICITH	m	Expressed	Expressed	Expressed	hydratase	25
	Alternate Carbon Metabolis				methylisoc	sps_RS099
MICITL	m	Expressed	Expressed	Expressed	itrate lyase	60
MLTAM	Alternate Carbon Metabolis m	Below	Below	Below	Alpha- Amylase (maltotetra ose)	sps_RS034 75
	Alternate Carbon Metabolis				glucoamyl ase (maltotrios	sps_RS032
MLTG1e	m	Below	Below	Below	e)	80

	1	1	1	1	1	
	Alternate				glucoamyl	
	Carbon				ase	
	Metabolis				(maltotetra	sps_RS032
MLTG2e	m	Below	Below	Below	ose)	80
	Alternate				glucoamyl	
	Carbon				ase	
	Metabolis				(maltopent	sps RS032
MLTG3e	m	Below	Below	Below	aose)	80
	Alternate				glucoamyl	
	Carbon				ase	
	Metabolis				(maltohexa	sps RS032
MLTG4e	m	Below	Below	Below	ose)	80
	Alternate				glucoamyl	
	Carbon				ase	
	Metabolis				(maltohept	sps RS032
MLTG5e	m	Below	Below	Below	aose)	80
	Alternate					
	Carbon					
	Metabolis					sps RS034
MLTS	m	Expressed	Below	Below	maltase	90
		-			maltase	
	Alternate				(periplasmi	
	Carbon				c), Alpha	
	Metabolis				glucosidas	sps RS033
MLTSp	m	Expressed	Expressed	Expressed	e	15
_	Alternate	_	_	_	2-	sps RS175
	Carbon				Oxobutano	80 and
	Metabolis				ate formate	sps_RS175
OBTFL	m	Expressed	Expressed	Expressed	lyase	75
	Alternate	_	_	_	phosphogl	
	Carbon				ycolate	
	Metabolis				phosphatas	sps RS265
PGLYCP	m	Expressed	Expressed	Expressed	e	95
	Alternate	-	-	-		
	Carbon					
	Metabolis				phosphogl	sps_RS038
PGMT	m	Expressed	Expressed	Expressed	ucomutase	45
	Alternate					sps_RS096
	Carbon				phosphom	35 or
	Metabolis				annomutas	sps_RS160
PMANM	m	Expressed	Below	Expressed	e	65
	Alternate					
	Carbon					
	Metabolis			Used_Belo	phosphope	sps_RS208
PPM	m	Expressed	Expressed	w	ntomutase	70

	Alternate				phosphope	
	Metabolis			Used Belo	(deoxvribo	sps RS208
PPM2	m	Expressed	Expressed		se)	70
	Alternate	_				
PULINAS	Metabolis				Neonullula	sps RS034
E	m	Below	Below	Below	nase	80
	Alternate					
	Carbon					
	Metabolis					sps_RS135
RBK	m	Expressed	Expressed	Expressed	ribokinase	30
	Alternate				S-	
	Carbon Motobolia				Formylglut	ma DS211
SEGTH	m	Fypressed	Fypressed	Expressed	hydralase	sps_K3211 40
51 5111	Alternate	LAPICOU	LAPICOU	Laprosou	serine-	
	Carbon				pyruvate	
	Metabolis				aminotrans	sps_RS154
SPA	m	Expressed	Expressed	Expressed	ferase,	05
	Alternate					
	Carbon				UDPgluco	D C100
	m	Expressed	Expressed	Expressed	se 4-	sps_K5180
UDI 04L	111	Expressed	Expressed	Expressed		00
					glucose-	
	Alternate				hexose-1-	
	Carbon				phosphate	
UDPHEX	Metabolis				uridylyltra	sps_RS035
URI	m	Below	Below	Expressed	nsferase	10
	Anapleroti				, ,	DC027
ICI	C Ponctions	Expressed	Expressed	Expressed	1socitrate	sps_RS037
	Reactions	Expressed	Expressed	Expressed	Tyase	sps RS189
						85 or
						sps_RS037
	Anapleroti					55 or
	c				malate	sps_RS088
MALS	Reactions	Expressed	Expressed	Expressed	synthase	60
	Anonlarati				malia	sps_KS218
	Anapierou				enzyme	sns RS263
ME2	Reactions	Expressed	Expressed	Expressed	(NADP)	75 rts205
	Anapleroti				())	
	c				phosphoen	sps_RS266
PPC	Reactions	Expressed	Expressed	Expressed	olpyruvate	95

					carboxylas	
					e	
					phosphoen	
	Anapleroti				olpyruvate	DC269
DDCK	C Reactions	Evpressed	Evpressed	Expressed	carboxykin	sps_K5208
FFCK	Reactions	Expressed	Expressed	Expressed		00
	Arginine				aminobuty	
	and Proline				rate	
	Metabolis				transamina	sps_RS139
ABTA	m	Expressed	Expressed	Expressed	se	00
	Arginine					
	and Proline				acetylgluta	DCOCC
ACCV	Metabolis	Emmand	Emmand	Example of	mate	sps_RS266
ACGK	M Argining	Expressed	Expressed	Expressed	Kinase	80
	and Proline				IN- acetylaluta	
	Metabolis				mate	sps_RS162
ACGS	m	Expressed	Expressed	Expressed	synthase	60
	Arginine			· ·	acetylornit	
	and Proline				hine	
	Metabolis				deacetylas	sps_RS266
ACODA	m	Expressed	Expressed	Expressed	e	90
	Arginine				acetylornit	
	And Proline				troncomino	ang PS 240
ΑСОТА	m	Expressed	Expressed	Expressed	se	50 sps_R3249
	Arginine	Expressed	Expressed	Lapressea	Adenosvl	
	and Proline				methionine	
	Metabolis				decarboxyl	sps_RS066
ADMDC	m	Expressed	Expressed	Expressed	ase	20
	Arginine					
	and Proline				Agmatine	DCOCC
AGMAHY	Metabolis	Everaged	Everaged	Expressed	ureonydrol	sps_RS066
D	111	Expressed	Expressed	Expressed	N_acetyl_	15
	Arginine				σ-	
	and Proline				glutamyl-	
	Metabolis				phosphate	sps_RS266
AGPR	m	Expressed	Expressed	Expressed	reductase	85
	Arginine					
	and Proline				Aminopept	Davaa
AMPIAS	ivietabolis	Evenessed	Dalarr	Errange and 1	Idase (pro-	sps_KS028
EFG	111	Expressed	Delow	Expressed	giy)	00

	Arginine and Proline				arginine	
	Metabolis				decarboxyl	sps RS066
ARGDC	m	Expressed	Expressed	Expressed	ase	25
ARGSL	Arginine and Proline Metabolis m	Expressed	Expressed	Expressed	argininosu ccinate lyase	sps_RS266 65
ARGSS	Arginine and Proline Metabolis m	Expressed	Expressed	Expressed	argininosu ccinate synthase	sps_RS266 70
ARGTRS	Arginine and Proline Metabolis m	Expressed	Expressed	Expressed	Arginyl- tRNA synthetase	sps_RS264 00
ACT	Arginine and Proline Metabolis	Emmand	Emmand	Evenerad	Arginine succinyltra	sps_RS249
A31	Arginine and Proline Metabolis	Expressed	Expressed	Expressed	carbamoyl- phosphate synthase (glutamine - hydrolysin	sps_RS210 35 and sps_RS210
CBPS	m	Expressed	Expressed	Expressed	g)	30
G5SD	Arginine and Proline Metabolis m	Expressed	Expressed	Expressed	glutamate- 5- semialdehy de dehydroge nase	sps_RS211 10
GGLUGA BDH	Arginine and Proline Metabolis m	Expressed	Expressed	Expressed	gammaglut amyl- gamma- aminobuty raldehyde dehydroge nase	sps_RS139 05
GGLUGA BH	Arginine and Proline Metabolis m	Expressed	Expressed	Expressed	gammaglut amyl- gamma- aminobuty rate hydrolase	sps_RS125 85

	Arginine				gammaglut	
CCLUDT	Motobolic				amyi	ong DS125
O	m	Below	Below	Relow	ovidase	sps_K3123
0	Δrginine	DCIOW	DCIOW	DCIOW	gammaglut	55
	and Proline				amvl	
	Metabolis				putrescine	sps_RS125
GGLUPTS	m	Expressed	Expressed	Expressed	synthetase	80
	Arginine	1	1	1		
	and Proline					
	Metabolis				glutamate	sps_RS211
GLU5K	m	Expressed	Expressed	Expressed	5-kinase	15
	Arginine				methylthio	
	and Proline				adenosine	
	Metabolis	F 1	F 1	F 1	nucleosida	sps_RS120
MIAN	m	Expressed	Expressed	Expressed	se	90
	Arginine				amithing	
	Metabolis				carbamovit	sps PS266
OCBT	m	Expressed	Expressed	Expressed	ransferase	sps_R3200 75
	111	Expressed	Expressed	Expressed	Tunisteruse	sps_RS217
						00 or
	Arginine					sps RS236
	and Proline				ornithine	25 or
	Metabolis		Used_Belo		cyclodeam	sps_RS054
ORNCD	m	Expressed	W	Expressed	inase	20
					1-	
					pyrroline-	
					5-	
	Arginine				carboxylat	
	and Proline				e dahudra aa	ang DS247
P5CD	m	Evpressed	Evpressed	Fypressed	nase	sps_K5247
1 300	Arginine	LAPICSSCU	LAPICSSCU	LAPICSSCU	nvrroline-	50
	and Proline				5-	
	Metabolis				carboxvlat	sps RS115
P5CR	m	Expressed	Expressed	Expressed	e reductase	05
	Arginine	•	•	•		
	and Proline					
	Metabolis				proline	sps_RS247
PRO1q	m	Expressed	Expressed	Expressed	oxidase	30
	Arginine					
	and Proline				Prolyl-	Dates
	Metabolis				tRNA	sps_RS103
PROTRS	m	Expressed	Expressed	Expressed	synthetase	45

	Arginine				Succinylar	
	and Proline				ginine	DC001
SADU	Metabolis	Evenessed	Everaged	Everaged	dinydrolas	sps_KS081
SADH	m Angining	Expressed	Expressed	Expressed	e Succievial	43
	Arginine and Prolina				succinyigi	
	Metabolis				desuccinvl	ene RS038
SGDS	m	Fypressed	Expressed	Expressed	ase	sps_R5050
5525	111	LAPICSSCG	Expressed	LApressed	Succinvlol	55
					utamic	
	Arginine				semialdehy	
	and Proline				de	
	Metabolis				dehydroge	sps_RS249
SGSAD	m	Expressed	Expressed	Expressed	nase	40
	Arginine				Succinylor	
	and Proline				nithine	
	Metabolis				transamina	sps_RS249
SOTA	m	Expressed	Expressed	Expressed	se	50
	Arginine					
	and Proline					D.C.2.4.(
CDMC	Metabolis	Used_Belo	Used_Belo	F 1	spermidine	sps_RS246
SPMS	m A nainin a	W	W	Expressed	synthase	80
	Arginine and Prolina					
	Metabolis				spermine	sns RS246
SPRS	m	Below	Below	Expressed	synthase	80
	111	Delow	Delow	LAPICSSCU	succinate-	
					semialdehv	
	Arginine				de	
	and Proline				dehydroge	
	Metabolis				nase	sps_RS126
SSALx	m	Expressed	Expressed	Expressed	(NAD)	05
Biomass_					biomass	
WP2	Biomass	Expressed	Expressed	Expressed	1gDW	Biomass
					DNA	
DNA_SY					synthesis	
NTHESIS	Biomass	Expressed	Expressed	Expressed	lg	Biomass
GLYCOG					Glycogen	
EN_SYNI	D:	F 1	F 1	F 1	Synthesis	D:
HESIS	BIOMASS	Expressed	Expressed	Expressed	WP2(lg)	ыomass
					Phospholip	
I IPID SV					Synthesis	
NTHESIS	Biomass	Expressed	Expressed	Expressed	WP2 (1g)	Biomass

					LPS	
LPS_SYN					synthesis	
THESIS	Biomass	Expressed	Expressed	Expressed	WP2 (1g)	Biomass
					Lipid	
PASYN_					Synthesis	
WP2	Biomass	Expressed	Expressed	Expressed	WP2 (1g)	Biomass
PEPTIDO						
_SYNTHE					peptidogly	
SIS	Biomass	Expressed	Expressed	Expressed	can 1gDW	Biomass
					Protein	
PROT_SY				_	synthesis	
NTHESIS	Biomass	Expressed	Expressed	Expressed	lg	Biomass
					RNA	
RNA_SY				_	synthesis	
NTHESIS	Biomass	Expressed	Expressed	Expressed	lg	Biomass
					Irace	
TRACE_E					Element	
LEMENI	D.	F 1	F 1	F 1	Synthesis	D'
5	Biomass	Expressed	Expressed	Expressed	WP2 (1g)	Biomass
	C - 11				acyi-lacyi-	DC2(7
	Cell Envilance				carrier-	sps_KS20/
	Envelope				proteinj	$a_{\rm max}$ DS067
A A CDS10	Biosynthes	Everaged	Polow	Everaged	(n C14.0)	sps_K5007
AACISIU	15	Expressed	Delow	Expressed	$(\Pi - C I 4.0)$	10
	Cell				acyl-lacyl-	sps RS267
	Envelope				protein]	sps_R3207
	Biosynthes				synthetase	sps RS067
AACPS11	is	Expressed	Below	Expressed	(n-C15:0)	10
		Lipressea	Deleti	Lipiessea	acyl-[acyl-	10
	Cell				carrier-	sps_RS267
	Envelope				protein]	65 and
	Biosynthes				synthetase	sps RS067
AACPS12	is	Expressed	Below	Expressed	(n-C16:0)	10
		1			acyl-[acyl-	
	Cell				carrier-	sps RS267
	Envelope				protein]	65 and
	Biosynthes				synthetase	sps_RS067
AACPS13	is	Expressed	Below	Expressed	(n-C17:0)	10
					acyl-[acyl-	
	Cell				carrier-	sps_RS267
	Envelope				protein]	65 and
	1				. 1 .	ana DCOG7
	Biosynthes				synthetase	sps_KS007
AACPS14	Biosynthes is	Expressed	Below	Expressed	(n-C15:1)	sps_KS067 10
AACPS14	Biosynthes is Cell	Expressed	Below	Expressed	(n-C15:1) acyl-[acyl-	sps_RS067 10 sps_RS267

	Biosynthes				protein]	sps_RS067
	15				synthetase $(n-C17\cdot1)$	10
					acyl-facyl-	
	Cell				carrier-	sps RS267
	Envelope				protein]	65 and
	Biosynthes				synthetase	sps_RS067
AACPS16	is	Expressed	Below	Expressed	(n-C18:1)	10
	G 11				acyl-[acyl-	DCACT
	Cell				carrier-	sps_RS26/
	Biosynthes				synthetase	$\frac{0.5}{2}$ and $\frac{0.5}{2}$ RS067
AACPS3	is	Expressed	Below	Expressed	(n-C16:0)	10
		2	2010 11	2	acyl-[acyl-	10
	Cell				carrier-	sps_RS267
	Envelope				protein]	65 and
	Biosynthes				synthetase	sps_RS067
AACPS4	is	Expressed	Below	Expressed	(n-C16:1)	10
	C -11				acyl-[acyl-	DC2(7
	Cell				carrier-	sps_RS26/
	Biosynthes				synthetase	$rac{0.5}{ranu}$ sps RS067
AACPS5	is	Expressed	Below	Expressed	(n-C18:1)	10
		Empressea	Beleti	Enpressea	acyl-[acyl-	10
	Cell				carrier-	sps RS267
	Envelope				protein]	65 and
	Biosynthes				synthetase	sps_RS067
AACPS6	is	Expressed	Below	Expressed	(n-C15:0)	10
	C -11				acyl-[acyl-	
	Cell				carrier-	sps_KS20/
	Biosynthes				synthetase	sps $RS067$
AACPS7	is	Expressed	Below	Expressed	(n-C17:0)	10
		1		1	acyl-[acyl-	-
	Cell				carrier-	sps_RS267
	Envelope				protein]	65 and
	Biosynthes		- 1		synthetase	sps_RS067
AACPS8	15	Expressed	Below	Expressed	(n-C18:0)	10
	Call				acyi-lacyi-	and DC267
	Envelope				protein]	sps_15207 65 and
	Biosynthes				synthetase	sps RS067
AACPS9	is	Expressed	Below	Expressed	(n-C13:0)	10
		-		•	acyl-[acyl-	
AACPSFA	Cell				carrier-	sps_RS267
130OH	Envelope	Expressed	Below	Expressed	protein]	65 and

	Biosynthes				synthetase	sps_RS067
	is				(n-C14:0)	10
AACPSFA 1718	Cell Envelope Biosynthes is	Expressed	Below	Expressed	acyl-[acyl- carrier- protein] synthetase (n-C14:0)	sps_RS267 65 and sps_RS067 10
AACPSFA 1817	Cell Envelope Biosynthes is	Expressed	Below	Expressed	acyl-[acyl- carrier- protein] synthetase (n-C14:0)	sps_RS267 65 and sps_RS067 10
ACNAMS	Cell Envelope Biosynthes is	Expressed	Expressed	Expressed	N- acetylneur aminate synthase	sps_RS184 15
ALAALA	Cell Envelope Biosynthes is	Expressed	Expressed	Expressed	D-alanine D-alanine ligase (reversible)	sps_RS061 70 or sps_RS215 95
CDDC4/D	Cell Envelope Biosynthes				CDP- glucose 4,6- dehydratas	sps_RS183
CKDOAS	Cell Envelope Biosynthes is	Expressed	Expressed	Expressed	e CMP-8- amino-3,8- dideoxy- D-manno- oct-2- ulosonic acid synthase	Gap
DACK	Cell Envelope Biosynthes				diacylglyc	sps_RS067
DAGK	1S Call	Expressed	Below	Expressed	erol kinase	93
DASYN	Envelope Biosynthes is	Used_Belo w	Used_Belo w	Used_Belo w	nosphatid ate cytidylyltr ansferase	sps_RS104 55
DMOCT	Cell Envelope Biosynthes	Fypressed	Fypressed	Fynressed	3-deoxy- manno- octulosona	sps_RS031
	10	LAPICSSCU	LAPICSSCU	LAPICSSCU		70

					cytidylyltr	
					ansferase	
					Endotoxin	
	Cell				Synthesis	sps_RS138
	Envelope				(lauroyl	25 and
	Biosynthes	Used_Belo	Used_Belo		transferase	sps_RS067
EDTXS5	is	W	W	Expressed)	10
					Endotoxin	
	Cell				Synthesis	sps_RS065
	Envelope				(myristoyl	45 and
	Biosynthes	Used_Belo			transferase	sps_RS067
EDTXS6	15	W	Expressed	Expressed)	10
					glucosami	
	G 11				ne-1-	
	Cell				phosphate	
	Envelope				IN-	ana DC279
C1DACT	Biosynthes	Evenessed	Everaged	Everaged	forego	sps_K5278
UIFACI	IS Coll	Expressed	Expressed	Expressed	alucoso 1	30
	Envelope				glucose-1-	
	Biosynthes				cytidylyltr	sns RS183
GIPCT	is	Expressed	Expressed	Below	ansferase	40
	Cell	LAPICSSEd	LAPICSSCA	Delow	glucose-1-	10
	Envelope				phosphate	
	Biosynthes				thymidylyl	sps RS182
G1PTMT	is	Expressed	Below	Expressed	transferase	00
		1		1	glutamine-	
	Cell				fructose-6-	
	Envelope				phosphate	
	Biosynthes				transamina	sps_RS278
GF6PTA	is	Below	Below	Below	se	15
	Cell					
	Envelope					
	Biosynthes				glutamate	sps_RS267
GLUR	is	Expressed	Expressed	Expressed	racemase	35
					D-glycero-	
					D-manno-	
	Cell				hepose 1-	
	Envelope				phosphate	Dance
GMHEPA	Biosynthes				adenyltran	sps_RS008
1	15	Expressed	Expressed	Expressed	sterase	US
	Call				D-glycero-	
	Cell Envilant				D-manno-	
	Diogymthes				nepiose /-	and DCUU0
GMUEDV		Expressed	Expressed	Expressed	kinasa	sps_r.5008
UNITERN	15	Lapiesseu	Expressed	DAPIESSEU	KIIIdSC	05

					D-glycero-	
					D-manno-	
					heptose	
					1,7-	
	Cell				bisphospha	
	Envelope				te	
GMHEPP	Biosynthes				phosphatas	sps_RS166
А	is	Expressed	Expressed	Expressed	e	60
					Glyceroph	
					osphodiest	
					er	
					phosphodi	
	Cell				esterase	
	Envelope				(Glyceroph	
	Biosynthes				osphoethan	sps_RS250
GPDDA2	18	Expressed	Expressed	Expressed	olamine)	85
					Glyceroph	
					osphodiest	
					er	
	C 11				phosphodi	
					esterase	
	Envelope				(Glyceroph	DC250
	Biosynthes	E	E	E	osphoglyce	sps_K5230
GPDDA4	15	Expressed	Expressed	Expressed	rol)	85
					5-deoxy-	
	Call				nianno-	
	Envelope				te-8-	
	Biosynthes				nhosnhatas	sns RS256
KDOPP	is	Expressed	Expressed	Expressed	e	05
					2-dehvdro-	
	Cell				3-deoxy-	
	Envelope				phosphooc	
	Biosynthes				tonate	sps RS213
KDOPS	is	Expressed	Expressed	Expressed	aldolase	75
	Cell	_	_	_		
	Envelope				Lipid A	
	Biosynthes				disaccaride	sps_RS104
LPADSS	is	Expressed	Expressed	Expressed	synthase	15
	Cell					
	Envelope				LPS	
LPSSYN_	Biosynthes	Used_Belo			synthesis	sps_RS007
core	15	W	Expressed	Expressed	(general)	30
	G 11				mannose-	Data
	Cell	-			1-	sps_RS160
MAN1PT2	Envelope	Expressed	Expressed	Expressed	phosphate	60

	Biosynthes				guanylyltra	
	18				nsferase (GDP)	
	Cell				(ODI) mvo-	
	Envelope				inositol 1-	
	Biosynthes				phosphatas	sps_RS177
MI1PP	is	Expressed	Expressed	Expressed	e	35
					8-amino	
					3,8-	
	Call				dideoxy-	
	Envelope				octulosoni	
	Biosynthes	Used Belo	Used Belo	Used Belo	c acid	sps RS007
MOAT3	is	W	W	W	transferase	25
	Cell				phosphatid	
	Envelope				ic acid	
	Biosynthes	Used_Belo	Used_Belo	Used_Belo	phosphatas	sps_RS153
PAP	15	W	W	W	e 1 1	75
					phospho- N-	
					acetylmura	
					moyl-	
					pentapepti	
					de-	
	Cell				transferase	
	Envelope	U. 1 D.1.			(meso-2,6-	DC1(1
D Λ DDT 3	Biosynthes	Used_Belo	Evpressed	Evpressed	alaminopi melate)	sps_K5101
TATTIS	18 Cell	W	Expressed	Expressed	Pentidogly	30
	Envelope				an subunit	
PEPTIDO	Biosynthes				crosslinkin	
Xe	is	Expressed	Expressed	Expressed	g reaction	Gap
	Cell					
	Envelope				phosphogl	
	Biosynthes	Used_Belo	г 1	F 1	ucosamine	sps_RS209
PGAMI	15	W	Expressed	Expressed	Dhoophatid	/5
	Cell				vlolvceron	sps RS153
	Envelope				hosphate	75 or
	Biosynthes	Used Belo	Used Belo	Used Belo	phosphohy	sps RS203
PGPPH	is	w	w	w	drolase	10
					CDPdiacyl	
	Cell				glycerol:sn	
	Envelope				-glycerol-	D COOO
DCSA	Biosynthes	Used_Belo	Used_Belo	Used_Belo	3-	sps_KS029
rusa	15	W	W	W	phosphate	0.0

					3_	
					nhosnhotid	
					yitransiera	
					se	
	Cell					
	Envelope				Peptidogly	
	Biosynthes				can subunit	
PPTGSe	is	Expressed	Expressed	Expressed	synthesis	Gap
	Cell				Phosphatid	
	Envolono				vlaarina	
	Envelope					DC250
	Biosynthes	- 1	- 1		decarboxyl	sps_RS250
PSD	15	Expressed	Expressed	Expressed	ase	70
					CDPdiacyl	
					glycerol-	
	Cell				serine O-	sps RS040
	Envelope				nhosnhatid	60 or
	Diogunthag				vltronsforo	$p_{\rm cmc}$ DS 216
DCCA	Biosynthes	D	F	F 1	ymansiera	sps_K3210
PSSA	1S	Expressed	Expressed	Expressed	se	<u> </u>
	Cell				sedoheptul	sps_RS265
	Envelope				ose 7-	65 or
	Biosynthes				phosphate	sps_RS173
S7PI	is	Expressed	Expressed	Expressed	isomerase	75
			4		dTDP-3-	
					amino-3.6-	
					didoovy	
	G 11				alpha-D-	
	Cell				galactopyr	
	Envelope				anose	
TDP3AAA	Biosynthes				transamina	sps_RS183
Т	is	Expressed	Expressed	Expressed	se	50
	Cell				dTDP-4-	
	Envelope				dehvdrorha	
	Biosynthes				mnose 3 5-	sps RS007
TOPORE	is	Evpressed	Evpressed	Expressed	enimerase	45
	Call	Lapressed	Lapressed	LAPICSSCU		
					u1DP-4-	sps_K500/
	Envelope				dehydrorha	55 or
	Biosynthes				mnose	sps_RS147
TDPDRR	is	Expressed	Expressed	Expressed	reductase	45
	Cell				dTDPgluc	
	Envelope				ose 4,6-	
	Biosynthes				dehvdratas	sps RS183
TDPGDH	is	Expressed	Expressed	Expressed	e	85
	Call	LAPICOUC	LAPICOUC	Lipiosod	-	
	Cell Envil				Tatura 11'	
	Envelope					DCAGA
	Biosynthes	Used_Belo	Used_Belo	Used_Belo	saccharide	sps_RS080
TDSK	15	W	W	W	4'kinase	55

					UDP-3-O-	
					(3-	
					(S hydroxym	
	C -11				inyuroxyin	
					yristoyi)gi	sps_KS104
	Envelope				ucosamine	30 and
	Biosynthes				acyltransfe	sps_RS067
U23GAAT	is	Expressed	Expressed	Expressed	rase	10
					UDP-N-	
					acetylmura	
					movl-L-	
					alanvl-D-	
					glutamyl-	
	Cell				meso 2.6	
	Envilance				diaminani	
	Discontinue				diaminopi	DC1(1
	Biosynthes	F 1	F 1	D 1	melate	sps_KS161
UAAGDS	15	Expressed	Expressed	Expressed	synthetase	60
					UDP-N-	
	Cell				acetylgluc	sps_RS104
	Envelope				osamine	20 and
	Biosynthes				acyltransfe	sps_RS067
UAGAAT	is	Expressed	Expressed	Expressed	rase	10
		-			UDP-N-	
					acetylgluc	
	Cell				osamine 1-	
	Envelope				carboxyvin	
	Biosynthes				vltransfera	sns RS255
UAGCVT	is	Evpressed	Expressed	Expressed	ynnansiera	5p5_R5255
UNUCVI	15	Expressed	Expressed	Expressed		00
	C-11				UDP-IN-	
					acetyigiuc	
	Envelope				osamine	D 0000
	Biosynthes			_	diphosphor	sps_RS278
UAGDP	is	Expressed	Expressed	Expressed	ylase	30
					UDP-N-	
					acetylgluc	
					osamine-	
					N-	
					acetylmura	
					mvl-	
					(pentapenti	
					de)pvronh	
					osphoryl-	
					undecanre	
	Cell				nol N	
	Envolono				nor in-	
	Diographia				accivigitue	and DOIGI
	Biosynthes	F 1	F 1	F 1	osamme	sps_K5101
UAGP13	18	Expressed	Expressed	Expressed	transferase	55

					UDP-N-	
					acetylmura	
	Cell				moyl-L-	
	Envelope				alanyl-D-	
	Biosynthes				glutamate	sps RS161
UAMAGS	is	Expressed	Expressed	Expressed	synthetase	45
		1	1	1	UDP-N-	
	Cell				acetvlmura	
	Envelope				movl-L-	
	Biosynthes				alanine	sps RS161
UAMAS	is	Expressed	Expressed	Expressed	synthetase	30^{-1}
		F	F		UDP-N-	
	Cell				acetylenol	
	Envelope				pyruvovlgl	
	Biosynthes		Used Belo	Used Belo	ucosamine	sps_RS017
UAPGR	is	Expressed	w	w	reductase	05
	Cell	Lipresee			undecapre	
	Envelope				nvl-	
	Biosynthes	Used Belo	Used Belo		diphosphat	sps_RS125
UDCPDP	is	w	w	Expressed	ase	05
				Lipressea	LIDP-N-	
					acetylmura	
					movl_L_	
					alanyl_D_	
					alutomyl	
					giutaniyi-	
					diaminoni	
	Call				melovi D	
	Envelope				alanyl_D_	
	Biosynthes				alaning	ene PS161
UGMDDS	is	Expressed	Evpressed	Expressed	synthetase	55_K5101
OGMDD3	15	Expressed	Expressed	Expressed		55
					acyl N	
	Call				acyr n-	
	Envolono				acetyigiue	
	Discurthes				depentular	and DS161
	Biosynthes	Evenessed	Everaged	Everaged	deacetylas	sps_K5101
UNGADA	15 Call	Expressed	Expressed	Expressed	e	10
	Envolana					
	Envelope Diagunth a					and DOOO
	Biosynthes	Evenes 1	Evenes 1	Exercise 1	UDP-sugar	sps_KS092
USHD	IS Citer t	Expressed	Expressed	Expressed	nyurolase	03
	Citrate					DCCC
	Cycle	F 1	F 1	F 1	•.	sps_RS264
ACONT	(TCA)	Expressed	Expressed	Expressed	aconitase	25

					_	sps_RS264
					2-	55 and
	Citrata				oxoglutarat	sps_RS0/9
	Curate				e debydroge	73 and
AKGD	(TCA)	Expressed	Expressed	Expressed	nase	80
	Citrate	Lipressea	Lipressea	Lipressea		
	Cycle				citrate	sps RS080
CS	(TCA)	Expressed	Expressed	Expressed	synthase	05
	Citrate					
	Cycle	_	_	_		sps_RS037
FUM	(TCA)	Expressed	Expressed	Expressed	fumarase	15
	Citrata				1socitrate	
	Curate				nase	sps RS100
ICDHxi	(TCA)	Expressed	Expressed	Expressed	(NAD)	85
	(1011)	2	2	2	isocitrate	
	Citrate				dehydroge	
	Cycle				nase	sps_RS027
ICDHy	(TCA)	Expressed	Expressed	Expressed	(NADP)	55
	Citrate				malate	D.G.1.0.0
MDH	Cycle	F 1	F 1	F 1	dehydroge	sps_RS132
MDH	(ICA)	Expressed	Expressed	Expressed	nase	/J
						sps_R3079 85 and
						sps RS079
						95 and
						sps_RS079
	Citrate				Succinate	90 and
CLICD7	Cycle	F 1	F 1	F 1	Dehydroge	sps_RS080
SUCD/	(ICA)	Expressed	Expressed	Expressed	nase	00
					Succinyi-	sps RS070
	Citrate				synthetase	65 and
	Cycle				(ADP-	sps RS079
SUCOAS	(TCA)	Expressed	Expressed	Expressed	forming)	70
					2-Methyl-	
	Cofactor				4-amino-5-	
	and				hydroxyme	
	Group				dine	
	Biosynthes	Used Belo	Used Belo	Used Belo	dinhosnhat	sps_RS027
2MAHMP	is	W	W	W	ase	45
	Cofactor				4-	
	and				hydroxybe	sps_RS206
4HBTE	Prosthetic	Expressed	Below	Expressed	nzoyl-CoA	00

	Group				thioesteras	
	Biosynthes				e	
	is					
	Cofactor					
	and				5'-	
	Prosthetic				deoxyaden	
	Group				osine	
	Biosynthes				nuclosidas	sps_RS120
5DOAN	is	Expressed	Expressed	Expressed	e	90
	Cofactor					
	and					
	Prosthetic				Adenosyl	
	Group				cobainami	
	Biosynthes	_		_	de GTP	sps_RS235
ACBIPGT	15	Expressed	Below	Below	transferase	45
	Cofactor					
	and				1	D G110
	Prosthetic				acyl-	sps_RS119
	Group				carrier	45 and
	Biosynthes	F 1	F 1	г 1	protein	sps_RS06/
ACPSI	1S	Expressed	Expressed	Expressed	synthase	10
	Cofactor				F1	
	and Dreath atio				[acyl-	ana DC179
	Crown				carrier-	sps_KS1/δ
	Group				protein]	00 and
ACDSo	Biosynthes	Everaged	Everaged	Everaged	phosphodi	sps_K5007
ACISC	15 Cofeeter	Expressed	Expressed	Expressed	esterase	10
	colacion					
	Brosthetic				1 amino 1	sps PS068
	Group				deoxychori	$\frac{\text{sps}_{\text{K}}}{45 \text{ or}}$
	Biosynthes				smate	$r_{\rm SDS} R S 068$
ADCI	is	Expressed	Expressed	Expressed	lvase	3ps_R5008 40
TIDEL	Cofactor	Expressed	LAPICSSCU	LAPICSSCG	Tydse	-10
	and					
	Prosthetic					
	Group				Adenosvl	
ADCOBA	Biosynthes				cobinamid	sps RS235
K	is	Expressed	Below	Below	e kinase	45
	Cofactor	p. 50004				
	and					
	Prosthetic				adenosvlco	
	Group				binamide-	
ADCOBA	Biosynthes				phosphate	sps RS120
S	is	Below	Below	Below	synthase	95

	Cofactor					
	and					
	Prosthetic				. 1 1	
	Group				adenosylco	and DS225
ADCOBI	Biosynthes	Dalaw	Palaw	Palow	byric acid	sps_K5255
EAS	18 Cofeeter	Delow	Delow	Delow	synthase	40
	colacion					
	Prosthetic				4-amino-4-	sps RS037
	Group				deoxychori	10 and
	Biosynthes	Used Belo	Used Belo	Used Belo	smate	sps RS249
ADCS	is	w	w	w	synthase	65
	Cofactor					
	and					
	Prosthetic					sps RS203
	Group				D-alanine	50 or
ALATA_	Biosynthes				transamina	sps_RS114
D2	is	Expressed	Expressed	Expressed	se	30
	Cofactor					
	and					
	Prosthetic					sps_RS203
	Group				alanine	50 or
ALATA_L	Biosynthes	F 1	F 1	F 1	transamina	sps_RS114
2	15	Expressed	Expressed	Expressed	se	30
	Cafaataa				adenosylm	
	Cofactor				ethionine-	
	Drosthetic				o-amino-/-	
	Group				ate	
	Biosynthes	Used Belo	Used Belo		transamina	sps_RS078
AMAOT	is	w	w	Expressed	se	65
					S-	
					adenosylm	
					ethione:2-	
	Cofactor				demthylme	
	and				naquinone	
	Prosthetic				methyltran	
	Group				sferase	
AMMQT7	Biosynthes				(menaquin	sps_RS150
_2	15	Expressed	Expressed	Expressed	one 7)	15
	Cofactor				4-amino-2-	
					.1 1 -	
	and				methyl-5-	
	and Prosthetic				methyl-5- phosphom	
	and Prosthetic Group		Land Data		methyl-5- phosphom ethylpyrim	and DC020
ΔΙΔΟΛΟΥ	and Prosthetic Group Biosynthes	Expressed	Used_Belo	Evpressed	methyl-5- phosphom ethylpyrim idine	sps_RS058

	Cofactor and				.	
	Prosthetic Group				8-amino-7-	
	Biosynthes	Used Belo	Used Belo		ate	sps RS078
AOXS	is	w	w	Expressed	synthase	55
APRAUR	Cofactor and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	5-amino-6- (5- phosphorib osylamino) uracil reductase	sps_RS203 40
	Cofactor and Prosthetic Group Biosynthes				L-aspartate	sps_RS120
ASPO3	1S	Expressed	Expressed	Expressed	oxidase	00
	Cofactor and Prosthetic Group Biosynthes				L-aspartate	sps_RS120
ASPO5	is	Expressed	Expressed	Expressed	oxidase	00
ASPO6	Cofactor and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	L-aspartate oxidase	sps_RS120 00
	Cofactor and Prosthetic Group Biosynthes				L-aspartate	sps_RS120
ASPO8	is	Expressed	Expressed	Expressed	oxidase	00
	Cofactor and Prosthetic Group Biosynthes				L-aspartate	sps_RS120
ASPO9	1S	Expressed	Expressed	Expressed	oxidase	00 DC070
	and Prosthetic				synthase condensed	sps_RS0/8 60 and sps_RS177
BTS4	Group	Expressed	Expressed	Expressed	reaction	15
	Biosynthes					
--------	------------	-----------	-----------	-----------	-------------	-----------
	is					
	Cofactor					
	and					
	Prosthetic				Cobinamid	
	Group				e	
	Biosynthes				adenyltran	sps RS235
CBIAT	is	Below	Below	Below	sferase	35
	Cofactor					
	and					
	Prosthetic				cob(I)alam	
	Group				in	
	Biosynthes	Used Belo	Used Belo	Used Belo	adenosyltr	sps RS235
CBLAT	is		w –		ansferase	35^{-}
					4-(cvtidine	
	Cofactor				5'-	
	and				diphospho)	
	Prosthetic				-2-C-	
	Group				methvl-D-	
	Biosynthes				ervthritol	sps RS214
CDPMEK	is	Expressed	Expressed	Expressed	kinase	25
	Cofactor	1	I	I		
	and					
	Prosthetic					
	Group				choline	
CHOLDH	Biosynthes				dehydroge	sps RS174
1	is	Expressed	Below	Below	nase	40
	Cofactor	1				
	and					
	Prosthetic					
	Group				choline	
CHOLDH	Biosynthes				dehvdroge	sps RS174
2	is	Expressed	Below	Below	nase	40
	Cofactor	1				
	and					
	Prosthetic					
	Group				choline	
CHOLDH	Biosynthes				dehydroge	sps RS174
3	is	Expressed	Below	Below	nase	40
	Cofactor	-				
	and					
	Prosthetic					
	Group				choline	
CHOLDH	Biosynthes				dehydroge	sps RS174
4	is	Expressed	Below	Below	nase	40

	Cofactor and					
	Prosthetic					
	Group				choline	
CHOLDH	Biosynthes				dehydroge	sps RS174
5	is	Expressed	Below	Below	nase	40
	Cofactor					
	and					
	Prosthetic					
	Group				chorismate	
	Biosynthes	Used_Belo	Used_Belo	Used_Belo	pyruvate	sps_RS272
CHRPL	is	W	W	W	lyase	20
	Cofactor					
	and					
	Prostnetic				cobalamin-	
	Group				J -	one PS235
CORPS	is	Below	Below	Below	synthase	sps_R3233
CODIS	Cofactor	Delow	Delow	Delow	synthase	50
	and					
	Prosthetic					
	Group				coproporp	
	Biosynthes				hyrinogen	sps_RS004
CPPPGO	is	Expressed	Expressed	Expressed	oxidase	00
	Cofactor				Oxygen	
	Cofactor and				Oxygen Independe	
	Cofactor and Prosthetic				Oxygen Independe nt	sps_RS006
	Cofactor and Prosthetic Group				Oxygen Independe nt coproporp	sps_RS006 60 or
CPPPGOA	Cofactor and Prosthetic Group Biosynthes	Eveneed	Eveneed	Eveneed	Oxygen Independe nt coproporp hyrinogen- UL avidase	sps_RS006 60 or sps_RS271
CPPPGOA N	Cofactor and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase	sps_RS006 60 or sps_RS271 15
CPPPGOA N	Cofactor and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dibydroxy	sps_RS006 60 or sps_RS271 15
CPPPGOA N	Cofactor and Prosthetic Group Biosynthes is Cofactor and	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2-	sps_RS006 60 or sps_RS271 15
CPPPGOA N	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone-	sps_RS006 60 or sps_RS271 15 sps_RS203
CPPPGOA N	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4-	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or
CPPPGOA N	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4- phosphate	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or sps_RS269
CPPPGOA N DB4PS	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4- phosphate synthase	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or sps_RS269 10
CPPPGOA N DB4PS	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is Cofactor	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4- phosphate synthase	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or sps_RS269 10
CPPPGOA N DB4PS	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is Cofactor and	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4- phosphate synthase	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or sps_RS269 10
CPPPGOA N DB4PS	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4- phosphate synthase	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or sps_RS269 10
CPPPGOA N DB4PS	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4- phosphate synthase	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or sps_RS269 10
CPPPGOA N DB4PS	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes	Expressed	Expressed	Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4- phosphate synthase dethiobioti	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or sps_RS269 10 sps_RS078
CPPPGOA N DB4PS DBTSr	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is	Expressed Expressed	Expressed Expressed	Expressed Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4- phosphate synthase dethiobioti n synthase	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or sps_RS269 10 sps_RS078 45
CPPPGOA N DB4PS DBTSr	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is	Expressed Expressed	Expressed Expressed	Expressed Expressed	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4- phosphate synthase dethiobioti n synthase	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or sps_RS269 10 sps_RS078 45
CPPPGOA N DB4PS DBTSr	Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes is Cofactor and Prosthetic Group Biosynthes	Expressed Expressed	Expressed Expressed Expressed Used_Belo	Expressed Expressed Expressed Used_Belo	Oxygen Independe nt coproporp hyrinogen- III oxidase 3,4- Dihydroxy -2- butanone- 4- phosphate synthase dethiobioti n synthase dihydrofol ate reductase	sps_RS006 60 or sps_RS271 15 sps_RS203 30 or sps_RS269 10 sps_RS269 10 sps_RS078 45 sps_RS132 40

	1	1	1	1	1	
	Group					
	is					
	Cofactor					
	and					
	Prosthetic					
	Group				dihydrofol	
	Biosynthes				ate	sps_RS086
DHFS	is	Expressed	Expressed	Expressed	synthase	00
	Cofactor				1,4-	
	and				dihydroxy-	
	Prosthetic				2-	
DINIAOT	Group				naphthoate	ama DC101
DHNAUT 7	biosynthes	Expressed	Expressed	Expressed	ransferase	30
	Cofactor	LAPICSSCU	LAPICSSCU	LAPICSSCU	Tansierase	50
	and					
	Prosthetic					
	Group				dihydroneo	
	Biosynthes		Used_Belo	Used_Belo	pterin	sps_RS125
DHNPA	is	Expressed	W	W	aldolase	15
	Cofactor				diaminohy	
	and				droxyphos	
	Prosthetic				phoribosyl	
	Group				aminopyri	ama DS202
	biosynthes	Expressed	Expressed	Expressed	deaminase	sps_K5205 40
DIIIIDAL	Cofactor	LAPICSSCU	LAPICSSCU	LAPICSSCU	dealiilliase	UTU
	and					
	Prosthetic					
	Group				dihydropte	
	Biosynthes				ridine	sps_RS224
DHPRx	is	Expressed	Expressed	Expressed	reductase	40
	Cofactor					
	and					
	Prosthetic				1.1 1	
	Group	Used Dele			dinydropte	ang DS200
рнрез	biosynthes	Useu_belo	Evpressed	Expressed	synthese	sps_K5209
2011105	Cofactor	••	LAPICSSCU	LAPICSSCU	synthase	00
	and				Dihydrone	
	Prosthetic				opterin	
	Group				triphosphat	
	Biosynthes				e 2'-	sps_RS176
DHPTPE	is	Expressed	Expressed	Expressed	epimerase	20

	Cofactor					
	and					
	Prosthetic					
	Group				dimethylall	
	Biosynthes				yltranstran	sps_RS110
DMATT	is	Expressed	Expressed	Expressed	sferase	35
					1-hydroxy-	
	Cofactor				2-methyl-	
	and				2-(E)-	
	Prosthetic				butenyl 4-	
	Group				diphosphat	
	Biosynthes			_	e reductase	sps_RS117
DMPPS	15	Expressed	Expressed	Expressed	(dmpp)	05
	Cofactor				3-	
	and				Dimethylu	
	Prosthetic				biquinonol	
	Group				3-	D C020
DMOMT	Biosynthes	Evenessed	Evenessed	Evenessed	methyltran	sps_KS039
DNQNI	IS Cofeeter	Expressed	Expressed	Expressed	Dibudeana	75
	Colactor				Dinydrone	
	Drosthatia				mononhos	
	Group				nhate	
	Biosynthes				denhosnho	
DNMPPA	is	Expressed	Expressed	Expressed	rylase	Gan
DIVINITI	Cofactor	LAPICSSEd	LAPICSSEd	Lapiessed	Dihydrone	Gup
	and				opterin	
	Prosthetic				triphosphat	
	Group				e	
	Biosynthes				pyrophosp	
DNTPPA	is	Expressed	Expressed	Expressed	hatase	Gap
	Cofactor	-	-	_		
	and					
	Prosthetic					
	Group				dephospho	
	Biosynthes				-CoA	sps_RS265
DPCOAK	is	Expressed	Expressed	Expressed	kinase	10
	Cofactor					
	and					
	Prosthetic				2-	sps_RS154
	Group				dehydropa	40 or
	Biosynthes				ntoate 2-	sps_RS213
DPR	1S	Expressed	Expressed	Expressed	reductase	35
	Cofactor				I-deoxy-	Data
DUPDI	and				D-	sps_RS104
DXPRI	Prosthetic	Expressed	Expressed	Expressed	xylulose-5-	50

	Group Biosynthes				phosphate reductoiso	
	is				merase	
DXPS	Cofactor and Prosthetic Group Biosynthes is	Fxpressed	Expressed	Expressed	1-deoxy- D-xylulose 5- phosphate synthase	sps_RS110 40
	Cofactor and Prosthetic Group Biosynthes	Zhpressed	Zipressed		Erythrose 4- phosphate dehydroge	sps_RS129
E4PD	is	Expressed	Expressed	Expressed	nase	90
FCLT	Cofactor and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	Heme B synthesis reaction	sps_RS081 65
FMNAT	Cofactor and Prosthetic Group Biosynthes is	Fynressed	Fxpressed	Fxpressed	FMN adenylyltra	sps_RS117 25
TIVIINAT	15 Cofactor	Expressed	Expressed	Expressed	lisiciase	23
FMNRx	and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	FMN reductase (NADH dependent)	sps_RS158 00
EDTT	Cofactor and Prosthetic Group Biosynthes	Everaged	Everaged	Everaged	farnesyltra nstransfera	sps_RS132
	15 Cofeeter	Expressed	Expressed	Expressed	se	70
G1SATi	and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	l- semialdehy de aminotrans ferase	sps_RS124 60 or sps_RS224 75

	Cofactor					
	and					
	Prosthetic					
	Group				geranylger	ana DC122
CCTT	Biosynthes	Evenessed	Evenessed	Evenessed	anyltranstr	sps_KS132
0011	IS Cofeeter	Expressed	Expressed	Expressed	ansierase	/0
	and					
	Prosthetic					
	Group				glutamate-	
GLUCYS	Biosynthes				cysteine	sps RS200
L	is	Expressed	Expressed	Expressed	ligase	75
	Cofactor	-	-	-		
	and					
	Prosthetic					
	Group				geranyltran	
	Biosynthes				stransferas	sps_RS110
GRTT	is	Expressed	Expressed	Expressed	e	35
	Cofactor					
	and					
	Prosthetic				- 1	
	Group				giulathione	and PS000
GTHRD	biosynthes	Expressed	Fypressed	Evpressed	-uisuillue	sps_K5009
UTIND	Cofactor	Expressed	Expressed	Expressed	Teductase	00
	and					
	Prosthetic					
	Group					
	Biosynthes				glutathione	sps RS142
GTHS	is	Expressed	Expressed	Expressed	synthase	75
	Cofactor					
	and					
	Prosthetic					
	Group				GTP	
OTDOI	Biosynthes	F 1	F 1	F 1	cyclohydro	sps_RS163
GTPCI	1S	Expressed	Expressed	Expressed	lase I	00
	Cofactor					
	Drosthatia					ang PS202
	Group				GTP	30 or
	Biosynthes				cyclohydro	sps RS088
GTPCII	is	Expressed	Expressed	Expressed	lase II	95
	Cofactor	1	1	1		
	and				4-	
	Prosthetic				hydroxybe	sps_RS154
HB7ODT	Group	Expressed	Expressed	Expressed	nzoate	80

	Biosynthes				octaprenylt	
	1S				ransferase	
	Cofactor					
	and					DC012
	Prosthetic					sps_RS012
	Group				II O	60 or
	Biosynthes	D 1	- 1	D 1	Heme O	sps_RS2//
HEMEOS	1S	Expressed	Expressed	Expressed	synthase	85
	Cofactor					
	and					
	Prosthetic				trans-	
	Group				heptapreny	DC122
UDDTT	Biosynthes	- 1	F 1	F 1	Itranstransf	sps_RS132
HEPIT	18	Expressed	Expressed	Expressed	erase	/0
	Cofactor					
	and					
	Prosthetic				trans-	
	Group				hexaprenyl	D.0122
	Biosynthes	F 1	F 1	D 1	transtransf	sps_RS132
HEXII	1S	Expressed	Expressed	Expressed	erase	/0
	Cofactor					
	and					
	Prosthetic				1 1	
	Group				hydroxyme	D.01.50
IDADC	Biosynthes	F 1	г 1	F 1	thylbilane	sps_RS152
HMBS	15	Expressed	Expressed	Expressed	synthase	05
					2-amino-4-	
	Cofactor				hydroxy-6-	
	and				hydroxyme	DC125
	Prostnetic				thyldinydr	sps_KS125
	Group				opteridine	10 or
LIDDIZ	Biosynthes	F 1	г 1	F 1	diphospho	sps_KS244
НРРК		Expressed	Expressed	Expressed	Kinase	90
	Coractor				4a-	
	and				nydroxytet	
	Prostnetic				ranydrobio	
	Group				pterin	D C100
מפתוודוו	Biosynthes		F 1	F 1	dehydratas	sps_KS180
HIHRAD		Expressed	Expressed	Expressed	e	00
	Cofactor					
	and					
	Prosthetic				т 1 .	
	Group				Isochorism	ana DOOO
ICHODA'	Biosynthes	D	E 1	F 1		sps_KS008
ICHORS1	18	Expressed	Expressed	Expressed	Synthase	80

	Cafastan				1-hydroxy-	
	Cofactor				2-metnyl-	
	and Due atheatic				2 - (E) - 1	
	Prostnetic				dimbographet	
	Group				aipnosphat	DC117
IDDDC	Biosynthes	г 1	г 1	г 1	e reductase	sps_KS11/
IPDPS	15	Expressed	Expressed	Expressed	(1pap)	05
					2C- methyl-D-	
	Cofactor				ervthritol	
	and				2 4	
	Prosthetic				cyclodipho	sps_RS189
	Group				sphate	05 and
MECDPD	Biosynthes				dehvdratas	sns RS038
Н	is	Expressed	Expressed	Expressed	e	20
		2	2	2	2-C-	
	Cofactor				methyl-D-	
	and				ervthritol	
	Prosthetic				2,4-	
	Group				cyclodipho	
	Biosynthes		Used Belo	Used Belo	sphate	sps RS202
MECDPS	is	Expressed	w	w	synthase	35
					2-C-	
	Cofactor				methyl-D-	
	and				erythritol	
	Prosthetic				4-	
	Group				phosphate	
	Biosynthes	Used_Belo	Used_Belo	Used_Belo	cytidylyltr	sps_RS202
MEPCT	is	W	W	W	ansferase	40
					3-methyl-	
	Cofactor				2-	
	and				oxobutano	
	Prostnetic				ate	
	Group				nydroxyme	DC244
MOUNT	Biosynthes	Evenessed	Evenessed	Evenessed	thyltransie	sps_K5244
	15 Cofeeter	Expressed	Expressed	Expressed	Tase	95
	and					
	Prosthetic					sps RS110
	Group					50 or
	Biosynthes				NAD	sns RS087
NADK	18	Expressed	Expressed	Expressed	kinase	30
	Cofactor					
	and				NAD	
	Prosthetic		Used Belo	Used Belo	synthase	sps RS021
NADS1	Group	Expressed	w	w	(nh4)	35

	Biosynthes					
	is					
NMNAT	Cofactor and Prosthetic Group Biosynthes is	Below	Below	Below	nicotinami de- nucleotide adenylyltra nsferase	sps_RS215 60
NNAT	Cofactor and Prosthetic Group Biosynthes is	Used_Belo	Used_Belo	Used_Belo	nicotinate- nucleotide adenylyltra nsferase	sps_RS215
NNDMBR	Cofactor and Prosthetic Group Biosynthes				nicotinate- nucleotide- dimethylbe nzimidazol e phosphorib osyltransfe	sps_RS235
Т	is	Below	Below	Below	rase	55
NNDPR	Cofactor and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	nicotinate- nucleotide diphosphor ylase (carboxylat ing)	sps_RS264 85
NPHS	Cofactor and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	naphthoate synthase	sps_RS277 55
	Cofactor and Prosthetic Group Biosynthes				O- Phospho- 4-hydroxy- L- threonine:2 - oxoglutarat e aminotrans	sps_RS039
OHPBAT	is	Expressed	Expressed	Expressed	ferase	85
	Cofactor				3-	sps_RS039
OHPHM	and	Expressed	Expressed	Expressed	demethylu	75

	Prosthetic				biquinol 3-	
	Group				0- ¹	
	Biosynthes				methvltran	
	is				sferase	
					2-	
	Cofactor				Octopropyl	
	colación				Cetapicity	
	anu Duo ath ati a				-0-	
	Prostnetic				methoxy-	
	Group				benzoquin	DC150
	Biosynthes	- 1	– 1	. .	ol	sps_RS150
OMBZLM	1S	Expressed	Expressed	Expressed	methylase	15
					2-	
					Octaprenyl	
					-3-methyl-	
					6-	
	Cofactor				methoxy-	
	and				1,4-	
	Prosthetic				benzoquin	
	Group				ol	
OMMBLH	Biosynthes				hydroxylas	sps_RS215
X	is	Expressed	Expressed	Expressed	e	00
		Lipressea	Lipressea	Liprebbeu	2_	
					Octaprenvl	
					3 methyl	
					-5-methyl-	
					0-	
	Cafaataa				memoxy-	
	Colactor				1,4-	
	and				benzoquin	
	Prosthetic				ol	
	Group				hydroxylas	
OMMBLH	Biosynthes				e	
XAN	is	Expressed	Expressed	Expressed	Anaerobic	Gap
					2-	
	Cofactor				octaprenyl-	
	and				6-	
	Prosthetic				methoxyph	
	Group				enol	
	Biosynthes				hydroxylas	sps RS238
OMPHHX	is	Expressed	Expressed	Expressed	e	50
	Cofactor	•		•	2-	
	and				octaprenvl-	
	Prosthetic				6-	
	Group				methovyph	
ОМРННУ	Biosynthee				enol	
	is	Expressed	Expressed	Expressed	hydroxylag	Gan
	15	Expressed	Expressed	Dybiessed	inyuruxyids	Jap

					e	
					Anaerobic	
OPHBDC	Cofactor and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	3- octaprenyl- 4- hydroxybe nzoate carboxy- lyase	sps_RS245 35 or sps_RS157 95
ОРННХ	Cofactor and Prosthetic Group Biosynthes is	Fxpressed	Expressed	Expressed	2- Octaprenyl phenol hydroxylas	sps_RS150
OPHHXA N	Cofactor and Prosthetic Group Biosynthes is	Expressed	Expressed	Expressed	2- Octaprenyl phenol hydroxylas e Anaerobic	Gap
OVCDC2	Cofactor and Prosthetic Group Biosynthes	Everyoggad	Everaged	Everaged	2- oxoglutarat e decarboxyl	sps_RS014
DAUDC2	Cofactor and Prosthetic Group Biosynthes	Expressed	Expressed	Expressed	pantothena	sps_RS245
PANTS	1S Cofactor and Prosthetic Group Biosynthes	Expressed	Expressed	Expressed	te synthase pyridoxine 5'- phosphate	sps_RS066
PDX5PO	is Cofactor and Prosthetic	Expressed	Expressed	Expressed	oxidase Pyridoxine 5'-	10 sps_RS119 50 and
PDX5PS	Biosynthes is	Expressed	Expressed	Expressed	phosphate synthase	sps_RS228

	Cofactor				Erythronat	
	and				e 4-	
	Prosthetic				phosphate	
	Group				(4per)	sps PS086
PFRD	is	Fypressed	Fypressed	Expressed	nase	20
	Cofactor	Expressed	Expressed	Expressed	nuse	20
	and					
	Prosthetic					
	Group				pyrimidine	
	Biosynthes				phosphatas	
PMDPHT	is	Expressed	Expressed	Expressed	e	Gap
	Cofactor					
	and				1 1	
	Prosthetic				phosphom	
	Group				idina	and DS058
рмрк	biosynthes	Below	Below	Below	kinase	sps_K3038 40
	Cofactor	Delow	Delow	Delow	KilldSC	10
	and					
	Prosthetic					
	Group					
	Biosynthes				pantothena	sps_RS017
PNTK	is	Expressed	Expressed	Expressed	te kinase	15
	Cofactor					
	and					
	Prostnetic				n amphabili	
	Biosynthes				porphobili	sps RS150
PPBNGS	is	Expressed	Expressed	Expressed	synthase	60
II DIVOD	Cofactor	Expressed	Expressed	LAPICSSCU	synthiose	
	and				phosphopa	
	Prosthetic				ntothenoyl	
	Group				cysteine	
	Biosynthes				decarboxyl	sps_RS162
PPCDC	is	Expressed	Expressed	Expressed	ase	80
	Cofactor					
	and Drogth atia				mh o ar h an -	
	Group				phosphopa	
	Biosynthes				cysteine	sps RS162
PPNCL	18	Expressed	Expressed	Expressed	ligase	80
	Cofactor			Lipiobed	protoporph	sps RS003
					, , , , , , , , , , , , , , , , , , ,	20
	and				yrinogen	30 or
	and Prosthetic				yrinogen synthesis	30 or sps_RS003

	Biosynthes					sps_RS137
	is					00
	Cofactor and					sps_RS003 30 or
	Prosthetic				protoporph	sps_RS003
	Group				yrinogen	20 or
N	Biosynthes	Everaged	Everaged	Everaged	synthesis	sps_KS137
1	18 Cofector	Expressed	Expressed	Expressed	anaerobic	
	and					30 or
	Prosthetic				protoporph	sps RS003
	Group				vrinogen	20 or
	Biosynthes				synthesis	sps RS137
PPPGNO3	is	Expressed	Expressed	Expressed	anaerobic	00
	Cofactor					sps_RS003
	and					30 or
	Prosthetic					sps_RS003
	Group				protoporph	20 or
	Biosynthes	_			yrinogen	sps_RS137
PPPGO	is	Expressed	Expressed	Expressed	oxidase	00
	Cofactor					
	and Description				4	
	Group				trans-	
	Biosynthes				ltronstronsf	ong DS122
рртт	biosynthes	Fypressed	Fypressed	Expressed	erase	sps_K3152 70
1111	Cofactor	LAPICISCU	LAPICISCU	LAPICSSCU	ciuse	70
	and				pantethein	
	Prosthetic				e-	
	Group				phosphate	
	Biosynthes				adenylyltra	sps_RS008
PTPATi	is	Expressed	Expressed	Expressed	nsferase	10
	Cofactor					
	and					
	Prosthetic				pyridoxam	
	Group				ine-	Dance
PYAM5P	Biosynthes	F 1	E 1	F 1	phosphate	sps_RS066
0	1S	Expressed	Expressed	Expressed	oxidase	10
	collactor					
	Prosthetic				Pyridoval	
	Group				5'-	
PYDXL5P	Biosynthes				phosphate	
SYN	is	Expressed	Expressed	Expressed	synthase	Gap
	Cofactor	1	1	1	quinolinate	sps RS038
QULNS	and	Expressed	Expressed	Expressed	synthase	75

	Prosthetic					
	Group					
	Biosynthes					
	is					
	Cofactor					
	and					
	Prosthetic					
	Group					
	Biosynthes				riboflavin	sps_RS117
RBFK	is	Expressed	Expressed	Expressed	kinase	25
	Cofactor				6,7-	
	and				dimethyl-	
	Prosthetic				8-	sps_RS053
	Group				ribitylluma	45 and
DDEC	Biosynthes	г 1	Used_Belo	г 1	zine	sps_RS203
RBFSa	1S	Expressed	W	Expressed	synthase	25
	Cofactor					
	and Due atle atio					
	Crown					
	Diogynthae				riboflavin	ong PS202
RBESH	biosynthes	Evpressed	Evpressed	Evpressed	synthese	sps_K3203
KDI'50	Cofactor	Expressed	Expressed	Expressed	synthase	33
	and					
	Prosthetic				alpha-	
	Group				ribazole-5-	
	Biosynthes				phosphatas	sps RS235
RBZP	is	Below	Below	Below	e	70
					2-succinyl-	
	Cofactor				6-hydroxy-	
	and				2,4-	
	Prosthetic				cyclohexad	sps_RS014
	Group				iene 1-	85 or
	Biosynthes				carboxylat	sps_RS014
SHCHCS2	is	Expressed	Expressed	Expressed	e synthase	80
	Cofactor					
	and				sirohydroc	
	Prosthetic				hlorin	
	Group				dehydroge	D.0177
SUCUDA	Biosynthes	Evenes 1	Evenes 1	Evenes 1	nase	sps_KS1//
SHCHD2	1S Cofeeter	Expressed	Expressed	Expressed	(NAD)	03
	Collactor				sironydroc	
	and Drosthatic				1110F111 forrochatel	and DC177
SHCHE	Group	Evpressed	Evpressed	Evpressed		sps_r.51//
SHUIIF	oroup	Expressed	Expressed	Expressed	asc	05

	Biosynthes					
	is					
	Cofactor and Prosthetic Group				o- succinylbe	
SUCBZL	Biosynthes is	Used_Belo w	Used_Belo w	Used_Belo w	nzoate- CoA ligase	sps_RS014 70
SUCBZS	Cofactor and Prosthetic Group Biosynthes is	Used_Belo w	Used_Belo w	Used_Belo w	O- succinylbe nzoate- CoA synthase	sps_RS014 75
TDP	Cofactor and Prosthetic Group Biosynthes is	Below	Below	Below	Thiamin pyrophosp hatase	sps_RS027 45
	Cofactor and Prosthetic Group Biosynthes	Used Belo	Used Belo	Used Belo	thiazole phosphate	sps_RS177 15 and sps_RS058 35 and sps_RS058 25 and sps_RS058 30 and sps_RS110 15 and sps_RS058
THZPSN	is Cofeeter	W	W	W	synthesis	20
TMPKr	and Prosthetic Group Biosynthes	Fynressed	Used_Belo	Used_Belo	thiamine- phosphate kinase	sps_RS203
1 1711 131	Cofactor	LAPICOU	••	••	Millube	1.0
TMPPP	and Prosthetic Group Biosynthes is	Used_Belo w	Used_Belo w	Used_Belo w	thiamine- phosphate diphosphor ylase	sps_RS058 40
	Cofactor	Used_Belo	Used_Belo	Used_Belo	Undecapre	sps_RS104
UDCPDPS	and	W	W	W	nyl	60

	Prosthetic				diphosphat	
	Group				e synthase	
	Biosynthes					
	is					
	Cofactor					
	and					
	Prosthetic				uroporphyr	sps RS152
	Group				inogen	15 or
	Biosynthes				methvltran	sps RS137
UPP3MT	is	Expressed	Expressed	Expressed	sferase	35
	Cofactor and Prosthetic					
	Group				uroporphyr	
	Biosynthes				inogen-III	sns RS152
LIDD3S	biosynthes	Expressed	Expressed	Evpressed	synthase	sps_K5152
01135	15	Expressed	Expressed	Expressed	synthase	10
	Cafastan				uroporphyr	
	Colactor				doogen	
	and Dragthatic				decarboxyr	
	Prostnetic				ase	
	Group				(uroporphy	DC157
	Biosynthes	F 1	F 1	F 1	rinogen	sps_KSI5/
UPPDCI	1S	Expressed	Expressed	Expressed	111)	15
	Cysteine				adenyiyi-	D C100
	Metabolis	. .	F 1	- 1	sulfate	sps_RS182
ADSK	m	Expressed	Expressed	Expressed	kinase	15
	Cysteine				Aminopept	Dana
AMPTAS	Metabolis	- 1	5.1	- 1	idase (cys-	sps_RS028
ECG	m	Expressed	Below	Expressed	gly)	85
						sps_RS044
	Cysteine				aspartate	90 or
	Metabolis				transamina	sps_RS039
ASPTA4	m	Expressed	Expressed	Expressed	se	90
	Crysteine				3',5'- bisphospha	
	Cysteine Matalialia					and DOOG
DDNT	Metabolis	Evenessed	Evenessed	Evenessed	nucleotidas	sps_K5207
Drivi	111	Expressed	Expressed	Expressed	C	/U
						sps_RS1/4 70 or
						sps_RS031
	Cysteine					60 or
	Metabolis				cysteine	sps_RS056
CYSS	m	Expressed	Expressed	Expressed	synthase	10

	Cysteine					
CVSTI	Metabolis	Evpressed	Expressed	Evpressed	cystathioni	sps_RS028
	Cysteine	Expressed	Expressed	Expressed	Cysteinyl-	15
	Metabolis				tRNA	sps RS092
CYSTRS	m	Expressed	Expressed	Expressed	synthetase	55
PAPSR	Cysteine Metabolis m	Expressed	Expressed	Expressed	phosphoad enylyl- sulfate reductase (thioredoxi n)	sps_RS137 80
	111	LAPICSSCU	LAPICSSCU	LAPICSSCU	11)	sps_RS182
SADT2	Cysteine Metabolis m	Expressed	Expressed	Expressed	sulfate adenylyltra nsferase	25 and sps_RS182
		2	Lupresse	Linpicere	O-acetyl-	
SLCYSS	Cysteine Metabolis m	Expressed	Expressed	Expressed	L-serine sulfhydryla se	sps_RS145 65
					sulfite	sps_RS137
	Cysteine				reductase	85 and
SULR	m	Expressed	Expressed	Expressed	(NADPH2	sps_KS157 90
ARSRD2	Energy Metabolis m	Below	Below	Below	arsenate reductase (glutaredo xin)	sps_RS025 60 and sps_RS030 80
ATPS4r	Energy Metabolis m	Expressed	Expressed	Expressed	ATP synthase (four protons for one ATP) and swp 5161	sps_RS278 45 and sps_RS278 50 and sps_RS278 55 and sps_RS278 60 and sps_RS278 65 and sps_RS278 70 and sps_RS278 75 and sps_RS278 85 and sps_RS278 85 and sps_RS278 85 and sps_RS278 85 and

	_				-	sps_RS070
	Energy				cytochrom	25 or
CYCPOe	m	Fypressed	Below	Below	e-c peroxidase	sps_K5248 25
		LAPICISCU	Delow	Delow	peroxiduse	(sps_RS01 285 and
						sps_RS012
						sps RS013
						00) or
						(sps_RS04 545 and
					cytochrom	sps_RS045
					e-c oxidase	50 and sps RS045
	Energy				translocate	55 and
	Metabolis				d) and	sps_RS045
CYOO2	m	Expressed	Expressed	Expressed	swp_2572)	60)
					e-c	
					reductase	sps_RS249
					(ubiquinol	90 and
	Energy				8:4 protons	sps_K5249 80 and
	Metabolis				translocate	sps_RS249
CYOR7	m	Expressed	Expressed	Expressed	d)	85
					cytochrom	
					bd	sps RS188
	Energy				(ubiquinol-	40 and
OVTDD	Metabolis	F 1	F 1	F 1	8:2	sps_RS188
CYIBD	m	Expressed	Expressed	Expressed	protons)	55 sns RS278
						00 and
						sps_RS277
						95 and
						90 and
					cytochrom	sps_RS278
CVTDO2	Energy				e bo3	05 and
4 CY IBO3_	ivietabolis	Below	Below	Below	ubiquinol oxidase	sps_KS000 35
		2010 11	2010 1	2010 1	Formate	(sps RS27
	Energy				Dehydroge	125 and
	Metabolis	D	D	D 1	nase	sps_RS271
rdh10	m	Expressed	Expressed	Expressed	(methylme	30 and

					naquinone-	sps_RS271
					7:1	20 and
					protons)	sps_RS2/1
						95) or
						(sps_K327)
						$r_{\rm SDS}$ and $r_{\rm SDS}$ RS271
						5ps_R3271 60 and
						sns RS271
						65 and
						sps RS271
						95)
						(sps_RS27
						125 and
						sps_RS271
						30 and
						$sps_RS2/1$
						20 and $p_{S} p_{S} 271$
						$\frac{95}{0}$ or
						(sns RS27)
						155 and
					Formate	sps RS271
					Dehvdroge	60 and
					nase	sps RS271
	Energy				(menaquin	65 and
	Metabolis				one-7: 1	sps RS271
FDH9	m	Expressed	Expressed	Expressed	protons)	95)
	-				0 1 .	sps_RS225
	Energy				terredoxin-	15 and
ENOD	Metabolis	F 1	F 1	F 1	NADP	sps_RS038
FNOR	m	Expressed	Expressed	Expressed	reductase	20
						sps_10101 35 and
					succinate	sns RS151
					dehydroge	30 and
					nase	sns RS151
	Energy				(menaduin	40 and
	Metabolis	Used Belo			ol 7:0	sps RS151
FRD10	m	W	Expressed	Expressed	proton)	45
			1	1	succinate	sps RS151
					dehydroge	35 and
					nase	sps RS151
	Energy				(methylme	30 and
	Metabolis				naquinol 7:	sps_RS151
FRD11	m	Below	Expressed	Expressed	Oproton)	40 and

						sps_RS151 45
FRD8	Energy Metabolis m	Below	Below	Below	succinate dehydroge nase (menaquin ol 7:0 proton)	sps_RS013 95 and sps_RS243 15
FRD9	Energy Metabolis m	Below	Below	Below	succinate dehydroge nase (methylme naquinol 7: 0proton)	sps_RS013 95 and sps_RS243 15
G3PD4	Energy Metabolis	Expressed	Below	Expressed	glycerol-3- phosphate dehydroge nase (menaquin one 7)	sps_RS241
G3PD4	Energy Metabolis m	Expressed	Below	Expressed	glycerol-3- phosphate dehydroge nase (methylme naquinone 7)	sps_RS241 75
GSHPO	Energy Metabolis m	Expressed	Below	Below	glutathione	sps_RS113 15
	Energy Metabolis	Palary	Used_Belo	Used_Belo	NADH dehydroge nase (ubiquinon e-8 and 4	sps_RS174 85 and sps_RS174 90 and sps_RS174 95 and sps_RS175 00 and sps_RS175 05 and sps_RS175 10 and sps_RS175 15 and sps_RS175 20 and
NADHII	111	Delow	W	W	protons)	20 and

						sps_RS175 25 and sps_RS175 30 and (sps_RS02 420 or sps_RS024 30) and sps_RS175 40 and sps_RS175 45
NADH12	Energy Metabolis m	Expressed	Expressed	Expressed	NADH dehydroge nase (ubiquinon e-8)	sps_RS064
NADH13	Energy Metabolis m	Below	Used_Belo	Used_Belo	NADH dehydroge nase (menaquin one-7 and 4 protons)	sps_RS174 85 and sps_RS174 90 and sps_RS174 95 and sps_RS175 00 and sps_RS175 05 and sps_RS175 10 and sps_RS175 15 and sps_RS175 20 and sps_RS175 20 and sps_RS175 25 and sps_RS175 30 and (sps_RS02 420 or sps_RS024 30) and sps_RS175 40 and sps_RS175 45

					NADH	
					dehydroge	
					nase	
					(methylme	
	Enonex				(intentiyinte	
	Energy				naquinone	DCO(4
	Metabolis	- 1	- 1		/ & no	sps_RS064
NADH14	m	Expressed	Expressed	Expressed	proton)	15
						sps_RS174
						85 and
						sps_RS174
						90 and
						sps RS174
						95 and
						sns RS175
						00 and
						cmc DS175
						$sps_K31/3$
						$sps_KS1/5$
						10 and
						sps_RS175
						15 and
						sps_RS175
						20 and
						sps RS175
						25 and
						sps RS175
						30 and
						(sps RS02
					NADH	420 or
					dehvdroge	sps RS024
					nase	30) and
					(mothylmo	SO = DS175
	Enorey				neurynne	sps_K31/3
	Litergy				naquinone-	40 all u
	Metabolis	D 1	D 1	D 1	/ and 4	sps_KS1/5
NADH16	m	Below	Below	Below	protons)	45
					NADH	
					dehydroge	
					nase	
	Energy				(Menaquin	
	Metabolis				one 7 & no	sps_RS064
NADH4	m	Expressed	Expressed	Expressed	proton)	15
		•		•	ammonium	sps RS077
	Energy				-	95 and
NH4HNA	Metabolis				hydroxide	sps_RS078
DOR	m	Below	Below	Below	NAD+	00
DOK	111	DCIOW	DUIUW	DCIOW		00

					oxidoreduc	
					tase .	
					ammonium	
					- hydroxido:	and DS077
	Fnergy				NADP+	sps_K30// 95 and
NH4HNA	Metabolis				oxidoreduc	$s_{\rm DS} = RS078$
DPOR	m	Below	Below	Below	tase	00
DION	Energy	Below	Denom	Dellow	nitric oxide	
	Metabolis				dioxygenas	sps RS132
NODOx	m	Expressed	Expressed	Expressed	e	00
	Energy				nitric oxide	
	Metabolis				dioxygenas	sps_RS132
NODOy	m	Expressed	Expressed	Expressed	e	00
						((sps_RS1
						4135 and
						sps_RS141
						40) or (sp_{0}, \mathbf{PS})
						205 and
						sps RS062
	Energy					(00) and
	Metabolis				nitrate	sps_RS061
NTR4	m	Expressed	Expressed	Expressed	reductase	95
						((sps_RS1
						4135 and
						sps_RS141
						40) or $(and BSOC)$
					nitrate	(sps_KS00)
					reductase	sns RS062
	Energy				(methylme	(00)) and
	Metabolis				naquinone-	sps RS061
NTR5	m	Expressed	Expressed	Expressed	7)	95
						sps_RS168
	Energy				NAD(P)	90 and
TUDA	Metabolis	D 1	F 1	D 1	transhydro	sps_RS168
THD2	m	Expressed	Expressed	Expressed	genase	8)
	Energy				ΝΑΒ	sps_KS108
	Metabolis				transhvdro	sns RS168
THD5	m	Expressed	Expressed	Expressed	genase	85
11120	Energy	LAPICOUC	LAPICOUC	Lipiobed	thioredoxi	
	Metabolis				n reductase	sps RS053
		Emmand	Evenessed	Evenaged		<u>.</u>

						(sps_RS21
						215 and sns RS212
						20 and
						sps RS212
						100 and
						sps RS212
						10 and
						sps_RS212
						05 and
						sps_RS212 25) or
						(sps_RS11
						130 and
						sps RS111
						25 and
						sps_RS111
					NADH-	05 and
					Ubiquinon	sps_RS111
					e	20 and
	Energy				Oxidoredu	sps_RS111
	Energy				translocati	13 and
LIOOR	m	Expressed	Fypressed	Fypressed	ng)	sps_KS111
UUUUK	1111					
		Lipressea	Lipressea	Lipressea	115)	sps RS142
		Lipiecoea	Lipiocou	Lipiocou	115)	sps_RS142 40 and
			Lipresseu		acetyl-	sps_RS142 40 and sps_RS149
		LAPICSOU	LAPICSSCA	Laprossed	acetyl- CoA	sps_RS142 40 and sps_RS149 40 and
	Fatty Acid	Used_Belo	Used_Belo	Used_Belo	acetyl- CoA carboxylas	sps_RS142 40 and sps_RS149 40 and sps_RS149
ACCOAC	Fatty Acid Synthesis	Used_Belo	Used_Belo	Used_Belo	acetyl- CoA carboxylas e	sps_RS142 40 and sps_RS149 40 and sps_RS149 45
ACCOAC	Fatty Acid Synthesis	Used_Belo w	Used_Belo w	Used_Belo w	acetyl- CoA carboxylas e Acyl-	sps_RS142 40 and sps_RS149 40 and sps_RS149 45
ACCOAC	Fatty Acid Synthesis	Used_Belo	Used_Belo	Used_Belo	acetyl- CoA carboxylas e Acyl- [acyl-	sps_RS142 40 and sps_RS149 40 and sps_RS149 45
ACCOAC	Fatty Acid Synthesis	Used_Belo w	Used_Belo w	Used_Belo w	acetyl- CoA carboxylas e Acyl- [acyl- carrier-	sps_RS142 40 and sps_RS149 40 and sps_RS149 45
ACCOAC	Fatty Acid Synthesis	Used_Belo w	Used_Belo w	Used_Belo w	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m	sps_RS142 40 and sps_RS149 40 and sps_RS149 45
ACCOAC	Fatty Acid Synthesis	Used_Belo w	Used_Belo w	Used_Belo w	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m alonyl- [acyl-	sps_RS142 40 and sps_RS149 40 and sps_RS149 45 (sps_RS08 695 and
ACCOAC	Fatty Acid Synthesis	Used_Belo w	Used_Belo w	Used_Belo w	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m alonyl- [acyl- carrier-	sps_RS142 40 and sps_RS149 40 and sps_RS149 45 (sps_RS08 695 and sps_RS067
ACCOAC	Fatty Acid Synthesis	Used_Belo w	Used_Belo w	Used_Belo w	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m alonyl- [acyl- carrier- protein] C-	sps_RS142 40 and sps_RS149 40 and sps_RS149 45 (sps_RS08 695 and sps_RS067 10) or
ACCOAC	Fatty Acid Synthesis	Used_Belo w	Used_Belo w	Used_Belo w	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m alonyl- [acyl- carrier- protein] C- acyltransfe	sps_RS142 40 and sps_RS149 40 and sps_RS149 45 (sps_RS08 695 and sps_RS067 10) or (sps_RS06
ACCOAC	Fatty Acid Synthesis	Used_Belo w	Used_Belo w	Used_Belo w	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m alonyl- [acyl- carrier- protein] C- acyltransfe rase	sps_RS142 40 and sps_RS149 40 and sps_RS149 45 (sps_RS08 695 and sps_RS067 10) or (sps_RS06 705 and
ACCOAC	Fatty Acid Synthesis Fatty Acid	Used_Belo w	Used_Belo w	Used_Belo w	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m alonyl- [acyl- carrier- protein] C- acyltransfe rase (decarboxy	sps_RS142 40 and sps_RS149 40 and sps_RS149 45 (sps_RS08 695 and sps_RS067 10) or (sps_RS06 705 and sps_RS067
ACCOAC ACMAT1	Fatty Acid Synthesis Fatty Acid Synthesis	Used_Belo w	Used_Belo w	Used_Belo w	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m alonyl- [acyl- carrier- protein] C- acyltransfe rase (decarboxy lating)	sps_RS142 40 and sps_RS149 40 and sps_RS149 45 (sps_RS08 695 and sps_RS067 10) or (sps_RS06 705 and sps_RS067 10)
ACCOAC ACMAT1	Fatty Acid Synthesis Fatty Acid Synthesis	Used_Belo w Expressed	Used_Belo w Expressed	Used_Belo w Expressed	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m alonyl- [acyl- carrier- protein] C- acyltransfe rase (decarboxy lating) Acetyl-	sps_RS142 40 and sps_RS149 40 and sps_RS149 45 (sps_RS08 695 and sps_RS067 10) or (sps_RS06 705 and sps_RS067 10) (sps_RS09
ACCOAC	Fatty Acid Synthesis Fatty Acid Synthesis	Used_Belo w	Used_Belo w Expressed	Used_Belo w Expressed	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m alonyl- [acyl- carrier- protein] C- acyltransfe rase (decarboxy lating) Acetyl- CoA ACP	sps_RS142 40 and sps_RS149 40 and sps_RS149 45 (sps_RS08 695 and sps_RS067 10) or (sps_RS06 705 and sps_RS067 10) (sps_RS09 695 and
ACCOAC ACMAT1	Fatty Acid Synthesis Fatty Acid Synthesis	Used_Belo w Expressed	Used_Belo w Expressed	Used_Belo w Expressed	acetyl- CoA carboxylas e Acyl- [acyl- carrier- protein]:m alonyl- [acyl- carrier- protein] C- acyltransfe rase (decarboxy lating) Acetyl- CoA ACP transacylas	sps_RS142 40 and sps_RS149 40 and sps_RS149 45 (sps_RS08 695 and sps_RS067 10) or (sps_RS06 705 and sps_RS067 10) (sps_RS09 695 and sps_RS067

						(sps_RS16 795 and
						sps_RS067 10)
AGPEPH OS	Fatty Acid Synthesis	Below	Below	Below	Lysophosp holipase	sps_RS006 50
AGPEPH OS	Fatty Acid Synthesis	Below	Below	Below	Lysophosp holipase	sps_RS006 50 (sps_RS02 955 and sps_RS067 15 and sps_RS067 05 and sps_RS091 90 and sps_RS067 10) or (sps_RS06 715 and sps_RS066 715 and sps_RS086 95 and sps_RS104 25 and sps_RS091 90 and sps_RS091 90 and sps_RS067 10) or
	Fatty Acid				and swp_3510 and swp_3256) or (swp_2802 and swp_3121 and swp_3045 and	(sps_RS02 955 and sps_RS086 95 and sps_RS067 15 and sps_RS091 90 and sps_RS067 10) or (sps_RS06 715 and sps_RS104 25 and sps_RS067 05 and sps_RS091 90 and sps_RS091 90 and sps_RS067
C120SN	Synthesis	Expressed	Expressed	Expressed	swp_3256)	10)

						(and DCO2
						(sps_KS02
						955 and
						sps_RS067
						15 and
						sps_RS067
						05 and
						sps_RS091
						90 and
						sps RS067
						10) or
						(sps RS06
						715 and
						sps RS086
						95 and
						sps RS104
						25 and
						25 and $\mathbf{PS}(0)$
					h Irata avri	sps_KS091
					D-Keloacyl	90 and $\mathbf{P} = \mathbf{P} = \mathbf{P} + \mathbf{P} = \mathbf{P} + $
					synthetase	sps_K500/
					(ISO-	10) or
					C13:0) and	(sps_RS02
					swp_3510	955 and
					and	sps_RS086
					swp_3256)	95 and
					or	sps_RS067
					(swp_2802	15 and
					and	sps_RS091
					swp_3121	90 and
					and	sps_RS067
					swp_3045	10) or
					and	(sps_RS06
					swp_3256)	715 and
					or	sps RS104
					(swp 3045	25 and
					and	sps RS067
					swp 3510	05 and
					and	sps RS091
					swp 3042	90 and
	Fatty Acid				and	sps RS067
C130ISN	Synthesis	Expressed	Expressed	Expressed	swn 3256)	10)
	~	Lipicobea	Laprosou	Laprosou	b-ketoacyl	sps RS020
					synthetase	55 and
					(Iso	SS and
					(150 - (12.0) = 1	sps_rsuo0
CI20OUIC	Fotty A and	Ugad Dala			(15.0) and (2510)	spa DS067
CI300HIS	rany Acid	Usea_Belo	F 1	D	swp_3310	sps_K500/
IN	Synthesis	W	Expressed	Expressed	and	15 and

					swp_3256) or (swp_2802 and swp_3121 and swp_3045 and swp_3256) or (swp_3045 and swp_3510 and swp_3042 and swp_3256)	sps_RS104 25 and sps_RS067 05 and sps_RS091 90 and sps_RS067 10
C140ISN	Fatty Acid Synthesis	Expressed	Expressed	Expressed	b-ketoacyl synthetase (Iso- C14:0) and swp_3510 and swp_3256) or (swp_2802 and swp_3121 and swp_3045 and swp_3045 and swp_3045 and swp_3045 and swp_3042 and swp_3042 and swp_3256)	(sps_RS02 955 and sps_RS067 15 and sps_RS067 05 and sps_RS091 90 and sps_RS067 10) or (sps_RS06 715 and sps_RS086 95 and sps_RS104 25 and sps_RS091 90 and sps_RS067 10) or (sps_RS02 955 and sps_RS086 95 and sps_RS086 95 and sps_RS086 95 and sps_RS086 95 and sps_RS086 95 and sps_RS086 95 and sps_RS087 15 and sps_RS091 90 and sps_RS091 90 and sps_RS091 90 and sps_RS091 90 and sps_RS091 90 and

						10) or
						(sps_RS06
						715 and
						sps_RS104
						25 and
						sps_RS067
						05 and
						sps_RS091
						90 and
						sps_RS067
						10)
						(sps_RS02
						955 and
						sps_RS067
						15 and
						sps_RS06/
						03 and
						sps_K3091
						sps $RS067$
						10 or
						(sps_RS06
						715 and
					Fatty acid	sps RS086
					biosynthesi	95 and
					s (n-C14:0)	sps RS104
					and	25 and
					swp_3510	sps_RS091
					and	90 and
					swp_3256)	sps_RS067
					or	10) or
					(swp_2802	(sps_RS02
					and	955 and
					swp_3121	sps_KSU86
					and and and	93 and
					swp_3043	sps_1500/
					swn 3256)	sns RSA01
					or	90 and
					(swp 3045	sps RS067
					and	10) or
					swp 3510	(sps RS06
					and	715 and
					swp_3042	sps_RS104
	Fatty Acid				and	25 and
C140SN	Synthesis	Expressed	Expressed	Expressed	swp_3256)	sps_RS067

						05 and
						sps RS091
						90 and
						sps RS067
						10)
						$(\mathbf{D} \mathbf{C} \mathbf{O} \mathbf{C})$
						(sps_RS02
						955 and
						sps_RS067
						15 and
						sps_RS067
						05 and
						sps RS091
						90 and
						sps RS067
						10 or
						$(and \mathbf{PS0})$
						(sps_K500
						/15 and
						sps_RS086
						95 and
						sps_RS104
						25 and
						sps_RS091
					b-ketoacyl	90 and
					synthetase	sps RS067
					(Íso-	10) or
					C15:0) and	(sps_RS02
					swn 3510	955 and
					and	sns RS086
					swn 3256)	95 and
					swp_3230)	
						sps_K500/
					(swp_2802	15 and
					and	sps_RS091
					swp_3121	90 and
					and	sps_RS067
					swp_3045	10) or
					and	(sps_RS06
					swp 3256)	715 and
					or	sps RS104
					(swp 3045	25 and
					and	sps RS067
					swp 3510	05 and
					and	sps RS001
					allu allu 2042	sps_K3031
	Eatter A .: 1				swp_3042	
C1 COTON	ratty Acid	F 1	-	F 1	and	sps_KS06/
CISUISN	Synthesis	Expressed	Expressed	Expressed	swp_3256)	10)

						(and DCO)
						(sps_K502
						955 and
						sps_RS067
						15 and
						sps_RS067
						05 and
						sps_RS091
						90 and
						sps_RS067
						10) or
						(sps_RS06
						715 and
						sps_RS086
						95 and
						sps_RS104
						25 and
						sps RS091
					b-ketoacyl	90 and
					synthetase	sps RS067
					(C15:0)	10) or
					and	(sps RS02
					swp 3510	955 and
					and	sps RS086
					swp 3256)	95 and
					or	sps RS067
					(swp 2802	15 and
					and	sps RS091
					swp 3121	90 and
					and	sps RS067
					swp 3045	10 or
					and	(sps_RS06
					swp 3256)	715 and
					or	sps RS104
					(swp 3045	25 and
					and	sps RS067
					swn 3510	05 and
					and	sns RS001
					swn 30/2	ops_100091
	Fatty A aid				and	spe RS067
C150GN	Synthesis	Everaged	Everaged	Everaged	allu allu 2256)	sps_1.3007
CIDUDIN	synthesis	Expressed	Expressed	Expressed	swp_3230)	$\frac{10}{(and DGO)}$
						(sps_KS02
						935 and
					F (1 1	sps_KS086
					Fatty acid	95 and
0151001	Fatty Acid	D 1			biosynthesi	sps_KS067
CI5ISN	Synthesis	Below	Expressed	Expressed	s (n-C15:1)	15 and

						one DC104
						sps_K3104
						25 and $\mathbf{PS067}$
						sps_KS007
						10) and $(ama DSO($
						(sps_K506
						705 and
						sps_RS091
						90 and
						sps_RS06/
						10)
						(sps_RS02
						955 and
						sps_RS067
						15 and
						sps_RS067
						05 and
						sps_RS091
						90 and
						sps_RS067
						10) or
						(sps_RS06
						715 and
						sps_RS086
					b-ketoacyl	95 and
					synthetase	sps_RS104
					(Iso-	25 and
					C16:0) and	sps_RS091
					swp_3510	90 and
					and	sps_RS067
					swp_3256)	10) or
					or	(sps_RS02
					(swp_2802	955 and
					and	sps_RS086
					swp_3121	95 and
					and	sps_RS067
					swp_3045	15 and
					and	sps_RS091
					swp_3256)	90 and
					or	sps_RS067
					(swp_3045	10) or
					and	(sps_RS06
					swp 3510	715 and
					and	sps RS104
					swp 3042	$\overline{25}$ and
	Fatty Acid				and	sps RS067
C160ISN	Synthesis	Expressed	Expressed	Expressed	swp_3256)	05 and

						sps_RS091 90 and
						sps_RS067 10)
						(sps_RS02
						955 and $\mathbf{D} \subseteq \mathbf{O}(7)$
						sps_KS00/
						sps RS067
						05 and
						sps RS091
						90 and
						sps_RS067
						10) or
						(sps_RS06
						715 and
						sps_RS086
						93 and sps $RS104$
						25 and
						sps RS091
					Fatty acid	90 and
					biosynthesi	sps_RS067
					s (n-C16:0)	10) or
					and	(sps_RS02
					swp_3510	955 and
					and	sps_RS086
					swp_3256)	95 and
					(swn 2802)	sps_K3007
					(swp_2002) and	sps RS091
					swp 3121	90 and
					and	sps RS067
					swp_3045	10) or
					and	(sps_RS06
					swp_3256)	715 and
					or	sps_RS104
					(swp_3045	23 and $\mathbf{PS047}$
					allu swp 3510	sps_KSU0/
					and	sps RS091
					swp 3042	90 and
	Fatty Acid				and	sps RS067
C160SN	Synthesis	Expressed	Expressed	Expressed	swp_3256)	10)

						sps_RS029
						55 and
						sps RS086
						95 and
						sps RS067
						15 and
						sps_RS104
						25 and
						sps_RS091
					Fatty acid	90 and
	Fatty Acid	Used_Belo			biosynthesi	sps_RS067
C161SN	Synthesis	W	Expressed	Expressed	s (n-C16:1)	10
						(sps_RS02
						955 and
						sps_RS067
						15 and
						sps_RS067
						05 and
						sps_RS091
						90 and
						sps_RS067
						10) or
					1 1 . 1	(sps_RS06
					b-ketoacyl	/15 and
					synthetase	sps_KS086
					(1SO- C17(0) and	95 and
					C1/(0) and 3510	sps_KS104
					swp_5510	23 and
					allu swp 3256)	$\frac{\text{sps}_\text{KS091}}{\text{90 and}}$
					swp_5250)	sps RS067
					(swn 2802)	10 or
					and	(sns RS02)
					swn 3121	955 and
					and	sps RS086
					swp 3045	95 and
					and	sps RS067
					swp 3256)	15 and
					or	sps RS091
					(swp 3045	90 and
					and	sps_RS067
					swp_3510	10) or
					and	(sps_RS06
					swp_3042	715 and
	Fatty Acid				and	sps_RS104
C170ISN	Synthesis	Expressed	Expressed	Expressed	swp 3256)	25 and

	1		1			
						sps_RS067
						05 and
						sps_KS091
						90 and $\mathbf{PS067}$
						sps_K5007
						(sps PS02)
						$(3ps_R302)$
						sps RS067
						15 and
						sps RS067
						05 and
						sps_RS091
						90 and
						sps_RS067
						10 and
						sps_RS067
						10) or
						(sps_RS06
						$/15$ and $P_{\rm SO}$
						sps_KSU80
						93 and
					h-ketoacyl	25 and
					synthetase	sps RS091
					(C17.0)	90 and
					and	sps RS067
					swp 3510	10) or
					and	(sps RS02
					swp_3256)	955 and
					or	sps_RS086
					(swp_2802	95 and
					and	sps_RS067
					swp_3121	15 and
					and	sps_RS091
					swp_3045	90 and $\mathbf{P}_{\mathbf{a}\mathbf{a}\mathbf{c}\mathbf{c}}$
					and	sps_RS067
					swp_3256)	10) or $(ama DCOC)$
					Or	(sps_K506 715 and
					(swp_3043	r_{1} and r_{2} and r_{3}
					swp 3510	sps_13104 25 and
					and	sns RS067
					swp 3042	05 and
	Fatty Acid				and	sps RS091
C170SN	Synthesis	Expressed	Expressed	Expressed	swp 3256)	90 and

						sps_RS067 10)
						sps_RS029 55 and
						sps_RS086
						95 and $\mathbf{D} \subseteq \mathbf{D} \subseteq \mathbf{C}$
						15 and
						sps_RS104
						25 and
						sps_RS067 05 and
						sps_RS091
	Fatty A aid	Used Dele			b-ketoacyl	90 and $PS067$
C171n8SN	Svnthesis	W	Expressed	Expressed	(C17:1)	sps_K5007
	,				()	sps_RS029
						55 and
						sps_RS086
						sps RS067
						15 and
						sps_RS104
						25 and sps RS067
						05 and
						sps_RS091
	Eatter A and				b-ketoacyl	90 and $\mathbf{P} = \mathbf{P} \mathbf{C} \mathbf{C} \mathbf{C}$
C171SN	Synthesis	Below	Expressed	Expressed	(C17:1)	sps_KS007
	Synthesis	Delow	Empressed	Empressed	Fatty acid	(sps RS02
					biosynthesi	955 and
					s (n-C18:0)	sps_RS067
					swp 3510	sps RS067
					and	05 and
					swp_3256)	sps_RS091
					or (swp. 2802	90 and $PS067$
					and	sps_K5007 10) or
					swp_3121	(sps_RS06
					and	715 and
					swp_3045	sps_RS086
	Fatty Acid				swp 3256)	sps RS104
C180SN	Synthesis	Expressed	Expressed	Expressed	or	25 and

					(2045	D COO1
					(swp_3045	sps_KS091
					and	90 and
					swp_3510	sps_RS067
					and	10) or
					swp_3042	(sps_RS02
					and	955 and
					swp_3256)	sps_RS086
						95 and
						sps_RS067
						15 and
						sps_RS091
						90 and
						sps_RS067
						10) or
						(sps_RS06
						715 and
						sps_RS104
						25 and
						sps_RS067
						05 and
						sps_RS091
						90 and
						sps_RS067
						10)
						sps_RS029
						55 and
						sps_RS086
						95 and
						sps_RS067
						15 and
						sps_RS104
						25 and
						sps_RS067
						05 and
						sps_RS091
	T (1 1 1				Fatty acid	90 and
G101 501	Fatty Acid	Used_Belo	D 1		biosynthesi	sps_RS067
CI8In/SN	Synthesis	W	Expressed	Expressed	s (n-C18:1)	10
						sps_RS029
						55 and
						sps_RS086
						95 and
						sps_RS067
	F (1 + · · ·				Fatty acid	15 and
G101537	Fatty Acid	5.1			biosynthesi	sps_RS104
C181SN	Synthesis	Below	Expressed	Expressed	s (n-C18:1)	25 and
						sps_RS067
--------	------------	------------	------------	------------	-------------	-----------------
						05 and
						sps_RS091
						90 and
						sps_RS067 10
					EPA	sps_RS107
					synthesis	50 and
	Fatty Acid				condensed	sps_RS107
C205SN	Synthesis	Expressed	Expressed	Expressed	reaction	40
					Fatty acid	(sps_RS09
					biosynthesi	695 and
					s (n-C5:0)	sps_RS067
					and	15 and
					swp_3045	sps_RS104
					and	25 and
					swp_3256)	sps_RS091
					or	90 and
					(swp_2802	sps_RS067
					and	10) or
					swp_3045	(sps_RS09
					and	695 and
					swp_3047	sps_RS029
					and	55 and
					swp_3256)	sps_RS067
					or	15 and
					(swp_3045	sps_RS091
					and	90 and
					swp_3510	sps_RS067
					and	10) or
					swp_3047	(sps_RS09
					and	190 and
					swp_3256)	sps_RS029
					or	55 and
					(swp_3256	sps_RS167
					and	95 and
					swp_2802	sps_RS067
					and	15 and
					swp_1980	sps_RS067
					and	10) or
					swp_3045)	(sps_RS06
					or	715 and
					(swp_3045	sps_KS104
					and	25 and
OF COL	Fatty Acid	. .	P 1	F 1	swp_3510	sps_KS167
C50SN	Synthesis	Expressed	Expressed	Expressed	and	95 and

					swp 1980	sps RS091
					and	90 and
					swp 3256)	sps RS067
					sp_5200)	10)
						(sns RS09)
					h-ketoacyl	(5p5_100)
					synthetase	$c_{\rm rns}$ RS067
					(Jac C6:0)	sps_KS007
					(150-C0.0)	15 and
						sps_KS104
					swp_3043	23 and $\mathbf{D}_{\rm SOO1}$
					and	sps_KS091
					swp_3256)	90 and
					or	sps_RS067
					(swp_2802	10) or
					and	(sps_RS09
					swp_3045	695 and
					and	sps_RS029
					swp_3047	55 and
					and	sps_RS067
					swp_3256)	15 and
					or	sps_RS091
					(swp_3045	90 and
					and	sps RS067
					swp 3510	10) or
					and	(sps RS09
					swp 3047	190 and
					and	sps RS029
					swp 3256)	55 and
					or	sps RS167
					(swn 3256	95 and
					and	sps RS067
					swp 2802	15 and
					swp_2002	$r_{\rm sps}$ RS067
					allu ave 1090	10 or
					swp_1960	10)01
					allu aura 2015)	(sps_K500
					swp_3043)	/15 and $DS104$
					OF	sps_KS104
					(swp_3045	25 and
					and	sps_KS167
					swp_3510	95 and
					and	sps_RS091
					swp_1980	90 and
	Fatty Acid				and	sps_RS067
C60ISN	Synthesis	Expressed	Expressed	Expressed	swp_3256)	10)
	Fatty Acid				b-ketoacyl	(sps_RS09
C70ISN	Synthesis	Expressed	Expressed	Expressed	synthetase	695 and

					(Iso-C7:0)	sps RS067
					and	15 and
					swp 3045	sps RS104
					and	25 and
					swp 3256)	sps RS091
					or	90 and
					(swp 2802	sps RS067
					and	10) or
					swp_3045	(sps_RS09
					and	695 and
					swp_3047	sps_RS029
					and	55 and
					swp_3256)	sps_RS067
					or	15 and
					(swp_3045	sps_RS091
					and	90 and
					swp_3510	sps_RS067
					and	10) or
					swp_3047	(sps_RS09
					and	190 and
					swp_3256)	sps_RS029
					or	55 and
					(swp_3256	sps_RS16/
					and	95 and
					swp_2802	sps_RS06/
					and	15 and $\mathbf{D} = \mathbf{D} \mathbf{C} \mathbf{O} (7)$
					swp_1980	$sps_RS00/$
					and	(sp_{0}, \mathbf{PS})
					swp_5045)	(sps_KS00)
					(swn 30/15)	713 and sps RS104
					(swp_50+5	25 and
					swp 3510	sps RS167
					and	95 and
					swp 1980	sps RS091
					and	90 and
					swp 3256)	sps RS067
					1_ /	10)
						sps_RS096
						95 or
						sps_RS167
						95 and
	Fatty Acid				b-ketoacyl	sps_RS067
KAS15	Synthesis	Expressed	Expressed	Expressed	synthase	10
	Fatty Acid				3-hydroxy-	(sps_RS06
KAS16	Synthesis	Expressed	Expressed	Expressed	myristoyl-	715 and

					ACP	sps_RS086
					synthesis	95 and
						sps_RS067
						10) or $(and PSO6)$
						(sps_K300) 715 and
						sps RS067
						05 and
						sps_RS067
						10)
					Malonyl-	
	Fatty Acid				decarboxyl	sps_RS086
MACPD	Synthesis	Expressed	Expressed	Expressed	ase	95
		1	1	1	Malonyl-	sps_RS067
					CoA-ACP	20 and
	Fatty Acid				transacylas	sps_RS067
MCOATA	Synthesis	Expressed	Expressed	Expressed	e	10
	D 1 /				Methionyl-	
	Folate Matabalia				tRNA	
EMETTDS	m	Expressed	Evpressed	Expressed	formyltran	sps_KS003
TWILTING	111	Expressed	Expressed	Expressed	formultetra	00
					hydrofolat	
	Folate				e	
	Metabolis				deformylas	sps RS105
FTHFD	m	Expressed	Expressed	Expressed	e	20
	Folate				formate-	
	Metabolis	- 1	- 1		tetrahydrof	sps_RS260
FTHFL	m	Expressed	Expressed	Expressed	olate ligase	70
	Folata				Glycolalde	
	rolate Metabolis				nyue dehydroge	
GCALDD	m	Expressed	Expressed	Expressed	nase	Gap
201200			p. 30004			sps RS238
						40 and
						sps_RS264
						55 and
	- 1					sps_RS238
	Folate				Glycine	30 and
GIVCI	m	Expressed	Expressed	Expressed	Cleavage	sps_K8238 35
ULICL	111	Expressed	Expressed	Expressed	Glycolate	55
	Folate				dehvdroge	
GLYCLT	Metabolis				nase	sps RS228
DXR	m	Expressed	Expressed	Expressed	(NAD)	25

					methenylte trahydrofol	
	Folate				ate	
	Metabolis				cyclohydro	sps_RS092
MTHFC	m	Expressed	Expressed	Expressed	lase	50
	Folate				methylenet etrahydrof olate dehydroge	
	Metabolis				nase	sps_RS092
MTHFD	m	Expressed	Expressed	Expressed	(NADP)	50
MTHFR2	Folate Metabolis m	Expressed	Expressed	Expressed	5,10- methylenet etrahydrof olate reductase (NADH)	sps_RS145
	111	LAPICSSCU	LAPICSSCU	Expressed		sps_RS165
GLNS	Glutamate Metabolis m	Expressed	Expressed	Expressed	glutamine synthetase	70 or sps_RS064 00 or sps_RS125 80
	Glutamate	1	1	1	Glutaminyl	
GLNTRS	Metabolis m	Expressed	Expressed	Expressed	-tRNA synthetase	sps_RS092 85
	Glutamate Metabolis				glutamate dehydroge nase	sps_RS029
GLUDx	m	Expressed	Expressed	Expressed	(NAD)	15
CLINI	Glutamate Metabolis	D 1	D 1	F 1	glutaminas	sps_RS115
GLUN	m	Below	Below	Expressed	e	45 and DS120
	Glutamate Metabolis				glutamate synthase	sps_RS120 80 and sps_RS120 85 and sps_RS079
GLUSy	m	Expressed	Expressed	Expressed	(NADPH)	55
GLUTRR	Glutamate Metabolis m	Expressed	Expressed	Expressed	glutamyl- tRNA reductase	sps_RS214 15
	Glutamate Metabolis			-	Glutamyl- tRNA	sps_RS179
GLUTRS	m	Expressed	Expressed	Expressed	synthetase	80

	Glycine				betaine-	
	and Serine				aldehvde	
BETALD	Metabolis				dehvdroge	sps RS174
Hx	m	Below	Below	Below	nase	35
	Glycine				betaine-	
	and Serine				aldehvde	
BETALD	Metabolis				dehvdroge	sps_RS174
Hv	m	Below	Below	Below	nase	35
	Glycine	2010.11		2010	glycine	
	and Serine				hydroxyme	
	Metabolis				thyltransfe	sps_RS203
GHMT	m	Expressed	Expressed	Expressed	rase	50
	Glycine	Lipresee	2	p	1.0.0	
	and Serine				glycine C-	
	Metabolis				acetvltrans	sps_RS007
GLYAT	m	Expressed	Expressed	Expressed	ferase	15
	Glycine					sps_RS002
	and Serine				Glycyl-	55 and
	Metabolis				tRNA	sps RS002
GLYTRS	m	Expressed	Expressed	Expressed	synthetase	50
GETTRS	Glycine	LAPICSSCA	Expressed	Expressed	nhosnhogl	50
	and Serine				vcerate	
	Metabolis				dehydroge	sps RS140
PGCD	m	Expressed	Expressed	Expressed	nase	45
TGCD	Glycine	LAPICSSCA	Expressed	Expressed	nhosphoser	15
	and Serine				ine	
	Metabolis				transamina	sns RS039
PSERT	m	Expressed	Expressed	Expressed	se	85
ISERI	111	LAPICSSCA	Expressed	Expressed	nhosnhoser	05
	Glycine				ine	
	and Serine				nhosnhatas	
	Metabolis		Used Belo		e (I -	sps RS208
DSD I	m	Expressed	w	Expressed	c (L-	55 Sps_R5200
	Glycine	LAPICSSCU	**	LAPICSSCU	501110)	sps RS177
	and Serine				serine O-	25 or
	Metabolis				acetultrane	sns RS15/
SERAT	m	Expressed	Expressed	Expressed	ferase	3ps_R5154
	Glycine	LAPICSSCU	LAPICSSCU	LAPICSSCU	101050	00
	and Serine					
	Metabolis				D-serine	sns RS204
SERD D	m	Below	Below	Below	deaminase	30 ³ 204
	Glycine	DCIOW	DCIOW	DCIOW	acammase	sne RSARI
	and Serine					$\frac{3}{25}$ or
	Metabolis				I_serine	2501
SERDI	m	Fynressed	Expressed	Expressed	deaminase	sps_K3150 50
SLKD_L	111	LAPICSSCU	Lapresseu	LAPICSSCU	acammase	50

	Glycine and Serine				Serine-	
SERGLY	Metabolis				transamina	sps_RS154
X	m	Expressed	Expressed	Expressed	se	05
SERTRS	Glycine and Serine Metabolis m	Expressed	Expressed	Expressed	Seryl- tRNA synthetase	sps_RS052 70
THRD	Glycine and Serine Metabolis m	Expressed	Expressed	Expressed	L- threonine dehydroge nase (w/ AOBUTDs)	sps_RS007 10
מרו סמרו א	Glycolysis/ Gluconeog	Palaw	Palaw	Palow	ADP ribose diphosphot	sps_RS251 40 and sps_RS267 75
ADEKDE	Glycolygig/	DCIOW	DEIOM	DEIOM	ast	15
FNO	Gluconeog	Fypressed	Fypressed	Fypressed	enolase	sps_RS202
LINO	Glycolysis/	LAPICSSCU	LAPICSSCU	LAPICSSCU	fructose-	50
FBA	Gluconeog enesis	Expressed	Expressed	Expressed	bisphospha te aldolase	sps_RS129 80
FBP	Glycolysis/ Gluconeog enesis	Expressed	Expressed	Expressed	fructose- bisphospha tase	sps_RS243
	Glycolysis/ Gluconeog	Lapressed	Lapressed	Empressed	glyceralde hyde-3- phosphate dehydroge nase	sps_RS044 50 or sps_RS261 80 or sps_RS044 60 or sps_RS207
GAPD	enesis	Expressed	Expressed	Expressed	(NAD)	35
GLCP	Glycolysis/ Gluconeog enesis	Below	Expressed	Expressed	glycogen phosphoryl ase	sps_RS113 40 or sps_RS113 45
GLCS1	Glycolysis/ Gluconeog enesis	Used_Belo w	Expressed	Expressed	glycogen synthase (ADPGlc)	sps_RS113 30
	Glycolysis/ Gluconeog				glucose-1- phosphate adenylyltra	sps_RS113
GLGC	enesis	Expressed	Expressed	Expressed	nsferase	35

	Glycolysis/					D C101
HEX1	Gluconeog enesis	Expressed	Expressed	Expressed	hexokinase	sps_RS181 05
PDH	Glycolysis/ Gluconeog enesis	Expressed	Expressed	Expressed	pyruvate dehydroge nase	sps_RS264 60 and sps_RS264 65 and sps_RS264 55
PGI	Glycolysis/ Gluconeog enesis	Expressed	Expressed	Expressed	glucose-6- phosphate isomerase	sps_RS117 80
PGK	Glycolysis/ Gluconeog enesis	Expressed	Expressed	Expressed	phosphogl ycerate kinase	sps_RS129 85
PGM	Glycolysis/ Gluconeog enesis	Expressed	Expressed	Expressed	phosphogl ycerate mutase	sps_RS276 85
PPS	Glycolysis/ Gluconeog enesis	Expressed	Expressed	Expressed	phosphoen olpyruvate synthase	sps_RS026 25
РҮК	Glycolysis/ Gluconeog enesis	Expressed	Expressed	Expressed	pyruvate kinase	sps_RS055 45
TPI	Glycolysis/ Gluconeog enesis	Expressed	Expressed	Expressed	triose- phosphate isomerase	sps_RS209 70
ATPPRT	Histidine Metabolis m	Expressed	Expressed	Expressed	ATP phosphorib osyltransfe rase	sps_RS064 90
FGLU	Histidine Metabolis m	Expressed	Expressed	Expressed	formimido ylglutamas e	sps_RS150 10
HISD1	Histidine Metabolis m	Expressed	Expressed	Expressed	Histadine Ammonia Lyase	sps_RS274 80
HISTD	Histidine Metabolis m	Expressed	Expressed	Expressed	histidinol dehydroge nase	sps_RS064 95
HISTP	Histidine Metabolis m	Expressed	Expressed	Expressed	histidinol- phosphatas e	sps_RS065 05
HISTRS	Histidine Metabolis m	Expressed	Expressed	Expressed	Histidyl- tRNA synthetase	sps_RS189 00

					histidinol-	
	Histidine				phosphate	
	Metabolis				transamina	sps_RS065
HSTPT	m	Expressed	Expressed	Expressed	se	00
					Imidazole-	sps_RS065
	Histidine				glycerol-3-	20 and
	Metabolis				phosphate	sps_RS065
IG3PS	m	Expressed	Expressed	Expressed	synthase	10
					imidazoleg	
					lycerol-	
	Histidine				phosphate	
	Metabolis			_	dehydratas	sps_RS065
IGPDH	m	Expressed	Expressed	Expressed	e	05
	Histidine				imidazolon	
	Metabolis	 1	D 1	D 1	epropionas	sps_RS274
IZPN	m	Expressed	Expressed	Expressed	e	95
	TT 1.				phosphorib	
	Histidine				osyl-AMP	DCO(5
	Metabolis	Evenessed	Evenessed	Evenessed	cyclonydro	sps_K5065
FRAMIL	111	Expressed	Expressed	Expressed	nhoanhorih	23
	Uistidino				phosphorid	
	Metabolis				osyl-Alf	sps PS065
PRATPP	m	Expressed	Expressed	Expressed	hatase	25 Sps_R5005
	111	LAPICSSEd	LAPICSSE	Lapressed	1_(5_	25
					phosphorib	
					osvl)-5-	
					[(5-	
					phosphorib	
					osylamino)	
					methyliden	
					eamino)im	
					idazole-4-	
					carboxami	
					de	
	Histidine				isomerase	
	Metabolis				(irreversibl	sps_RS065
PRMICIi	m	Expressed	Expressed	Expressed	e)	15
	TT				phosphorib	
	Histidine				osylpyroph	Deat
סמתמת	Metabolis				osphate	sps_RS214
РКРРЗ	m	Expressed	Expressed	Expressed	synthetase	30
	Histidine Motobalia					and DCOTA
LIDCN	m	Everaged	Everaged	Evenessad	11700070000	sps_K52/4
UKUN	111	Expressed	Expressed	Expressed	urocanase	03

	Methionin				adenosylho	
	e				mocysteine	
AHCYSN	Metabolis				nucleosida	sps_RS120
S	m	Expressed	Expressed	Expressed	se	90
					2,3-diketo- 5-	
					methylthio	
	Methionin				phosphope	
	e				ntane	
DKMPPD	Metabolis	– 1	– 1	D 1	degradatio	a
3	m	Expressed	Expressed	Expressed	n reaction	Gap
	Methionin				homoserin	
	e				e O-	D C100
UCCT	Metabolis	F 1	F 1	F 1	succinyltra	sps_RS100
H551	m	Expressed	Expressed	Expressed	nsterase	/5
)- N - 41141- : -	
					Methylthio	
					-3-deoxy-	
	Mathianin					
					1- nhosnhate	
	C Metabolis				dehydratas	
MDRPD	m	Expressed	Expressed	Expressed	e	Gan
	Methionin	Lapiessed	LAPICSSEd	Lapiessed	C	Gap
	e				methionine	
	e Metabolis				adenosyltr	sps RS130
METAT	m	Expressed	Expressed	Expressed	ansferase	00
	Methionin	LAPICOUC	LAPICODE	Lapresseu	unsteruse	
	e					
	Metabolis				methionine	sps_RS091
METGL	m	Expressed	Below	Expressed	g-lvase	30
	Methionin	1		1	tetrahvdrof	sps RS235
	e				olate	85 or
	Metabolis				methyltran	sps RS220
METS	m	Expressed	Expressed	Expressed	sferase	50
	Methionin	-	-	_		
	e				Methionyl-	
	Metabolis				tRNA	sps_RS068
METTRS	m	Expressed	Expressed	Expressed	synthetase	15
					5-	
				1	1	
					methyltetra	
	Methionin				methyltetra hydroptero	
	Methionin e				methyltetra hydroptero yltriglutam	
MTHPTG	Methionin e Metabolis				methyltetra hydroptero yltriglutam ate	sps_RS220

					ine S-	
					methyltran	
					sforoso	
					5101250	
	N 1 · · ·				5-	
	Methionin				methylthio	
	e				ribose-1-	
	Metabolis				phosphate	
MTRI	m	Expressed	Expressed	Expressed	isomerase	Gap
	Methionin				5-	
	e				methylthio	
	Metabolis				ribose	
MTRK	m	Expressed	Expressed	Expressed	kinase	Gap
		2	Lipicce	2	S-	
	Methionin				ribosylhom	
					noosymon	
					ocysteme	DC212
DUCCE	Metabolis	F 1	F 1	D 1	cleavage	sps_KS212
RHCCE	m	Expressed	Expressed	Expressed	enzyme	30
					O-	
	Methionin				succinylho	
	e				moserine	
	Metabolis				lyase (L-	sps RS145
SHSL1	m	Expressed	Expressed	Expressed	cysteine)	65
		1	1		2-keto-4-	
	Methionin				methylthio	
					huturata	
	C Matahalia				tuanaanina	
IDHZO	Metabolis	F 1	F 1	F 1	transamina	C
UNK3	m	Expressed	Expressed	Expressed	tion	Gap
					OHCU	
	Purine and				Decarboxy	
	Pyrimidine				lase	
5HPUDIC	Metabolis				(spontaneo	spontaneou
DCr	m	Expressed	Expressed	Expressed	us)	S
	Purine and	-	-	•	Í	
	Pyrimidine				OHCU	
5HPUDIC	Metabolis				Decarboyy	sps RS054
	m	Evenessed	Dalaw	Dalaw	lasa	sps_K5054
DCS		Expressed	Delow	Delow	lase	03
	Purine and					
	Pyrimidine					
ALLNRA	Metabolis				Allantoin	
С	m	Expressed	Expressed	Expressed	Racemase	Gap
	Purine and					
	Pyrimidine					
	Metabolis				Allantoicas	sps RS054
ALLTC	m	Expressed	Below	Below	e	70
	Purine and		2010 11	2010 //	Allantoina	
ALITN	Durimiding	Expressed	Expressed	Expressed	s a since in a second	Gan
ALLIN	r yr maine	Expressed	Expressed	Expressed	20	Jap

	Metabolis					
	m					
	Purine and					
	Pyrimidine				hydroxyiso	
	Metabolis				urate	sps_RS054
HIUH	m	Below	Below	Below	hydrolase	60
	Purine and					
	Pyrimidine				TT · 1 1	
UDDOLV	Metabolis	D 1	D 1	D 1	Ureidoglyc	sps_RS054
URDGLY	m D · 1	Below	Below	Below	olate lyase	55 DC054
	Purine and				TT /	sps_RS054
	Pyrimidine				Urate	80 and $\mathbf{D} \subseteq \mathbf{D} \subseteq \mathbf{D}$
OKHYDR	Metabolis	E	E	E	Hydroxyla	sps_K5054
0X	M	Expressed	Expressed	Expressed	se	83
	Nucleotide				Adamagina	mg DS219
	Dathwaye	Everaged	Everaged	Everaged	Adeniosine	sps_K5216
ADA	Nucleatide	Expressed	Expressed	Expressed	ucammase	30
	Salvage				adanvlata	sps PS081
ADK1	Pathways	Expressed	Expressed	Expressed	kinase	5ps_K5081
	Nucleotide	Expressed	Expressed	Lapiessed	guanylate	10
	Salvage				kinase	sns RS081
ADK3	Pathways	Expressed	Expressed	Expressed	(aMP:gTP)	70
	Nucleotide			2	adentvlate	
	Salvage				kinase	sps RS081
ADK4	Pathways	Expressed	Expressed	Expressed	(ITP)	70
	2	-	-	_		sps RS158
						65 or
						sps_RS120
						55 or
						sps_RS152
	Nucleotide					00 or
	Salvage				adenylate	sps_RS247
ADNCYC	Pathways	Expressed	Expressed	Expressed	cyclase	10
	Nucleotide					
	Salvage				adenosine	sps_RS081
ADNKI	Pathways	Expressed	Expressed	Expressed	kınase	70
					adenine	
	Nucleotide				phosphorib	DCOOC
A DDT	Salvage	Evenessed	Evenessed	Exercise 1	osyltransie	sps_KSU82
ADPI	rainways	Expressed	Expressed	Expressed	rase	00
	Nucleotide				$DIS(\mathcal{I} - \mathbf{n})$	
	Salvage				tetraphosp	sns RS228
ΔΡΔΔΗ	Pathwave	Below	Below	Below	hatase	75 rts220
1 11 TI 11	1 au ways				natuse	15

	Nucleotide					
	Salvage				Ap5A	sps RS228
AP5AH	Pathways	Below	Below	Below	hydrolase	75
	Nucleotide					
	Salvage				cytidine	sps_RS066
CYTD	Pathways	Expressed	Expressed	Expressed	deaminase	85
	Nucleotide					
	Salvage	_			Cytodine	sps_RS098
CYTDH	Pathways	Expressed	Expressed	Expressed	Hydrolase	20
	Nucleotide				cytidine	
	Salvage	- 1	F 1	F 1	kinase	sps_RS068
CYTDKI	Pathways	Expressed	Expressed	Expressed	(ATP)	50
	Nucleotide				cytidine	DCOCO
OVTDVA	Salvage	F 1	F 1	F 1	Kinase	sps_RS068
CYIDK2	Pathways	Expressed	Expressed	Expressed	(GIP)	50
	Nucleotide				cytidine	ma DCOCO
CVTDV2	Dathwaya	Evenessed	Everaged	Evenessed	(ITD)	sps_K5008
CTIDKS	Nucleatide	Expressed	Expressed	Expressed	(IIF)	30
	Salvage				kinase	sps PS040
CVTK1	Pathways	Expressed	Expressed	Expressed	(CMP)	sps_K3040
	Nucleotide	Lapiessed	LAPICSSEd	LAPICSSEd	cytidylate	00
	Salvage				kinase	sps RS040
CYTK2	Pathways	Expressed	Expressed	Expressed	(dCMP)	00
	Nucleotide				deoxvaden	
	Salvage				osine	sps RS218
DADA	Pathways	Expressed	Expressed	Expressed	deaminase	50
	Nucleotide	-	-	-	deoxyaden	
	Salvage				ylate	sps_RS081
DADK	Pathways	Expressed	Expressed	Expressed	kinase	70
	Nucleotide				deoxycytid	
	Salvage				ine	sps_RS066
DCYTD	Pathways	Expressed	Expressed	Expressed	deaminase	85
					deoxyguan	
					ylate	
	Nucleotide				kinase	
	Salvage				(dGMP:A	sps_RS163
DGKI	Pathways	Expressed	Expressed	Expressed	TP)	55
	Nucleotide					DCACO
	Salvage	Usea_Belo	Usea_Belo	Usea_Belo	a I MP	sps_KS068
DIMPK	rainways	W	W	W	kinase	33
	Nucleatide				ueoxyuridi	
	Salvage				$(\Delta T P \cdot D_{P})$	sps RS102
DURIK 1	Pathways	Expressed	Expressed	Expressed	xviiridine)	90
~ ~		- rr cooca	- rr cooca	- mr. cooca		

					purine- nucleoside	
	Nucleotide				phosphatas	
DURIPP	Salvage Pathways	Expressed	Expressed	Expressed	(deoxyurid ine)	sps_RS208 75
DUTPDP	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	dUTP diphosphat ase	sps_RS162 85
GK1	Nucleotide Salvage	Evpressed	Evpressed	Evpressed	guanylate kinase (GMP:AT P)	sps_RS163
UKI	Nucleotide	Expressed	Expressed	Expressed	1)	55
GP4GH	Salvage Pathways	Below	Below	Below	Gp4G hydrolase	sps_RS228 75
GSNK	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	guanosine kinase	sps_RS081 60
GTPDPK	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	GTP diphospho kinase	sps_RS202 65
	Nucleotide			· · · ·		
GUAD	Salvage Pathwavs	Expressed	Used_Belo w	Used_Belo w	Guanine deaminase	sps_RS054 50
GUAPRT	Nucleotide Salvage	Evpressed	Evpressed	Evpressed	guanine phosphorib osyltransfe	sps_RS245 30 or sps_RS128 40
JUAINI	Tallways	Lapressed	Lapressed	Lapressed	hypoxanthi ne phosphorib	TU DC245
	Nucleotide Salvage				osyltransfe rase (Hypoxant	sps_RS245 30 or sps_RS128
HXPRT	Pathways	Expressed	Expressed	Expressed	hine)	40
INSK	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	inosine kinase	sps_RS081 60
NIDDV 1	Nucleotide Salvage	Everenced	Everenced	Every	nucleoside - diphosphat e kinase (ATP:GDP	sps_RS176
NDFKI	1 aniways	Expressed	Expressed	Expressed)	00

					nucleoside	
					-	
	Nucleotide				e kinase	
	Salvage				(ATP:UDP	sps_RS176
NDPK2	Pathways	Expressed	Expressed	Expressed)	80
					nucleoside	
					- diphosphat	
	Nucleotide				e kinase	
	Salvage				(ATP:CDP	sps_RS176
NDPK3	Pathways	Expressed	Expressed	Expressed) muoloogido	80
					-	
					diphosphat	
	Nucleotide				e kinase	
NDPKA	Salvage	Evpressed	Evpressed	Expressed	(ATP:dTD	sps_RS176
	1 attiways	Expressed	Expressed	Expressed	nucleoside	00
					-	
	NT 1 1				diphosphat	
	Nucleotide Salvage				e kinase $(\Delta TP \cdot dGD)$	sps RS176
NDPK5	Pathways	Expressed	Expressed	Expressed	(A11.dOD P)	80
			-	-	nucleoside	
					- dinhoanhot	
	Nucleotide				e kinase	
	Salvage				(ATP:dUD	sps_RS176
NDPK6	Pathways	Expressed	Expressed	Expressed	P)	80
					nucleoside	
					diphosphat	
	Nucleotide				e kinase	
NIDDU7	Salvage	D	D	F 1	(ATP:dCD	sps_RS176
NDPK/	ratnways	Expressed	Expressed	Expressed	r) nucleoside	80
					-	
					diphosphat	
	Nucleotide				e kinase	and DC174
NDPK8	Pathwavs	Expressed	Expressed	Expressed	(AIF.uAD)	sps_K3170 80
	· <i>j</i> =	1	1		,	sps_RS069
	Nucleotide				5'-	45 or
NTD1	Salvage Pathways	Expressed	Expressed	Fypressed	nucleotidas	sps_RS157 45 or
	1 aurways	LAPICSSCU	LAPICSSCU	Lapicsocu		7J UI

						sps_RS037 95
	Nucleotide				5'-	D CO(O
NTD10	Salvage Pathways	Expressed	Expressed	Expressed	e (XMP)	sps_RS069 45
	Nucleotide				51	sps_RS069
	Salvage				nucleotidas	sps_RS267
NTD11	Pathways	Expressed	Expressed	Expressed	e (IMP)	80
	Nucleotide Salvage				5' nucleotidas	sps_RS037
NTD12	Pathways	Expressed	Below	Below	e (dIMP)	95
	Nucleotide				5'-	sps_RS069 45 or
	Salvage				nucleotidas	sps_RS157
NTD2	Pathways	Expressed	Expressed	Expressed	e (UMP)	45
	Nucleotide				5'-	sps_K5069 45 or
	Salvage				nucleotidas	sps_RS037
NTD3	Pathways	Expressed	Expressed	Expressed	e (dCMP)	95 DG0(0
	Nucleotide				5'	sps_RS069 45 or
	Salvage				Nucleotida	sps RS037
NTD3_P	Pathways	Expressed	Expressed	Expressed	se (dCMP)	95
	Nucleotide				5'-	ana DSO(0
NTD4	Pathways	Expressed	Expressed	Expressed	e (CMP)	sps_K5009 45
		ł		A		sps_RS069
						45 or
	Nucleotide				5'-	45 or
	Salvage				nucleotidas	sps_RS037
NTD5	Pathways	Expressed	Expressed	Expressed	e (dTMP)	95 DC0(0
						sps_RS069 45 or
	Nucleotide				5'	sps_RS157 45 or
	Salvage				Nucleotida	sps RS037
NTD5_P	Pathways	Expressed	Expressed	Expressed	se (dTMP)	95
	Nucleotide				5'-	sps_RS069 45 or
	Salvage				nucleotidas	sps_RS037
NTD6	Pathways	Expressed	Expressed	Expressed	e (dAMP)	95
	Nucleotide				5' Nucleatide	and DCOLO
NTD6_P	Pathways	Expressed	Expressed	Expressed	se (dAMP)	45 or

						sps_RS037 95
NTD7	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	5'- nucleotidas e (AMP)	sps_RS069 45
NTD8	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	5'- nucleotidas e (dGMP)	sps_RS069 45 or sps_RS037 95
NTD8 P	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	5' Nucleotida se (dGMP)	sps_RS069 45 or sps_RS037 95
NTD9	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	5'- nucleotidas e (GMP)	sps_RS069 45 or sps_RS267 80
NTPP1	Nucleotide Salvage Pathways	Below	Below	Below	Nucleoside triphosphat e pyrophosp horylase (dgtp)	sps_RS202 60
NTPP10	Nucleotide Salvage Pathways	Expressed	Below	Expressed	Nucleoside triphosphat e pyrophosp horylase (dITP)	sps_RS115 20
NTPP11	Nucleotide Salvage Pathways	Expressed	Below	Expressed	Nucleoside triphosphat e pyrophosp horylase (xtp)	sps_RS115 20
NTPP2	Nucleotide Salvage Pathways	Below	Below	Below	Nucleoside triphosphat e pyrophosp horylase (gtp)	sps_RS202 60
NTPP3	Nucleotide Salvage Pathways	Below	Below	Below	dCTP diphosphat ase	sps_RS202 60

PUNP2	Salvage Pathways	Expressed	Expressed	Expressed	phosphoryl ase	sps_RS208 65
	Nucleotide				purine- nucleoside	sps_RS204 40 or
PUNP1	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	phosphoryl ase (Adenosin e)	sps_RS204 40 or sps_RS208 65
					purine- nucleoside	
NTPP9	Nucleotide Salvage Pathways	Expressed	Below	Expressed	Nucleoside triphosphat e pyrophosp horylase (ITP)	sps_RS115 20
NTPP8	Nucleotide Salvage Pathways	Below	Below	Below	Nucleoside triphosphat e pyrophosp horylase (utp)	sps_RS202 60
NTPP7	Nucleotide Salvage Pathways	Below	Below	Below	Nucleoside triphosphat e pyrophosp horylase (dttp)	sps_RS202 60
NTPP6	Nucleotide Salvage Pathways	Below	Below	Below	Nucleoside triphosphat e pyrophosp horylase (atp)	sps_RS202 60
NTPP5	Nucleotide Salvage Pathways	Below	Below	Below	Nucleoside triphosphat e pyrophosp horylase (datp)	sps_RS202 60
NTPP4	Nucleotide Salvage Pathways	Below	Below	Below	Nucleoside triphosphat e pyrophosp horylase (ctp)	sps_RS202 60

					(Deoxyade	
					nosine)	
	Nucleotide Salvage				purine- nucleoside phosphoryl ase (Guanosin	sps_RS204 40 or sps_RS208
PUNP3	Pathways	Expressed	Expressed	Expressed	e) .	65
PUNP4	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	purine- nucleoside phosphoryl ase (Deoxygua nosine)	sps_RS204 40 or sps_RS208 65
PUNP5	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	purine- nucleoside phosphoryl ase (Inosine)	sps_RS204 40 or sps_RS208 65
PUNP6	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	purine- nucleoside phosphoryl ase (Deoxyino sine)	sps_RS204 40 or sps_RS208 65
PUNP7	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	purine- nucleoside phosphoryl ase (Xanthosin e)	sps_RS204 40 or sps_RS208 65
PYNP2	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	pyrimidine - nucleoside phosphoryl ase (uracil)	sps_RS155 25
RNDR1	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	ribonucleo side- diphosphat e reductase (ADP)	sps_RS039 55 and sps_RS039 65 and sps_RS038 20
RNDR2	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	ribonucleo side- diphosphat	sps_RS039 55 and sps_RS039 65 and

					e reductase (GDP)	sps_RS038 20
RNDR3	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	ribonucleo side- diphosphat e reductase (CDP)	sps_RS039 55 and sps_RS039 65 and sps_RS038 20
RNDR4	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	ribonucleo side- diphosphat e reductase (UDP)	sps_RS039 55 and sps_RS039 65 and sps_RS038 20
RNTR1	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	ribonucleo side- triphosphat e reductase (ATP)	sps_RS089 10 and sps_RS038 20
RNTR2	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	ribonucleo side- triphosphat e reductase (GTP)	sps_RS089 10 and sps_RS038 20
RNTR3	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	ribonucleo side- triphosphat e reductase (CTP)	sps_RS089 10 and sps_RS038 20
RNTR4	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	ribonucleo side- triphosphat e reductase (UTP)	sps_RS089 10 and sps_RS038 20
TMDK1	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	thymidine kinase (ATP:thym idine)	sps_RS102 90
TMDPP	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	thymidine phosphoryl ase	sps_RS208 75
TMDS	Nucleotide Salvage Pathways	Expressed	Expressed	Expressed	thymidylat e synthase	sps_RS120 30

	Nucleotide					
	Salvage		Used Belo	Used Belo	UMP	sps RS104
UMPK	Pathways	Expressed	w	w	kinase	70
	2	-			uracil	
	Nucleotide				phosphorib	
	Salvage				osvltransfe	sps_RS024
UPPRT	Pathways	Expressed	Expressed	Expressed	rase	60
	Nucleotide	Liproce	Liprosee	Lipicco	uridylate	
	Salvage	Used Belo	Used Belo	Used Belo	kinase	sns RS068
LIRIDK2	Pathways	w	w	w	(dUMP)	35
	1 univay5				uridine	55
	Nucleotide				kinase	
	Salvage				(ATD. Urid	sps PS068
	Dathways	Expressed	Expressed	Expressed	(All .Olld	50
UKIKI	1 alliways	Expressed	Expressed	Expressed	unidin a	50
	Nucleatide				linago	
	Nucleotide				(CTD.LL.: 1	ana DCOCO
	Dathuyaya	Evenessed	Evenessed	Evenessed	(GIP:Ond	sps_K5008
URIKZ	Pathways	Expressed	Expressed	Expressed	ine)	30
	Nucleatide				uridine	
	Nucleotide				(ITD.I.I.: 1)	
	Salvage	F 1	F 1	F 1	(IIP:Uridi	sps_KS068
URIK3	Pathways	Expressed	Expressed	Expressed	ne)	50
					2-dehydro-	
					3-deoxy-	
	Pentose				phosphogl	
	Phosphate	- 1	- 1	- 1	uconate	sps_RS055
EDA	Pathway	Expressed	Expressed	Expressed	aldolase	20
					glucose 6-	
	Pentose				phosphate	
	Phosphate				dehydroge	sps_RS055
G6PDHy	Pathway	Expressed	Expressed	Expressed	nase	35
					phosphogl	
	Pentose				uconate	
	Phosphate				dehydroge	sps_RS102
PGDH	Pathway	Expressed	Expressed	Expressed	nase	05
					phosphogl	
	Pentose				uconate	
	Phosphate				dehydratas	sps_RS055
PGDHY	Pathway	Expressed	Expressed	Expressed	e	25
					6-	
	Pentose				phosphogl	
	Phosphate				uconolacto	sps_RS055
PGL	Pathway	Expressed	Expressed	Expressed	nase	30
	Pentose					
	Phosphate				Phosphorib	sps_RS249
PRKIN	Pathway	Expressed	Expressed	Expressed	ulokinase	05

					ribulose 5-	
	Pentose				phosphate	
	Phosphate				3-	sps_RS266
RPE	Pathway	Expressed	Expressed	Expressed	epimerase	00
	Pentose			_	ribose-5-	
	Phosphate				phosphate	sps RS128
RPI	Pathway	Expressed	Expressed	Expressed	isomerase	80
	Pentose			_		
	Phosphate				transaldola	sps_RS117
TAL	Pathway	Expressed	Expressed	Expressed	se	75
	Pentose			_		
	Phosphate				transketola	sps RS129
TKT1	Pathway	Expressed	Expressed	Expressed	se	95
	Pentose					
	Phosphate				transketola	sps RS129
TKT2	Pathway	Expressed	Expressed	Expressed	se	95
					Xylulose-	
					5-	
	Pentose				phosphate	
	Phosphate				phosphoke	sps_RS117
ХРК	Pathway	Expressed	Expressed	Expressed	tolase	65
	Purine and					
	Pyrimidine				adenosylho	
ADHMCY	Metabolis				mocysteina	
SSYN	m	Expressed	Expressed	Expressed	se	Gap
	Purine and					
	Pyrimidine					
	Metabolis				adenylsucc	sps_RS027
ADSL1r	m	Expressed	Expressed	Expressed	inate lyase	30
	Purine and					
	Pyrimidine				adenylosuc	
	Metabolis		_	_	cinate	sps_RS027
ADSL2r	m	Expressed	Expressed	Expressed	lyase	30
	Purine and					sps_RS255
	Pyrimidine				adenylosuc	20 or
	Metabolis	- 1		F 1	cınate	sps_RS042
ADSS	m	Expressed	Expressed	Expressed	synthetase	70
					phosphorib	
	D · 1				osylaminoi	
	Purine and				midazoleca	
	Pyrimidine				rboxamide	DCICC
	Metabolis	E 1	E 1	F 1	tormyltran	sps_KS156
AICART	m	Expressed	Expressed	Expressed	sterase	/3
	Deni 1				pnosphorib	
	Purine and	F 1			osylaminoi	C
AIKC2	Pyrimidine	Expressed	Expressed	Expressed	midazole	Gap

	Metabolis				carboxylas	
	m				e	
AIRC3	Purine and Pyrimidine Metabolis m	Expressed	Expressed	Expressed	phosphorib osylaminoi midazole carboxylas e (mutase rxn)	sps_RS200 35
ASPCT	Purine and Pyrimidine Metabolis	Everaged	Expressed	Expressed	aspartate carbamoylt	sps_RS191 35 or sps_RS191 30
ASPCI	Purine and Pyrimidine	Expressed	Expressed	Expressed	ransierase	30
CampHydr olyase	Metabolis m	Expressed	Expressed	Expressed	Camp Hydrolase	sps_RS251 30
	Purine and Pyrimidine Metabolis	-	-	- 1	Cytosine	sps_RS062
CSND	m	Expressed	Expressed	Expressed	deaminase	25
CTPS2	Purine and Pyrimidine Metabolis m	Expressed	Expressed	Expressed	CTP synthase (glutamine	sps_RS202
	Purine and Pyrimidine Metabolis				dihydoorot ic acid dehydroge nase	sps RS029
DHORD2	m	Expressed	Expressed	Expressed	(quinone8)	20
	Purine and Pyrimidine Metabolis				dihydrooro tate dehydroge	sps_RS029
DHORD4i	m	Expressed	Expressed	Expressed	nase	20
	Purine and Pyrimidine Metabolis	Evpressed	Evoressed	Evpressed	dihydrooro tate dehydroge	sps_RS029
DHOKD0	III During and	Expressed	Expressed	Expressed	11450	20
DHORTS	Pyrimidine Metabolis m	Expressed	Expressed	Expressed	dihydrooro tase	sps_RS223 05
	Purine and Pyrimidine Metabolis				guanosine pentaphosp	sps_RS151
EPPP2	m	Expressed	Expressed	Expressed	hatase	05

G35DP	Purine and Pyrimidine Metabolis m	Expressed	Expressed	Expressed	guanosine- 3',5'- bis(diphos phate) 3'- diphosphat ase	sps_RS163 65
GARFT	Purine and Pyrimidine Metabolis m	Expressed	Expressed	Expressed	phosphorib osylglycin amide formyltran sferase	sps_RS024 50
GLUPRT	Purine and Pyrimidine Metabolis m	Expressed	Expressed	Expressed	glutamine phosphorib osyldiphos phate amidotrans ferase	sps_RS085 85
	Purine and Pyrimidine Metabolis				GMP synthase (glutamine - hydrolysin	sps_RS188 65 and sps_RS188 60 and sps_RS258
GMPS2	m	Below	Below	Below	g)	50
IMPC	Purine and Pyrimidine Metabolis m	Expressed	Expressed	Expressed	IMP cyclohydro lase	sps_RS156 75
IMPD	Purine and Pyrimidine Metabolis m	Expressed	Expressed	Expressed	IMP dehydroge nase	sps_RS188 65
OMPDC	Purine and Pyrimidine Metabolis m	Expressed	Expressed	Expressed	orotidine- 5'- phosphate decarboxyl ase	sps_RS040 25
ORPT	Purine and Pyrimidine Metabolis m	Expressed	Expressed	Expressed	orotate phosphorib osyltransfe rase	sps_RS163
PRAGS	Purine and Pyrimidine Metabolis m	Expressed	Expressed	Expressed	phosphorib osylglycin amide synthetase	sps_RS156
	Purine and				nhosnhorih	sns RS024
PRAIS	Pyrimidine	Expressed	Expressed	Expressed	osylaminoi	55

	Metabolis				midazole	
	m				synthetase	
					phosphorib	
					osylaminoi	
	Purine and				midazolesu	
	Pyrimidine				ccinocarbo	
	Metabolis				xamide	sps_RS065
PRASCS	m	Expressed	Expressed	Expressed	synthase	35
					phosphorib	
	Purine and				osylformyl	
	Pyrimidine				glycinamid	
	Metabolis				ine	sps_RS188
PRFGS	m	Expressed	Expressed	Expressed	synthase	45
						sps_RS086
						05 and
						sps_RS067
						55 and
	Purine and				1 . 1	sps_RS082
	Pyrimidine				pseudourid	55 and
DELIDE	Metabolis	Evenessed	Evenessed	Evenessed	ylate	sps_KS216
PSUDS	m Duning and	Expressed	Expressed	Expressed	synthase	80
	Purine and					
	Matabalia				uridina	cmc DS008
прп	m	Everaged	Everaged	Everaged	hydrologo	sps_K3098
UKIII	III Purine and	Expressed	Expressed	Expressed	ilyulolase	20
	Pyrimidine				vanthine	
	Metabolis				dehydroge	sns RS044
XAND	m	Expressed	Expressed	Expressed	nase	60
	111	Expressed	Expressed	LAPICSSCU	acetaldehy	00
					de	
					dehvdroge	
	Pvruvate				nase	
	Metabolis				(acetvlatin	sps RS037
ACALDi	m	Expressed	Expressed	Expressed	g)	65
	Pyruvate	-	-	-		
	Metabolis				acetate	sps RS175
ACKr	m	Expressed	Expressed	Expressed	kinase	90
	Pyruvate	-	-	•	acetyl-	
	Metabolis				CoÁ	sps RS025
ACS	m	Expressed	Expressed	Expressed	synthetase	70
	Pyruvate	-	-	-	D-lactate	
	Metabolis				dehydroge	sps_RS242
LDH_Dir	m	Expressed	Expressed	Expressed	nase	40

						sps_RS201
					avalaastat	35 and
	Pyruvate				oxaloacetat	sps_K3201
	Metabolis				decarboxyl	sps RS201
OAADC	m	Expressed	Expressed	Expressed	ase	25
	Pyruvate				Formate C-	
	Metabolis				acetyltrans	sps_RS175
PFL	m	Expressed	Expressed	Expressed	ferase	75
	Pyruvate				1 1 4	DC175
DT A "	Metabolis	Everaged	Everaged	Everaged	phosphotra	sps_KS1/5
PIAſ	III	Expressed	Expressed	Expressed	aspartate	95
	Threonine				semialdehv	
	and Lysine				de	
	Metabolis				dehydroge	sps RS086
ASAD	m	Expressed	Expressed	Expressed	nase	15
						sps_RS118
						25 or
	Threonine					sps_RS145
	and Lysine					60 or
	Metabolis	D 1	T 1	F 1	aspartate	sps_RS242
ASPK	m Thursting	Expressed	Expressed	Expressed	kinase	90
	I nreonine				diaminopi	sps_KS151
	Metabolis				decarboxyl	$\frac{90.01}{\text{sps}}$
DAPDC	m	Expressed	Expressed	Expressed	ase	sps_R3275
DINDE	Threonine	Empressea	Empressed	Enpressea	use	
	and Lysine				diaminopi	
	Metabolis				melate	sps RS151
DAPE	m	Expressed	Expressed	Expressed	epimerase	85
	Threonine				dihydrodip	
	and Lysine				icolinate	
DUDDD	Metabolis	F 1	F 1	D 1	reductase	sps_RS210
DHDPRy	m ·	Expressed	Expressed	Expressed	(NADPH)	40
	I hreonine				dibuduadia	
	Metabolis				icolinate	sps RS031
DHDPS	m	Fypressed	Fypressed	Expressed	synthase	20
DIIDIS	111	LAPICSSCU	LAPICSSCU	LAPICSSCU	homoserin	20
	Threonine				e	sps RS118
	and Lysine				dehydroge	25 or
	Metabolis				nase	sps_RS145
HSDy	m	Expressed	Expressed	Expressed	(NADPH)	60
	Threonine				homoserin	sps_RS118
HSK	and Lysine	Expressed	Expressed	Expressed	e kinase	20

	Metabolis					
	m					
	Threonine					
	and Lysine				Lysyl-	
	Metabolis			_	tRNA	sps_RS241
LYSTRS	m	Expressed	Expressed	Expressed	synthetase	55
					succinyl-	
	I hreonine				diaminopi	
	And Lysine				doguooinvi	mg DS032
SUDDS	metabolis	Everaged	Everaged	Everaged	desuccinyi	sps_K5052
SDFDS	111	Expressed	Expressed	Expressed	ase	10
	Threenine				minopimel	
	and Lysine				ate	
	Metabolis				transamina	sns RS249
SDPTA	m	Expressed	Expressed	Expressed	se	50
	Threonine	2	Luproces	Linpiteste	tetrahvdro	
	and Lysine				picolinate	
	Metabolis				succinylas	sps RS104
THDPS	m	Expressed	Expressed	Expressed	e	95
	Threonine	-	-	-		sps RS203
	and Lysine					50 or
	Metabolis				threonine	sps_RS114
THRA	m	Expressed	Expressed	Expressed	aldolase	30
	Threonine					
	and Lysine				L-allo-	
	Metabolis	- 1	D 1	– 1	threonine	sps_RS114
THRLAD	m ·	Expressed	Expressed	Expressed	aldolase	30
	Threonine					
	and Lysine					D C110
TUDC	Metabolis	F 1	F 1	F 1	threonine	sps_RS118
IHKS	m Thus an in a	Expressed	Expressed	Expressed	synthase	15
	I nreonine				Throopyl	
	Metabolis				THEOHYI-	sps PS053
THRTRS	m	Expressed	Expressed	Evpressed	synthetase	sps_K3033
TIIRTRS	111	Expressed	Expressed	Expressed	Acetoaceta	23
	Transport				te transport	
	Extracellul				via proton	sps_RS062
ACACt2	ar	Below	Below	Below	symport	95
					N-Acetvl-	-
					D-	
	Transport,				glucosami	
	Extracellul				ne	sps_RS116
ACGAt2	ar	Expressed	Expressed	Expressed	transport	00

					via proton	
					symport	
					acetate	
					transport	
	Transport,				in/out via	
	Extracellul	Used_Belo	Used_Belo	Used_Belo	proton	sps_RS169
ACt6	ar	W	W	W	symport	25
					adenosine	
	Transport,				transport in	
	Extracellul				via proton	sps_RS208
ADNt2	ar	Expressed	Expressed	Expressed	symport	90
						sps_RS261
						65 or
						sps_RS243
	Transport,				D-Alanine-	65 or
	Extracellul				Sodium	sps_RS117
ALA_Dt4	ar	Expressed	Expressed	Expressed	symporter	60
						sps_RS261
						65 or
						sps_RS243
	Transport,				Alanine-	65 or
	Extracellul				Sodium	sps_RS117
ALAt4	ar	Expressed	Expressed	Expressed	symporter	60
						sps_RS135
					L-	35 and
					arabinose	sps_RS135
	Transport,				transport	45 and
	Extracellul				via ABC	sps_RS135
ARBABC	ar	Below	Below	Expressed	system	40
	Transport,				arsenite	
	Extracellul				transporter	sps_RS261
ARSt1	ar	Below	Below	Below	via uniport	85
	Transport,				L-	
	Extracellul				Aspartate	sps_RS081
ASPt2	ar	Expressed	Expressed	Expressed	transport	55
	Transport,					
	Extracellul				butyrate	sps_RS062
BUT_T	ar	Below	Below	Below	symporter	95
						sps_RS235
					Cob(1)ala	65 and
					min	sps_RS235
	Transport,				transport	60 and
	Extracellul	Used_Belo	Used_Belo	Used_Belo	via ABC	sps_RS235
CBL1abc	ar	w	W	W	system	25

						sps_RS174 45 or
						sps RS114
	Transport,				choline-	05 or
	Extracellul				sodium	sps_RS097
CHOLt4	ar	Expressed	Expressed	Expressed	symporter	20
					Citrate transport	sps_RS217 75 and sps_RS217
	Transport,				via	70 and
	Extracellul				succinate	sps_RS217
CITT7	ar	Below	Below	Below	antiport	80
	Transport, Extracellul		Used Belo		chloride ion	sps RS124
Clt	ar	Expressed	w –	Expressed	transport	15
					CO2	
	Transport,				transport	
	Extracellul				out via	
CO2t	ar	Expressed	Expressed	Expressed	diffusion	Diffusion
					cobalt	
	Tuonanout				transport	
COBALT	Extracellul				out via	ene RS215
3	ar	Expressed	Expressed	Expressed	antiporter	25 sps_R3213
		2	2	Zinprocess	cobalt	
					transport	
	Transport,				in/out via	
COBALTt	Extracellul				permease	sps_RS020
5	ar	Expressed	Expressed	Expressed	(no H+)	45
					chromate	
	T				transport	
	Transport,				in/out via	ang DS241
CRO4t6	exuacenui	Below	Below	Below	symport	sps_K5241 70
	di .	Delow	Delow	Delow	cytosine	/0
	Transport.				transport	
	Extracellul				via proton	sps RS062
CSNt2	ar	Expressed	Expressed	Expressed	symport	20
	Transport, Extracellul				Copper ABC	
CU2t	ar	Expressed	Expressed	Expressed	transport	Gap
	Transport.	Lipiessed	Lipiessea	2112100000	Copper	Jul
	Extracellul				export via	sps RS100
Cut1	ar	Below	Below	Below	ATPase	10

FE2abc	Extracellul ar	Expressed	Expressed	Expressed	iron (II) transport	sps_RS092 90
DURIt2	Transport, Extracellul ar	Expressed	Expressed	Expressed	ne transport in via proton symport	sps_RS208 90
DIPEPabc 13	Transport, Extracellul ar	Below	Below	Below	Dipeptide transport via ABC system (gly-asp) deoxyuridi	sps_RS091 65 and sps_RS091 75 and sps_RS091 70 and sps_RS091 85 and sps_RS091 80
DIPEPabc 10	Transport, Extracellul ar	Below	Below	Below	Dipeptide transport via ABC system (gly-glu)	sps_RS091 65 and sps_RS091 75 and sps_RS091 70 and sps_RS091 85 and sps_RS091 80
DCYTt2	Transport, Extracellul ar	Expressed	Expressed	Expressed	deoxycytid ine transport in via proton symport	sps_RS208 90
DADNt2	Transport, Extracellul ar	Expressed	Expressed	Expressed	deoxyaden osine transport in via proton symport	sps_RS208 90
D-LACt2	Transport, Extracellul ar	Below	Below	Below	D-lactate transport via proton symport	sps_RS084 80
CYTDt2	Transport, Extracellul ar	Expressed	Expressed	Expressed	cytidine transport in via proton symport	sps_RS208 90

					via ABC	
					system	
					iron (III)	sps_RS224 95 and sps_RS225
	Transport,				transport	00 and
FE3abc	ar	Below	Below	Below	system	o5
FOPt	Transport, Extracellul	Fypressed	Fypressed	Evpressed	formate	sps_RS175
PORt	Transport	Expressed	Expressed	Expressed	fumarate	70
	Extracellul	D -1	D -1	D - 1	via sodium	sps_RS165
FUMIt4_2	ar	Below	Below	Below	symport	80
	Transport,				L- glutamate transport in	sps_RS081 55 or sps_RS243
GLUt2	ar	Expressed	Fypressed	Expressed	symport	sps_R3243
GLOIZ	Transport	Expressed	Lapressed	Lapiessed	Na+/oluta	55
	Extracellul				mate	sps_RS269
GLUt4i	ar	Expressed	Expressed	Expressed	symport	85
	Transport,				betaine-	sps_RS174 45 or sps_RS114 05 or
	Extracellul				sodium	sps_RS097
GLYBt4	ar	Expressed	Expressed	Expressed	symporter	20
	Transport, Extracellul				Glycerol	sps_RS123
GLYC_T	ar	Expressed	Expressed	Expressed	Transport	90
GLYCLTt 2r	Transport, Extracellul ar	Below	Below	Below	glycolate transport via proton symport, reversible	sps_RS084 80
CI VCD+2	Transport, Extracellul	Relow	Balow	Evprogod	D- glycerate transport (proton	sps_RS094
OL I CRIZ	al	DUIUW	DCIUW	Expressed	alveine	0.0
CI V+4	Transport, Extracellul	Evenessed	Evenerad	Eunoaced	reversible transport via sodium	sps_RS243 65 or sps_RS117
UL I 14	ar	Expressed	Expressed	Expressed	symport	ou or

						sps_RS261 65
					Glutathion	sps_RS247
	Transport,				e export	45 and
GTHRDab	Extracellul				via ABC	sps_RS247
c	ar	Below	Below	Below	system	40
					H2O	
	Transport,				transport	
	Extracellul				via	sps_RS123
H2Ot5	ar	Expressed	Expressed	Expressed	Diffusion	90
						sps_RS206
	Transport,					55 or
	Extracellul				mercury	sps_RS206
HGT	ar	Below	Below	Below	transport	50
					homoserin	
	Transport,				e transport	
	Extracellul				via proton	sps_RS173
HOMt2	ar	Below	Below	Below	symport	85
	Transport,				Na+/Isoleu	
	Extracellul				cine-L	sps_RS129
ILEt4	ar	Expressed	Expressed	Expressed	symporter	25
					Indole	
					transport	
	Transport,				via proton	
	Extracellul				symport,	sps_RS013
INDOLEt2	ar	Below	Below	Expressed	reversible	20
						sps_RS003
						45 or
						sps_RS003
					potassium	15 or
					irreversible	sps_RS033
	Transport,				transport	70 or
TT : 01	Extracellul	- 1	D 1	- 1	via proton	sps_RS033
Kt21	ar	Expressed	Expressed	Expressed	symporter	65 DG100
					· .	sps_RS199
					potassium	25 or
	T (transport	sps_RS143
	I ransport,				out via	80 or
V+2		Erranse 1	Emman 1	Exercise 1	proton	sps_KS103
NIJ	ar	Expressed	Expressed	Expressed		90
					L-lactate	
	Tuonoris				reversible	
	Transport,				transport	and DCOOA
		Polow	Palow	Dolow	via proton	sps_K5084
L-LAUIZ	ai	DCIUW	DUIUW	DUIUW	sympon	00

	Transport,				Na+/Leuci	
	Extracellul				ne-L	sps_RS129
LEUt4	ar	Expressed	Expressed	Expressed	symporter	25
					L-lysine	
					transport	
	Transport,				out via	
	Extracellul				proton	sps_RS031
LYSt3	ar	Below	Expressed	Below	antiport	05
					L-	
					Methionin	
	Transport,				e Transport	
MET-	Extracellul				via ABC	
LABC	ar	Expressed	Expressed	Expressed	system	Gap
					magnesiu	
					m transport	
	Transport,				out via	
	Extracellul		_		proton	sps_RS215
MGt3	ar	Expressed	Expressed	Expressed	antiporter	25
					magnesiu	DGOOO
	T (m transport	sps_RS020
	I ransport,				1n/out via	45 or
MOLE	Extracellul	г 1	г 1	г 1	permease	sps_RS256
MGt5	ar	Expressed	Expressed	Expressed	(no H+)	50 DC2(0
	Transmont				Managanaga	sps_KS260
	Transport,		Used Dele	Ugad Dala	Tranganese	43 and
MNaha		Everaged	Useu_Belo	Useu_Belo	r	sps_K5200
Will abe	ai	Expressed	••	••	1	rom RS270
						30 and
					molybdate	sps RS270
	Transport				transport	35 and
	Extracellul	Used Belo	Used Belo	Used Belo	via ABC	sps RS270
MOBDabc	ar	w	w	w	system	40
					sodium	
					transport	sps RS276
	Transport,				out via	30 or
	Extracellul				ABC	sps RS276
NAabcO	ar	Expressed	Below	Below	system	25
						sps_RS063
						05 or
						sps_RS059
					sodium	00 or
					transport	sps_RS124
	Transport,				out via	70 or
	Extracellul				proton	sps_RS138
NAt3	ar	Expressed	Expressed	Expressed	antiport	80

					sodium	
	T				proton	
	I ransport,				(H.N.A. ic	ong DS120
NAt3 2	ar	Expressed	Expressed	Expressed	$(\Pi. NA IS 2)$	25 sps_K3120
	ui	LAPICSSCU	Expressed	LAPICSSCU	sodium	23
					transport	sps RS163
	Transport,				in/out via	90 or
	Extracellul		Used_Belo		calcium	sps_RS255
NAt9	ar	Expressed	W	Expressed	antiport	95
	Transport,					DGOOL
NILL /+	Extracellul	Used_Belo	Used_Belo	Used_Belo	ammonium	sps_RS225
<u>INП4</u> і	ar	W	W	W	ransport	/0
					transport	
	Transport.				in/out via	
	Extracellul				proton	sps RS215
NIt3	ar	Expressed	Expressed	Expressed	antiporter	25
	Transport,					
	Extracellul				NMN	sps_RS076
NMNP	ar	Below	Below	Below	permease	85
	Transport,				••.	D C0 77
NO2T7	Extracellul	Dalary	Dalaw	Dalaw	nitrite	sps_RS0/7
NUS1/	ar	Below	Below	Below		90
	Transport				transport in	
	Extracellul				via	
O2t	ar	Expressed	Expressed	Expressed	diffusion	Diffusion
		-		-		sps_RS109
						15 or
						sps_RS143
						50 or
						sps_RS143
					Acetate	45.01 sps RS113
					transport to	60 or
					periplasm	sps RS243
	Transport,				(ompF,	95 or
	Extracellul				ompC, or	sps_RS117
OMP_AC	ar	Expressed	Expressed	Expressed	oprF)	70
					N-Acetyl-	
					D-	
	Transport				glucosami	
OMP AC	Extracellul				transport to	sps_RS116
GAM	ar	Expressed	Expressed	Expressed	periplasm	50

					Adenosine	
	Transport,				transport to	
OMP_AD	Extracellul				periplasm	sps_RS208
N	ar	Expressed	Expressed	Below	(tsx)	85
						sps_RS109 15 or
						sps_RS143 50 or
						sps_RS143 45 or
					D-Alanine transport to	sps_RS113 60 or
	Transport				periplasm	sps_RS243
OMP_AL	Extracellul	Evpressed	Evpressed	Evpressed	ompC, or	sps_RS117
A-D	al	Expressed	Expressed	Expressed	opir)	sps RS109
						15 or
						sps_RS143
						50 or
						sps_RS143
						45 or
					L-Alanine	sps_RS113
					transport to	60 or
	T (periplasm	sps_RS243
	I ransport,				(ompF,	95 or
A-L	ar	Expressed	Expressed	Expressed	ompC, or oprF)	sps_KS117 70
						sps_RS109
						15 or
						sps_RS143
						50 or
					Τ_	45 or
					Aspartate	sps_RS113
					transport to	60 or
					periplasm	sps RS243
	Transport,				(ompF,	95 or
OMP_ASP	Extracellul				ompC, or	sps_RS117
-L	ar	Expressed	Expressed	Expressed	oprF)	70
	Transport,				cellobiose	
OMP_BG	Extracellul				transport to	sps_RS197
L	ar	Below	Below	Below	periplasm	50
	Transport,				Calcium	sps_RS109
	Extracellul				transport to	15 or
OMP_CA2	ar	Expressed	Expressed	Expressed	periplasm	sps_RS143

					(ompF,	50 or
					ompC, or	sps RS143
					oprF)	45 or
					1 /	sps RS113
						60 or
						sps_RS243
						95 or
						sps_RS117
						70
					Cob(I)ala	
					min	
	Transport,				transport to	
OMP_CB	Extracellul				periplasm	
L1	ar	Expressed	Expressed	Expressed	(btuB)	Gap
	Transport,				chitobiose	
OMP_CHI	Extracellul	F 1	F 1	F 1	transport to	sps_RS116
ТОВ	ar	Expressed	Expressed	Expressed	periplasm	50
						sps_RS109
						15 or
						sps_K5143
						50 or
						sps_KS143
					abolino	$\frac{43.01}{\text{cm}_{\text{c}}} = \mathbf{P} \mathbf{S} 112$
					transport to	sps_K3113
					nerinlasm	sns RS243
	Transport				(ompF	95 or
OMP CH	Extracellul				ompC or	sps RS117
OL_CIT	ar	Expressed	Expressed	Expressed	oprF)	70
					-F)	sps RS109
						15 or
						sps RS143
						50 or
						sps RS143
						45 or
					Chloride	sps_RS113
					transport to	60 or
					periplasm	sps_RS243
	Transport,				(ompF,	95 or
	Extracellul				ompC, or	sps_RS117
OMP_CL	ar	Expressed	Expressed	Expressed	oprF)	70
						sps_RS109
					CO2	15 or
	Transport,				transport to	sps_RS143
	Extracellul				periplasm	50 or
OMP_CO2	ar	Expressed	Expressed	Expressed	(ompF,	sps_RS143
					ompC, or	45 or
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					oprF)	sps_RS113
						60 or
						sps_RS243
						95 or
						70
						sps_RS109
						sps RS143
						50 or
						sps_RS143
						45 or
					Co2+	sps_RS113
					transport to	60 or
	Transport				periplasm (ompE	sps_K5245
OMP CO	Extracellul				ompC or	sns RS117
BALT2	ar	Expressed	Expressed	Expressed	oprF)	70
				-		sps_RS109
						15 or
						sps_RS143 50 or
						sps_RS143
					Cu^{2+}	45 01 sns RS113
					transport to	60 or
					periplasm	sps RS243
	Transport,				(ompF,	95 or
	Extracellul				ompC, or	sps_RS117
OMP_CU2	ar	Expressed	Expressed	Expressed	oprF)	70
	Tronge out				Cytidine	
OMP CV	Extracellul				nerinlasm	sns RS208
TD	ar	Expressed	Expressed	Below	(tsx)	85 85
		1	1		Deoxyaden	-
					osine	
	Transport,				transport to	
OMP_DA	Extracellul			D 1	periplasm	sps_RS208
D-2	ar	Expressed	Expressed	Below	(tsx)	85
	Tronge out				dAMP transport to	
	i ransport.			1	uransport to	
	Extracellul				nerinlasm	sns RS208

					dCMP	
	Transport,				transport to	
OMP_DC	Extracellul				periplasm	sps_RS208
MP	ar	Expressed	Expressed	Below	(tsx)	85
					Deoxycyti	
					dine	
	Transport,				transport to	
OMP_DC	Extracellul				periplasm	sps_RS208
YT	ar	Expressed	Expressed	Below	(tsx)	85
					dGMP	
	Transport,				transport to	
OMP_DG	Extracellul	F 1	- 1	5.1	periplasm	sps_RS208
MP	ar	Expressed	Expressed	Below	(tsx)	85
					Deoxygua	
	T (nosine	
	I ransport,				transport to	D C 200
OMP_DG	Extracellul	E	Emmand	Dalarr	periplasm	sps_K5208
SIN	ar	Expressed	Expressed	Below	(ISX)	03
						sps_KS109
						$r_{\rm SDS} RS143$
						50 or
						sns RS143
					Dimethyl	45 or
					sulfide	sps RS113
					transport to	60 or
					periplasm	sps RS243
	Transport,				(ompF,	95 or
OMP DM	Extracellul				ompC, or	sps RS117
s	ar	Expressed	Expressed	Expressed	oprF)	70
						sps_RS109
						15 or
						sps_RS143
						50 or
						sps_RS143
					Dimethyl	45 or
					sulfoxide	sps_RS113
					transport to	60 or
	Turn f				periplasm	sps_RS243
	I ransport,				(ompF,	95 Or
SO DMP_DM	Extracellul	Evenessed	Expressed	Expressed	ompC, or	sps_K511/
30	ar	Expressed	Expressed	Expressed	Oprr)	/U
	Transport				Douecanol	$\frac{\text{sps}_{\text{KS102}}}{00 \text{ or}}$
OMP DO	Extracellul				transport to	sne RSU88
	ar	Fynressed	Fypressed	Fypressed	nerinlasm	35_10000
DUA	นา	LAPICSSCU	Tubicosca	LAPICSSCU	Perphasin	55

					dTMP	
	Transport,				transport to	
OMP_DT	Extracellul				periplasm	sps_RS208
MP	ar	Expressed	Expressed	Below	(tsx)	85
					Deoxyuridi	
					ne	
	Transport,				transport to	
OMP_DU	Extracellul				periplasm	sps_RS208
RI	ar	Expressed	Expressed	Below	(tsx)	85
						sps_RS109
						15 or
						sps_RS143
						50 or
						sps_RS143
					E-2	45 or
					rez+	sps_KS115
					nerinlasm	sps RS2/3
	Transport				(ompF	95 or
	Extracellul				ompC, or	sps_RS117
OMP FE2	ar	Expressed	Expressed	Expressed	oprF)	70
					-F)	sps RS109
						15 or
						sps_RS143
						50 or
						sps_RS143
						45 or
					Formate	sps_RS113
					transport to	60 or
	-				periplasm	sps_RS243
	Transport,				(ompF,	95 or
OMP_FO	Extracellul	F 1	F 1	F 1	ompC, or	sps_RS117
ĸ	ar	Expressed	Expressed	Expressed	oprr)	/U
						sps_K5109
						$\frac{1501}{\text{sps}} RS1/12$
						50 or
						sps_RS143
						45 or
					Fumarate	sps RS113
					transport to	60 or
					periplasm	sps_RS243
	Transport,				(ompF,	95 or
OMP_FU	Extracellul				ompC, or	sps_RS117
M	ar	Expressed	Expressed	Expressed	oprF)	70

					D-	
					Galactose	
	Transport,				transport to	
OMP_GA	Extracellul				periplasm	sps_RS073
L	ar	Below	Below	Below	(oprB)	70
					Galactan	
	Transport,				transport to	
OMP_GA	Extracellul				periplasm	sps_RS073
LTAN	ar	Below	Below	Below	(oprB)	70
					D-Glucose	
	Transport,				transport to	
OMP_GL	Extracellul				periplasm	sps_RS073
C-D	ar	Below	Below	Below	(oprB)	70
						sps_RS109
						15 or
						sps_RS143
						50 or
					_	sps_RS143
					L-	45 or
					Glutamate	sps_RS113
					transport to	60 or
	T (periplasm	sps_RS243
	I ransport,				(ompF,	95 or
UMP_GL	Extracellul	Evenessed	Evenessed	Evenegad	ompC, or	sps_KS11/
U-L	ai	Expressed	Expressed	Expressed	opir)	70 smg PS100
						$\frac{\text{sps}_\text{K3109}}{15 \text{ or}}$
						sns RS143
						50 or
						sps RS143
						45 or
					Glycine	sps RS113
					transport to	60 or
					periplasm	sps RS243
	Transport,				(ompF,	95 or
OMP GL	Extracellul				ompC, or	sps RS117
Y _	ar	Expressed	Expressed	Expressed	oprF)	70
						sps_RS109
					glycyl-L-	15 or
					aspartic	sps_RS143
					acid	50 or
					transport to	sps_RS143
					periplasm	45 or
	Transport,				(ompF,	sps_RS113
OMP_GL	Extracellul				ompC, or	60 or
Y-ASP-L	ar	Expressed	Expressed	Expressed	oprF)	sps_RS243

						95 or
						sps_RS117 70
						sps_RS109 15 or
						sps_RS143 50 or
					glycyl-L- glutamic	sps_RS143 45 or
					acid	sps_RS113
	Transport.				periplasm	sps_RS243 95 or
OMP_GL Y-GLU-L	Extracellul ar	Expressed	Expressed	Expressed	ompC, or oprF)	sps_RS117 70
						sps_RS109
						sps_RS143 50 or
					Glucina	sps_RS143
					betaine	sps_RS113
					transport to periplasm	60 or sps_RS243
	Transport,				(ompF,	95 or
OMP_GL YB	ar	Expressed	Expressed	Expressed	ompC, or oprF)	sps_RS11/ 70
	Transport.				Glycerol transport to	
OMP_GL	Extracellul	Dalary	Deleve	Dalarry	periplasm	sps_RS073
<u>rc</u>	ar	Below	Below	Below	(OprB) (R)-	/0
	Transport				Glycerate	
OMP_GL	Extracellul				periplasm	sps_RS073
YC-R	ar	Below	Below	Below	(oprB)	70
						sps_KS109 15 or
						sps_RS143 50 or
					Glycolate	sps_RS143
					periplasm	sps_RS113
	Transport,				(ompF,	60 or
OMP_GL	Extracellul	Expressed	Expressed	Expressed	ompC, or oprF)	sps_RS243 95 or

	1	1		1	1	1
						sps_RS117 70
						sps_RS109 15 or
						sps_RS143 50 or
						sps_RS143
					Reduced	45 or
					transport to	sps_KS113
					periplasm	sps RS243
	Transport,				(ompF,	95 or
OMP_GT	Extracellul	E	E	E	ompC, or	sps_RS117
ΠΚD	ar	Expressed	Expressed	Expressed	oprr)	70 sps_RS109
						15 or
						sps_RS143
						50 or sps RS143
						45 or
					H+	sps_RS113
					transport to	60 or
	Transport,				(ompF,	95 or
	Extracellul				ompC, or	sps_RS117
OMP_H	ar	Expressed	Expressed	Expressed	oprF)	70
						15 or
						sps_RS143
						50 or
						sps_KS143 45 or
					H2	sps_RS113
					transport to	60 or
	Transport				periplasm (ompF	sps_K5243 95 or
	Extracellul				ompC, or	sps_RS117
OMP_H2	ar	Expressed	Expressed	Expressed	oprF)	70
						sps_RS109
					H2O	sps RS143
					transport to	50 or
	Tuonerset				periplasm	sps_RS143
OMP H2	Extracellul				(ompF, ompC, or	45 or sps RS113
0	ar	Expressed	Expressed	Expressed	oprF)	60 or

						sps_RS243 95 or
						sps_RS117 70 or
						sps_RS089 35
						sps_RS109
						sps_RS143
						50 or sps_RS143
					Hydrogen	45 or
					transport to	sps_KS115 60 or
	T (periplasm	sps_RS243
OMP H2	Transport, Extracellul				(ompF, ompC, or	95 or sps RS117
02	ar	Expressed	Expressed	Expressed	oprF)	70
						sps_RS109 15 or
						sps_RS143
						50 or sps RS143
					Hydrogen	45 or
					sulfide	sps_RS113
					periplasm	sps_RS243
	Transport,				(ompF,	95 or
OMP H2S	ar	Expressed	Expressed	Expressed	ompC, or oprF)	sps_KS117 70
			4		hexadecan	
	Transport				oate $(n-C16.0)$	sps_RS162
OMP_HD	Extracellul				transport to	sps_RS088
CA	ar	Expressed	Expressed	Expressed	periplasm	35 DC100
						sps_KS109 15 or
					L-	sps_RS143 50 or
					Isoleucine	sps_RS143
					transport to	45 or sns RS112
	Transport,				(ompF,	60 or
OMP_ILE-	Extracellul	Emer 1	Erre 1	Emeral 1	ompC, or	sps_RS243
L	ar	Expressed	Expressed	Expressed	oprr)	93 or

						sps_RS117 70
						sps_RS109 15 or
						sps_RS143 50 or
						sps_RS143 45 or
					Indole	sps_RS113
					periplasm	sps RS243
	Transport,				(ompF,	95 or
OMP_IND OLE	Extracellul	Expressed	Expressed	Expressed	ompC, or oprF)	sps_RS117 70
				2	-p)	sps_RS109
						15 or sps RS143
					myo-	50 or
					Inositol	sps_RS143
					sphate	sps RS113
					transport to	60 or
	Transport.				(ompF.	sps_RS243 95 or
OMP_INO	Extracellul	-	- 1	- 1	ompC, or	sps_RS117
SHP	ar	Expressed	Expressed	Expressed	oprF)	70 sps_RS109
						15 or
						sps_RS143 50 or
					10	sps_RS143
					1D-myo- inositol 1	45 or sps RS113
					transport to	60 or
	Transport				periplasm (ompF	sps_RS243 95 or
OMP_INO	Extracellul				ompC, or	sps_RS117
SPP1	ar	Expressed	Expressed	Expressed	oprF)	70
						sps_K5109 15 or
					K+	sps_RS143
					transport to	50 or sps RS143
	Transport,				(ompF,	45 or
OMP V	Extracellul	Expressed	Evpressed	Evpressed	ompC, or	sps_RS113
	aı	LAPICSSCU	DAPIESSEU	LAPICSSCU	opri j	10.00

						sps_RS243 95 or
						sps_RS117 70
						sps_RS109 15 or
						sps_RS143 50 or
						sps_RS143 45 or
					D-Lactate transport to	sps_RS113 60 or
	Transport.				periplasm (ompF.	sps_RS243 95 or
OMP_LA C-D	Extracellul ar	Expressed	Expressed	Expressed	ompC, or oprF)	sps_RS117 70
		1	1	1	1 /	sps_RS109
						15 or sps RS143
						50 or
						sps_RS143 45 or
					L-Lactate	sps RS113
					transport to	60 or
	-				periplasm	sps_RS243
	Transport,				(ompF,	95 or
C-L	ar	Expressed	Expressed	Expressed	ompC, or oprF)	sps_KS117 70
						sps_RS109
						15 or
						50 or
						sps_RS143
						45 or
					L-Leucine	sps_RS113
					transport to	60 or
	Transport				(ompF	sps_K5245 95 or
OMP LE	Extracellul				ompC, or	sps RS117
U-L	ar	Expressed	Expressed	Expressed	oprF)	70
					L-Lysine	sps_RS109
					transport to	15 or
	Trace				periplasm	sps_RS143
OMPIVS	Transport, Extracellul				(ompr,	SU OF
-L	ar	Expressed	Expressed	Expressed	oprF)	45 or

	1	1	1			
						sps_RS113
						60 or
						sps_K5243
						$\frac{9501}{\text{sps}}$
						70
						sps_RS109
						15 or
						sps_KS143
						$\frac{3000}{\text{spc}} \text{PS}1/3$
						45 or
					L-Malate	sns RS113
					transport to	60 or
					periplasm	sps RS243
	Transport,				(ompF,	95 or
OMP MA	Extracellul				ompC, or	sps RS117
L-L	ar	Expressed	Expressed	Expressed	oprF)	70
					Maltose	
					transport to	
	Transport,				periplasm	
OMP_MA	Extracellul	_		_	(lamB or	sps_RS034
LT	ar	Below	Below	Below	ompMal2)	85
					Maltohepta	
					ose	
	Transport				transport to	
OMP MA	Extracellul				(lamB or	sps RS034
	ar	Below	Below	Below	(lallib of ompMal2)	sps_13054
LIII	u	Delow	Delow	Delow	Maltotetra	
					ose	
					transport to	
	Transport,				periplasm	
OMP_MA	Extracellul				(lamB or	sps_RS034
LTTTR	ar	Below	Below	Below	ompMal2)	85
						sps_RS109
						15 or
					L-	sps_RS143
					Methionin	50 or
					e transport	sps_KS143
					10	43 OF
	Transport				(omp ^E	sps_KS113
OMP ME	Extracellul				ompC or	$\frac{10001}{\text{sps}}$
T-L	ar	Expressed	Expressed	Expressed	oprF)	95 or
					- r - /	

						sps_RS117 70
						sps_RS109 15 or
						sps_RS143 50 or
						sps_RS143 45 or
					Mg	sps_RS113
					transport to	60 or
	Transport,				periplasm (ompF,	sps_RS243 95 or
OMP_MG 2	Extracellul ar	Expressed	Expressed	Expressed	ompC, or oprF)	sps_RS117 70
						sps_RS109
						15 or
						sps_KS143
						sps RS143
						45 or
					Mn2+	sps_RS113
					transport to	60 or
	Transport				(ompF	sps_K5245 95 or
OMP MN	Extracellul				ompC, or	sps RS117
2 _	ar	Expressed	Expressed	Expressed	oprF)	70
						sps_RS109 15 or
						sps_RS143 50 or
						sps_RS143 45 or
					Molybdate	sps_RS113
					transport to	60 or
	Transport,				periplasm (ompF,	sps_RS243 95 or
OMP_MO	Extracellul	D 1	D 1		ompC, or	sps_RS117
BD	ar	Expressed	Expressed	Expressed	oprF)	70
						sps_K5109
					Sodium	sps RS143
					transport to	50 or
	-				periplasm	sps_RS143
	Transport,				(ompF,	45 or
OMD mal		Evpressed	Evpressed	Expressed	ompC, or	sps_K5113
UNVER DAL						

						sps_RS243 95 or
						sps_RS117 70
						sps_RS109 15 or
						sps_RS143 50 or
					Ammoniu	sps_RS143 45 or
					m transport to	sps_RS113 60 or
	Transport				periplasm	sps_RS243
OMP_NH	Extracellul	Emmand	E	Emmand	ompC, or	sps_RS117
4	ar	Expressed	Expressed	Expressed	oprr)	/U
						sps_RS109
						13 or
						50 or
						sps RS143
						45 or
					NMN	sps RS113
					transport to	60 or
					periplasm	sps_RS243
	Transport,				(ompF,	95 or
OMP_NM N	Extracellul ar	Expressed	Expressed	Expressed	ompC, or oprF)	sps_RS117 70
						sps_RS109
						15 or
						sps_RS143
						50 or
						sps_K5143
					Nitrite	$\frac{4501}{\text{sps}}$
					transport to	60 or
					periplasm	sps RS243
	Transport.				(ompF.	95 or
OMP NO	Extracellul				ompC, or	sps RS117
2	ar	Expressed	Expressed	Expressed	oprF)	70
					Nitrate	sps_RS109
					transport to	15 or
					periplasm	sps_RS143
	Transport,				(ompF,	50 or
OMP_NO	Extracellul		-		ompC, or	sps_RS143
3	ar	Expressed	Expressed	Expressed	oprF)	45 or

						sps_RS113 60 or
						sps_RS243 95 or
						sps_RS117 70
						sps_RS109 15 or
						sps_RS143 50 or
						sps_RS143 45 or
					O2 transport to	sps_RS113
	_				periplasm	sps_RS243
	Transport, Extracellul				(ompF, ompC, or	95 or sps RS117
OMP_O2	ar	Expressed	Expressed	Expressed	oprF)	70
					octadecano	DC1(2
	Transport				ate $(n - C_1 \otimes 0)$	sps_KS162
OMP OC	Extracellul				transport to	SDS R SO88
DCA	ar	Expressed	Expressed	Expressed	periplasm	35 35
			_		Phosphate	
	Transport,				transport to	
OMP PI	Extracellul ar	Used_Belo w	Used_Belo w	Used_Belo w	periplasm (oprP)	sps_RS217 85
						sps_RS109
						sps RS143
						50 or
						sps_RS143
					Pimeloyl-	45 or
					CoA	sps_RS113
					transport to	60 or
	Transport.				(ompF.	95 or
OMP PM	Extracellul				ompC, or	sps RS117
COA	ar	Expressed	Expressed	Expressed	oprF)	70
					D	sps_RS109
					Propionate	15 or
					nerinlasm	sps_K5143
	Transport.				(ompF.	sps RS143
	Extracellul				ompC, or	45 or
OMP_PPA	ar	Expressed	Expressed	Expressed	oprF)	sps_RS113

OMP_SER -L	Transport, Extracellul ar	Expressed	Expressed	Expressed	L-Serine transport to periplasm (ompF,	sps_RS109 15 or sps_RS143 50 or sps_RS143
OMP_PY R	Transport, Extracellul ar	Expressed	Expressed	Expressed	Pyruvate transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP_PTR C	Transport, Extracellul ar	Expressed	Expressed	Expressed	Putrescine transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP_PR O-L	Transport, Extracellul ar	Expressed	Expressed	Expressed	L-Proline transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
						60 or sps_RS243 95 or sps_RS117 70

					ompC, or oprF)	45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP SO3	Transport, Extracellul ar	Expressed	Expressed	Expressed	Sulfite transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP SO4	Transport, Extracellul ar	Expressed	Expressed	Expressed	Sulfate transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP_SU CC	Transport, Extracellul ar	Expressed	Expressed	Expressed	Succinate transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP_TH R-L	Transport, Extracellul ar	Expressed	Expressed	Expressed	L- Threonine transport to	sps_RS109 15 or sps_RS143

					periplasm (ompF, ompC, or oprF)	50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP_TH YMD	Transport, Extracellul ar	Expressed	Expressed	Below	transport to periplasm (tsx)	sps_RS208 85
OMP_TM A	Transport, Extracellul ar	Expressed	Expressed	Expressed	Trimethyla mine transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP_TM AO	Transport, Extracellul ar	Expressed	Expressed	Expressed	Trimethyla mine N- oxide transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP_TRP -L	Transport, Extracellul ar	Expressed	Expressed	Expressed	L- Tryptopha n transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243

						95 or
						sps_RS117 70
						sps_RS109 15 or
						sps_RS143 50 or
						sps_RS143 45 or
					Thiosulfate transport to	sps_RS113 60 or
	Transport,				periplasm (ompF,	sps_RS243 95 or
OMP_TSU L	Extracellul ar	Expressed	Expressed	Expressed	ompC, or oprF)	sps_RS117 70
		1	1	1	tetradecan	
					oate	sps_RS162
	Transport,				(C14:0)	00 or
OMP_TT DCA	Extracellul	Everaged	Everaged	Everaged	transport to	sps_RS088
DCA	ai	Expressed	Expressed	Expressed	peripiasin	SS
						15 or
						sps_RS143 50 or
					tetrathionat	sps_RS143
					e transport	sps RS113
					to	60 or
					periplasm	sps_RS243
	Transport,				(ompF,	95 or
OMP_TTT	Extracellul				ompC, or	sps_RS117
NT	ar	Expressed	Expressed	Expressed	oprF)	70
						sps_RS109
						sps RS143
						50 or
						sps RS143
						45 or
					L-Tyrosine	sps_RS113
					transport to	60 or
	-				periplasm	sps_RS243
	Transport,				(ompF,	95 or
	Extracellul	Evenessed	Evenessed	Evenessed	ompC, or $omrE$	sps_KS117
K-L	ar	Expressed	Expressed	Expressed	оргг)	/0

OMP_UR A	Transport, Extracellul ar	Expressed	Expressed	Expressed	Uracil transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP_UR EA	Transport, Extracellul ar	Expressed	Expressed	Expressed	Urea transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP URI	Transport, Extracellul ar	Expressed	Expressed	Below	Uridine transport to periplasm (tsx)	sps_RS208 85
OMP_VA L-L	Transport, Extracellul ar	Expressed	Expressed	Expressed	L-Valine transport to periplasm (ompF, ompC, or oprF)	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP_XA	Transport, Extracellul	Engeneral 1	English 1	Deleve	Xanthine transport to periplasm	sps_RS208
1N	ar	Expressed	Expressed	Delow	(ISX)	03

PTRCabc	ar	Below	Below	Below	system	70 and
	Transport, Extracellul				transport via ABC	75 and sps_RS125
	-	<u>F - 222 - 3</u>	<u>r</u> 222 2 4		putrescine	sps RS125
PROt4	Extracellul ar	Expressed	Expressed	Expressed	via sodium symport	sps_KS088 30
	Transport,				L-proline	DCOOC
PPAtNa	ar	Expressed	Expressed	Expressed	r r	30
	Transport, Extracellul				Propionate Transporte	sns RS088
PMCOAt	ar	Expressed	Expressed	Expressed	Transport	Gap
	Transport, Extracellul				Pimeloyl- CoA	
PIt6	ar	Expressed	Expressed	Expressed	symporter	sps_K524/ 20
	Transport,				phosphate transport in/out via	cpc DS247
PIabc	Extracellul ar	Expressed	Below	Below	and swp_5140)	sps_RS277 65)
	Transport,				phosphate transport via ABC system and swp_5141 and	900 and sps_RS097 35 and sps_RS097 30 and sps_RS097 40) or (sps_RS27 780 and sps_RS277 75 and sps_RS277 70 and sps_RS277
PHNabc	ar	Below	Below	Below	system	80 (sps_RS10
	Transport, Extracellul				phosphona te transport via ABC	85 and sps_RS020 90 and sps_RS020
	ai	Expressed	Expressed	Delow	Via ADC	sps_RS020
PHEMEab	Transport, Extracellul	Fypressed	Fypressed	Below	Protoheme transport via ABC	sps_RS019 60 and sps_RS019 45
						sps_RS019 55 and

						65 and
						sps_RS125 60
DVD+2	Transport, Extracellul	Evenessed	Eveneed	Evenessed	pyruvate reversible transport via proton	Can
PYRI2	ar	Expressed	Expressed	Expressed	symport	sps_RS135
RIBabc	Transport, Extracellul ar	Below	Below	Expressed	D-Ribose transport via ABC	35 and sps_RS135 45 and sps_RS135 40
SFRt4	Transport, Extracellul ar	Expressed	Expressed	Expressed	serine/thre onine:Na+ symporter, SstT	sps_RS179
SERI	a	Expressed	Expressed	Expressed	L-serine	00
SED+4	Transport, Extracellul	Everaged	Everaged	Everaged	transport in/out via proton	sps_RS130
SERIO	ar	Expressed	Expressed	Expressed	sulfate	33
SO4t2	Transport, Extracellul ar	Used_Belo w	Used_Belo w	Used_Belo w	transport in via proton symport	sps_RS067 65
SUCC _t 4	Transport, Extracellul	Below	Below	Below	succinate via sodium	sps_RS165
SUCCtex	Transport, Extracellul ar	Expressed	Expressed	Expressed	Succinate	Gap
THMabc	Transport, Extracellul ar	Below	Below	Below	thiamin transport via ABC system	sps_RS076 85
THMDt2	Transport, Extracellul ar	Expressed	Expressed	Expressed	thymidine transport in via proton symport	sps_RS208 90
THRHT	Transport, Extracellul ar	Below	Used_Belo w	Used_Belo w	L- Threonine Transport	sps_RS173 85

					L-	
					threonine	
					transport	
	Transport,				out via	
	Extracellul			_	proton	sps_RS021
THRt3	ar	Expressed	Below	Expressed	antiport	25
	-				serine/thre	
	Transport,				onine:Na+	DC170
	Extracellul	F 1	F 1	F 1	symporter,	sps_RS179
IHKt4	ar	Expressed	Expressed	Expressed	SSU I	00
					L-	
					transport	cmc DS012
	Transport				in/out via	sps_K3013
	Extracellul				nroton	2001 sps RS140
TR Pt6	ar	Below	Expressed	Expressed	symport	05
		Delow	LAPICODE	Lapresseu	L-tyrosine	
					transport	
	Transport,				in/out via	
	Extracellul				proton	sps RS140
TYRt6	ar	Below	Expressed	Expressed	symport	05
			-	_		sps RS030
					uracil	55 or
					transport	sps_RS211
	Transport,				in/out via	20 or
	Extracellul				proton	sps_RS207
URAt6	ar	Expressed	Expressed	Expressed	symport	30
	Transport,					
	Extracellul				Urea	
UreaExp	ar	Expressed	Expressed	Expressed	Diffusion	Diffusion
					uridine	
	Transport,				transport in	
	Extracellul			_	via proton	sps_RS208
URIt2	ar	Expressed	Expressed	Expressed	symport	90
	Transport,				Na+/Valin	D.G.1.00
TTATIA	Extracellul	 1	D 1	D 1	e-L	sps_RS129
VALt4	ar	Expressed	Expressed	Expressed	symporter	25
						sps_RS008
						55 and
	Transport					sps_K5008
	Fytracellul				tungstata	SU allu
WO4aba	ar	Fypresod	Expressed	Expressed	transportor	sps_150008 15
W Utabl	al Transport	Expressed	Expressed	Expressed	Vanthing	SDG DC211
	Extracellul				Transporte	3ps_15211 20 or
XANt	ar	Fynressed	Fynressed	Expressed	r	$rac{2001}{sns}$ RS207
2 3 2 3 1 1 1	41	LAPICSSCU	L'UNPICOSCU	LAPICSSCU	1	3P3_10207

						30 or
						sps_RS030 55
	Tyrosine,					
	Tryptopha				anthranilat	
	n, and Phenylalan				e	
	ine				phosphorib	
	Metabolis				osyltransfe	sps_RS082
ANPRT	m The state of the	Expressed	Expressed	Expressed	rase	90
	Tyrosine, Tryptopha					
	n, and					
	Phenylalan					sps_RS082
	ine					80 and
ANG 1	Metabolis	E	E	Emmand	anthranilat	sps_RS082
ANSI	m Tyrosine	Expressed	Expressed	Expressed	e synthase	83
	Tryptopha					
	n, and					
	Phenylalan					sps_RS118
	ine Metabolis				chorismate	60 and
CHORM	m	Expressed	Expressed	Expressed	mutase	85
	Tyrosine,		1	L		
	Tryptopha					
	n, and					
	ine					
	Metabolis				chorismate	sps RS087
CHORS	m	Expressed	Expressed	Expressed	synthase	40
						sps_RS118
	Tyrosine,				2 doory	60 or
	n, and				D-arabino-	sps_K5225 45 or
	Phenylalan				heptuloson	sps_RS026
	ine				ate 7-	15 or
DAUDO	Metabolis	F 1	F 1	F 1	phosphate	sps_RS118
DAHPS	m Tyrosine	Expressed	Expressed	Expressed	synthetase	90
	Tryptopha					
	n, and				3-	
	Phenylalan				dehydroqui	
	ine Motobalia		Hand D-1		nate	ang DC140
DHOD1	m	Expressed	w	Expressed	e	sps_K5149 35
2		- Pressed	l • •		<u> </u>	~~

	Tyrosine,					
	Tryptopha					
	n, and					
	Phenylalan				3-	
	ine				dehydroqui	
	Metabolis				nate	sps RS266
DHQS	m	Expressed	Expressed	Expressed	synthase	25
	Tyrosine,					
	Tryptopha					
	n, and					
	Phenylalan					
	ine					
	Metabolis				fumarylace	sps RS180
FUMACA	m	Expressed	Expressed	Expressed	toacetase	55
	Tyrosine,		A			
	Tryptopha				4-	
	n. and				hvdroxvph	
	Phenvlalan				envlpvruva	
	ine				te	
	Metabolis				dioxygenas	sps RS070
HPPDO1	m	Expressed	Below	Below	e	40
	Tvrosine.	I				
	Tryptopha					
	n. and					
	Phenylalan				indole-3-	
	ine				glycerol-	
	Metabolis				phosphate	sps RS082
IGPS	m	Expressed	Expressed	Expressed	synthase	95
	Tyrosine,	1	1	1		
	Tryptopha					
	n, and					
	Phenylalan					
	ine				maleylacet	
	Metabolis				oacetate	sps RS180
MLACI	m	Expressed	Below	Below	isomerase	50
	Tyrosine,	-				
	Tryptopha					
	n, and					
	Phenylalan				phenylalan	
	ine				ine 4-	
	Metabolis				monooxyg	sps RS180
PHE4MO	m	Expressed	Below	Below	enase	70
	Tyrosine,	-			phenylalan	
	Tryptopha				ine	
	n, and				ammonia-	sps RS164
PHEAL	Phenylalan	Expressed	Expressed	Expressed	lyase	60

indindindindindTyposine, Tryptopha n, andrandrandrandrandPhenylalan inemeransaminasps_RS044MetabolismExpressedExpressedexpressedPHETA1Tyrosine, Tryptopha n, andTyrosine, Tryptopha n, andsps_RS039PHETR5MetabolisExpressedExpressedExpressedPHETR5mExpressedExpressedsps_RS065PHETR5mExpressedExpressedExpressedsps_RS065PHETR5n, and phenylalan ineExpressedExpressedExpressedsps_RS065PHETR5mExpressedExpressedExpressedsps_RS065Phenylalan ineExpressedExpressedExpressedsps_RS065PHETR5mExpressedExpressedExpressedsps_RS065mExpressedExpressedExpressedExpressedsps_RS065Phenylalan ineExpressedExpressedExpressedsps_RS065Metabolis ineExpressedExpressedExpressedsps_RS065Phenylan ineExpressedExpressedExpressedsps_RS065Phenylan ineExpressedExpressedExpressedsps_RS065Phenylan ineExpressedExpressedExpressedsps_RS065Phenylan ineExpressedExpressedExpressedsps_RS065Phenylan ineExpressedExpressedEx		ine Metabolis					
Tyrosine, Tryptopha n, andTyrosine, Tryptopha 		m					
Tryptopha n, and Phenylalan inerryptopha n, and Phenylalan inephenylalan phenylalan inesps_RS044 90 or transamina sps_RS039PHETA1mExpressedExpressedExpressedse90Tyrosine, Tryptopha n, and Phenylalan ineTyrosine, Phenylalan inesps_RS065 60 and sps_RS065sps_RS065 60 and sps_RS065PHETRSmExpressedExpressedExpressedsps_RS065 (60 and sps_RS065PHETRSmExpressedExpressedsynthetase55PHETRSn, and Phenylalan n, and PhenylalanFigure 100 (100 (100 (100 (100 (100 (100 (100		Tyrosine,					
n, and Phenylalan inen, and Phenylalan inephenylalan sps_RS044 inesps_RS044 90 or transaminaPHETA1mExpressedExpressedExpressedse90PHETA1mExpressedExpressedExpressedse90PHETA1mExpressedExpressedExpressedse90PHETA1mExpressedExpressedse90PHETA1mExpressedExpressedse90PHETA1mExpressedExpressedse90PHETA1mExpressedExpressedse90PHETA1mExpressedExpressedse90PHETA1FrequenciesFrequenciesse90PHETA1FrequenciesFrequenciesse90PHETA1FrequenciesFrequenciessesePhenylalanFrequenciesFrequenciessesePHETRSmExpressedExpressedExpressedsePHETRSmExpressedExpressedsesePHETRSmExpressedExpressedsesePHETRSmExpressedExpressedsesePHETRSmExpressedExpressedsesePHETRSFrequenciesFrequenciessesesePHETRSFrequenciesFrequenciessesesePHETRSFrequenciesFrequenciesse		Tryptopha					
Phenylalan inespensylalan inesps_RS044 ineMetabolisMetabolisExpressedExpressedinePHETA1mExpressedExpressedExpressedseTyrosine, Tryptopha n, and Phenylalan ineTryptopha inesps_RS065 inesps_RS065 inePHETRSmExpressedExpressedExpressedsps_RS065 inePHETRSmExpressedExpressedExpressedsps_RS065 inePHETRSmExpressedExpressedExpressedsps_RS065 inePHETRSmExpressedExpressedExpressedsps_RS065 inePhenylalan ine ineineinesps_RS065 inesps_RS065 inePHETRSmExpressedExpressedExpressedsps_lencePHETRSmExpressedinesps_lencesps_lencePHETRSmExpressedinesps_lencesps_lencePHETRSmExpressedinesps_lencesps_lencePhenylalan in, and PhenylalanineineineinePhenylalanineineineineinePHETRSmExpressedineineinePhenylanineineineineinePhenylanineineineineinePhenylanineineineineinePhenylanineineineineine <td></td> <td>n, and</td> <td></td> <td></td> <td></td> <td></td> <td>D C 0 4 4</td>		n, and					D C 0 4 4
Ine Metabolis90 or transaminaPHETA1mExpressedExpressedExpressedse90Tyrosine, Tryptopha n, andTryptopha n, andFree State Phenylalan ineFree State Phenylalan ineFree State Phenylalan sps_RS065Se90PHETRSMExpressedExpressedExpressedSe90PHETRSMExpressedExpressedSe90PHETRSMExpressedExpressedSps_RS065PHETRSMExpressedExpressedSps_RS065Phenylalan n, and PhenylalanFree State Free StateSps_RS065Phenylalan n, and PhenylalanFree State Free StateSps_RS065PHETRSMExpressedExpressedSps_RS065State Free StateFree State Free StateSps_RS065Sps_RS065PHETRSMExpressedExpressedSps_RS065State Free StateFree State Free StateSps_RS065Sps_RS065State Free StateFree State Free StateState Free StateState <b< td=""><td></td><td>Phenylalan</td><td></td><td></td><td></td><td>phenylalan</td><td>sps_RS044</td></b<>		Phenylalan				phenylalan	sps_RS044
PHETA1mExpressedExpressedExpressedExpressedse90Tyrosine, Tryptopha n, and Phenylalan ineTryptopha phenylalan Metabolis <td< td=""><td></td><td>Metabolis</td><td></td><td></td><td></td><td>transamina</td><td>90.0r</td></td<>		Metabolis				transamina	90.0r
THETHYInExpressedExpressedExpressedExpressed50Tyrosine, Tryptopha n, and Phenylalan ineTryptopha inesps_RS065sps_RS065PHETRSmExpressedExpressedExpressedsynthetasePHETRSmExpressedExpressedSynthetase55Tyrosine, Tryptopha n, and PhenylalanTyrosine, Tryptopha n, and PhenylalanFunctional synthetase55	PHFTA1	m	Fypressed	Expressed	Expressed	se	sps_K3039
PHETRSTyrosine, Tryptopha n, and Phenylalan ineExpressedExpressedExpressedExpressedsps_RS065 synthetasePHETRSmExpressedExpressedExpressedsynthetase55Tyrosine, Tryptopha n, and PhenylalanTryptopha n, and Phenylalanineineine		Tyrosine	LAPICSSCU	LAPICSSCU	LAPICSSCU	30	70
PHETRSTypopha n, and Phenylalan ine MetabolisExpressedExpressedExpressedsps_RS065 phenylalan yl-tRNAPHETRSmExpressedExpressedExpressedsynthetaseTyrosine, Tryptopha n, and Phenylalanfor the second seco		Tryptopha					
Phenylalan ine MetabolisPhenylalan ine Metabolissps_RS065 60 and sps_RS065PHETRSmExpressedExpressedExpressedSps_RS065 synthetaseTyrosine, Tryptopha n, and PhenylalanTryptopha h, and PhenylalanImage: Comparison of the synthetaseSps_RS065 synthetase		n. and					
PHETRSImage: Normal ine ine Metabolis mExpressedExpressedExpressedPhenylalan60 and sps_RS065 synthetasePHETRSmExpressedExpressedExpressedSynthetase55Tyrosine, Tryptopha n, and Phenylalann, and PhenylalanImage: Normal information		Phenylalan					sps RS065
PHETRSMetabolis mExpressedExpressedExpressedyl-tRNA synthetasesps_RS065 55Tyrosine, Tryptopha n, and PhenylalanTyrosine, in and in any in an antipactorial participactorial participactorial in an antipactorial participactorial participactorial in an antipactorial participactorial participactorial in an antipactorial participactorial participactorial participactorial in an antipactorial participactorial participactorial participactorial in an antipactorial participactorial parti		ine				Phenylalan	60 and
PHETRSmExpressedExpressedExpressedsynthetase55Tyrosine, Tryptopha n, and Phenylalan		Metabolis				yl-tRNA	sps RS065
Tyrosine, Tryptopha n, and Phenylalan	PHETRS	m	Expressed	Expressed	Expressed	synthetase	55
Tryptopha n, and Phenylalan		Tyrosine,					
n, and Phenylalan		Tryptopha					
Phenylalan		n, and					
		Phenylalan					
ine prephenate		ine				prephenate	D C110
Metabolis dehydroge sps_RS118		Metabolis	F 1	F 1	г 1	dehydroge	sps_RS118
PPND m Expressed Expressed Expressed nase 85	PPND	m T ·	Expressed	Expressed	Expressed	nase	85
Tyrosine,		Tyrosine,					
n and		n and					
Phenylalan		n, and Phenylalan					
ine prephenate		ine				prephenate	
Metabolis dehvdratas sps RS118		Metabolis				dehydratas	sps_RS118
PPNDH m Expressed Expressed Expressed e 60	PPNDH	m	Expressed	Expressed	Expressed	e	60
Tyrosine,		Tyrosine,	1	1	1		
Tryptopha phosphorib		Tryptopha				phosphorib	
n, and osylanthra		n, and				osylanthra	
Phenylalan nilate		Phenylalan				nilate	
ine isomerase		ine				isomerase	
Metabolis (irreversibl sps_RS082		Metabolis				(irreversibl	sps_RS082
PRAIi m Expressed Expressed e) 95	PRAIi	m	Expressed	Expressed	Expressed	e)	95
Tyrosine,		Tyrosine,					
Iryptopha 3-		Tryptopha				3-	
n, and phosphoshi		n, and \mathbf{D}_{1}				phosphoshi	
rnenylalan Kimate I-		rnenylalan				kimate 1-	
Metabolis vitronsfore and DS020		Metabolia				vltransfore	sne DC020
PSCVT m Expressed Expressed Expressed se 05	PSCVT	m	Expressed	Expressed	Expressed	se	95 sps_1039

	Tyrosine,					
	Tryptopha					
	n, and					
	Phenylalan					
	ine				shikimate	
	Metabolis				dehydroge	sps RS004
SHK3D	m	Expressed	Expressed	Expressed	nase	10
	Tyrosine,					
	Tryptopha					
	n, and					
	Phenylalan					
	ine					
	Metabolis				shikimate	sps RS266
SHKK	m	Expressed	Expressed	Expressed	kinase	30
	Tyrosine,	-	-			
	Tryptopha					
	n, and					
	Phenylalan					
	ine				tryptophan	
	Metabolis				7-	sps RS116
TRPOR	m	Expressed	Expressed	Expressed	halogenase	40
	Tyrosine,	•	•	-		
	Tryptopha					
	n. and					
	Phenvlalan					
	ine				tryptophan	
	Metabolis				synthase	sps RS083
TRPS2	m	Expressed	Expressed	Expressed	(indole)	00^{-1}
	Tyrosine,					
	Tryptopha					
	n, and				tryptophan	
	Phenvlalan				synthase	
	ine				(indoleglyc	
	Metabolis				erol	sps RS083
TRPS3	m	Expressed	Expressed	Expressed	phosphate)	05
	Tyrosine,	-	-	-		
	Tryptopha					
	n, and					
	Phenylalan					
	ine				Tryptopha	
	Metabolis				nyl-tRNA	sps RS265
TRPTRS	m	Expressed	Expressed	Expressed	synthetase	90
	Tyrosine,	•	·	-	-	sps RS044
	Tryptopha				tyrosine	90 or
	n, and				transamina	sps RS039
TYRTA	Phenylalan	Expressed	Expressed	Expressed	se	90

	ine Matabalia					
	m					
	Tyrosine, Tryptopha n, and					
	Phenylalan				T1	
	ine Metabolis				1 yrosyl-	sps RS123
TYRTRS	m	Expressed	Expressed	Expressed	synthetase	60
		2	2	Ziipioooo	4HBA	
	Unassigne				compound	
4HBASink	d	Expressed	Expressed	Expressed	Sink	Sink
					5DRIB	
5DRIB_Si	Unassigne				compound	
nk	d	Expressed	Expressed	Expressed	Sink	Sink
	T T •				AMOB	
AMOB_S1		Emmand	E	E	compound	Cin1-
пк	a	Expressed	Expressed	Expressed	SINK	SINK
САТ	Unassigne d	Expressed	Expressed	Expressed	catalase	20 or sps_RS085 00 or sps_RS140 15
		Lapressea	LAPICSSCU	Empressed	chloramph	10
CLAT	Unassigne d	Below	Below	Below	enicol acetyltrans ferase	sps_RS042 65
					Coniferyl-	
CONFAL DD	Unassigne d	Expressed	Below	Expressed	aldehyde dehydroge nase	sps_RS234 40
		_		_	hydroxyac	
GLYOX	Unassigne d	Expressed	Expressed	Expressed	ylglutathio ne hydrolase	sps_RS059 45
					Biomass	
Growth	Unassigne	Everaged	Everaged	Everaged	Compound Sin ¹	Biomass
Giowill	u	Expressed	Expressed	Expressed	Glutathion	DIOIIIaSS
					e hydralase	
	Unassigne				(periplasmi	sps RS070
GTHRDH	d	Expressed	Expressed	Expressed	c)	55
	Unassigne	-	<u> </u>		carbonate	sps_RS031
HCO3E	d	Expressed	Expressed	Expressed	dehydratas	85

					e (HCO3	
					equilibrati	
					on	
					reaction)	
					lactoylglut	
	Unassigne				athione	sps_RS057
LGTHL	d	Below	Below	Below	lyase	05
					inorganic	
	Unassigne				diphosphat	sps_RS048
PPA	d	Expressed	Expressed	Expressed	ase	25
					Selenopho	
	Unassigne				sphate	sps_RS267
SELNPS	d	Expressed	Expressed	Expressed	synthase	55
	Unassigne				superoxide	sps_RS030
SOD	d	Expressed	Expressed	Expressed	dismutase	45
					thiosulfate	
	Unassigne				sulfurtrans	sps_RS007
TSULST	d	Expressed	Below	Expressed	ferase	05
	Valine,					
	Leucine,					
	and				acetyl-	
	Isoleucine				CoA C-	
	Metabolis				acetyltrans	sps_RS100
ACACCB	m	Expressed	Expressed	Expressed	ferase	60
	Valine,					
	Leucine,				acetyl-	
	and				CoA:aceto	sps_RS102
	Isoleucine				acetyl-	60 and
	Metabolis	- 1			CoA	sps_RS102
ACACCT	m	Expressed	Expressed	Expressed	transferase	65
					acetyl-	
	Valine,				CoA C-	
	Leucine,				acyltransfe	
	and				rase (2-	
	Isoleucine				Methyl-3-	Dana
ACACITO	Metabolis	F 1	F 1	– 1	acetoacetyl	sps_RS002
ĸ	m	Expressed	Expressed	Expressed	-CoA)	95
						(sps_RS15
	Valina					435 and
	vaime,					sps_KS154
	Leucine,					(an a D C O C)
	and				2-aceto-2-	(sps_KS06
	Isoleucine Matala lia				nyaroxybu	933 and
ACUDO	m	Evenesse	Evenesse	Evenesse	tanoate	sps_K5009
ACUDS	111	Expressed	Expressed	Expressed	synmase	30)

ACLS	Valine, Leucine, and Isoleucine Metabolis m	Expressed	Expressed	Expressed	acetolactat e synthase (Also catalyzes ACHBS)	(sps_RS15 435 and sps_RS154 30) or (sps_RS06 935 and sps_RS069 30)
ACOAD10	Valine, Leucine, and Isoleucine Metabolis m	Expressed	Expressed	Expressed	acyl-CoA dehydroge nase (2- methylbuta noyl-CoA)	sps_RS003 00
ACOAD8	Valine, Leucine, and Isoleucine Metabolis m	Below	Below	Expressed	acyl-CoA dehydroge nase (isovaleryl -CoA)	sps_RS102 30
	Valine, Leucine, and Isoleucine Metabolis				acyl-CoA dehydroge nase (isobutyryl	sps_RS003
ACOAD9	m Valine, Leucine, and Isoleucine Metabolis m	Expressed	Expressed	Expressed	-CoA) acetohydro xy acid isomerored uctase	00 sps_RS154 40
	Valine, Leucine, and Isoleucine Metabolis				dihydroxy- acid dehydratas e (2,3- dihydroxy- 3- methylbuta	sps_RS154
DHAD1	m Valine, Leucine, and Isoleucine Metabolis	Expressed	Expressed	Expressed	noate) Dihydroxy -acid dehydratas e (2,3- dihydroxy-	20 sps_RS154
DHAD2	m	Expressed	Expressed	Expressed	3-	20

					methylpent anoate)	
ECOAH2 C	Valine, Leucine, and Isoleucine Metabolis m	Expressed	Expressed	Expressed	enoyl-CoA hydratase, bacterial	sps_RS100 40 or sps_RS003 00
ЕСОАН9	Valine, Leucine, and Isoleucine Metabolis m	Expressed	Expressed	Expressed	2- Methylpro p-2-enoyl- CoA (2- Methylbut- 2-enoyl- CoA)	sps_RS100 40 or sps_RS003 00
HACD8	Valine, Leucine, and Isoleucine Metabolis m	Expressed	Expressed	Expressed	3- hydroxyac yl-CoA dehydroge nase (2- Methylacet oacetyl- CoA)	sps_RS058 95
HACOAD r	Valine, Leucine, and Isoleucine Metabolis m	Expressed	Used_Belo	Expressed	3- hydroxyac yl-CoA dehydroge nase	sps_RS100 35
HIBHR	Valine, Leucine, and Isoleucine Metabolis m	Expressed	Expressed	Expressed	3- hydroxyiso butyryl- CoA hydrolase	sps_RS002 95
HMGI	Valine, Leucine, and Isoleucine Metabolis	Evpressed	Below	Below	hydroxyme thylglutary l-CoA	sps_RS102
ILEDH2	Valine, Leucine, and Isoleucine	Expressed	Expressed	Expressed	isoleucine dehydroge nase	sps_RS026

	Metabolis					
	m					
	Valine,					
	Leucine,					
	and					
	Isoleucine				isoleucine	
	Metabolis				transamina	sps_RS159
ILETA	m	Expressed	Expressed	Expressed	se	30
	Valine,					
	Leucine,					
	and				T 1 1	
	Isoleucine				Isoleucyl-	D0117
II ETD C	Metabolis	D 1	– 1	 1	tRNA	sps_RS117
ILETRS	m	Expressed	Expressed	Expressed	synthetase	20
	Valine,				2	
	Leucine,				3- · 1	
	and				isopropyim	
	Isoleucine				alate	ana DC162
	metabolis	Everaged	Evenessed	Everaged	denydroge	sps_K5102
IFMD	III Valina	Expressed	Expressed	Expressed	nase	15
	Valine,				2	
	Leucine,				5-	and DS162
	Isoleucine				alate	sps_K3102
	Matabalia				dobydrotog	$\frac{0.5}{2}$ and $\frac{0.5}{2}$
IPPMIa	m	Expressed	Expressed	Expressed	e	sps_K3102
11 1 1/114	Valine	Lapressed	LAPICSSEd	Lapressed	C	10
	I eucine					
	and				2-	sps RS162
	Isoleucine				isopropylm	05 and
	Metabolis				alate	sps RS162
IPPMIb	m	Expressed	Expressed	Expressed	hydratase	10
	Valine.	Lapressea	Lipressea	Lipressea	ing anatabe	10
	Leucine.					
	and				2-	
	Isoleucine				isopropylm	
	Metabolis				alate	sps RS162
IPPS	m	Expressed	Expressed	Expressed	synthase	20
	Valine,	-	-	-	ketol-acid	
	Leucine,				reductoiso	
	and				merase (2-	
	Isoleucine				Aceto-2-	
	Metabolis				hydroxybu	sps_RS154
KARA2i	m	Expressed	Expressed	Expressed	tanoate)	40

	Valine,					
	Leucine,					
	and					sps RS159
	Isoleucine				leucine	30 or
	Metabolis				transamina	sps RS154
LEUTA	m	Expressed	Expressed	Expressed	se	25
	Valine	Lipressea	Lipressea	Liprebeea		
	I eucine					
	and					
	Isoleucine				Leucyl	
	Metabolis				tPNA	one PS215
IFUTDS	m	Everaged	Everaged	Evprogod	synthetase	sps_R3213
LEUIKS	III Valine	Expressed	Expressed	Expressed	synthetase	43
	Vallic,					
	and					
	Isoleucine				I_leucine	
	Metabolis				dehydroge	sps RS026
LIFUDr	m	Expressed	Expressed	Expressed	nase	sps_R3020
LLLODI	Valine	Expressed	LAPICSSEd	Expressed	nase	55
	Leucine					
	and				methylcrot	sps RS102
	Isoleucine				onovl-CoA	35 and
	Metabolis				carboxylas	sps RS102
MCCC	m	Below	Below	Below	e	45
	Valine	Deleti	Deleti	Deleti		
	Leucine.					
	and				methylglut	
	Isoleucine				aconvl-	
	Metabolis				CoA	sps RS102
MGCH	m	Expressed	Below	Below	hvdratase	40
					methylmal	
	Valine.				onate-	
	Leucine.				semialdehv	
	and				de	
	Isoleucine				dehvdroge	
	Metabolis		Used Belo		nase	sps RS100
MMSDHir	m	Expressed	w	Expressed	(acylating)	55
		-			2-	sps RS038
					oxoisovale	65 and
	Valine,				rate	sps_RS038
	Leucine,				dehydroge	70 and
	and				nase	sps_RS038
		1				
	Isoleucine				(acylating;	60 and
	Isoleucine Metabolis				(acylating; 4-methyl-	60 and sps_RS264

					oxopentao	
					ate)	
					2-	
					oxoisovale	
					rate	sps_RS038
					dehydroge	65 and
	Valine,				nase	sps_RS038
	Leucine,				(acylating;	70 and
	and				3-methyl-	sps_RS038
	Isoleucine				2-	60 and
	Metabolis	F 1	F 1	F 1	oxobutano	sps_RS264
OIVD2	m	Expressed	Expressed	Expressed	ate)	55
					2-	
					oxoisovale	and DS038
					dehydroge	sps_K3038
	Valine				nase	$s_{ns} RS038$
	Leucine				(acylating)	3p3_100000 70 and
	and				3-methyl-	sps RS038
	Isoleucine				2-	60 and
	Metabolis				oxopentan	sps RS264
OIVD3	m	Expressed	Expressed	Expressed	oate)	55
	Valine,				2-Oxo-4-	
	Leucine,				methyl-3-	
	and				carboxype	
	Isoleucine				ntanoate	
	Metabolis	- 1			decarboxyl	sps_RS162
OMCDC	m	Expressed	Expressed	Expressed	ation	15
	Valine,					
	Leucine,					
	and				т	
	Metabolis				L- threenine	ene RS15/
THRD I	m	Expressed	Expressed	Expressed	deaminase	3ps_R5154
	Valine	Expressed	LAPICSSCU	LAPICSSCU	dealimitase	15
	Leucine.					
	and				Valine	
	Isoleucine				Pyruvate	
VALALA	Metabolis				Transamin	sps RS089
MOB	m	Expressed	Expressed	Expressed	ase	85
	Valine,					
	Leucine,					
	and					
	Isoleucine				valine	
	Metabolis				dehydroge	sps_RS026
VALDHr	m	Expressed	Expressed	Expressed	nase	55

	Valine,					
	Leucine,					
	and					
	Isoleucine				valine	
	Metabolis				transamina	sps_RS159
VALTA	m	Expressed	Expressed	Expressed	se	30
	Valine,					
	Leucine,					
	and					
	Isoleucine				Valyl-	
	Metabolis				tRNA	sps RS226
VALTRS	m	Expressed	Expressed	Expressed	synthetase	50
					Dimethyl	
					sulfoxide	
	Energy				reductase	
	Metabolis				(Menaquin	sps RS061
DMSOR3e	m	Expressed	Expressed	Expressed	ol 7)	95
					Dimethyl	
					sulfoxide	
	Energy				reductase	
	Metabolis				(methylme	sps RS061
DMSOR4e	m	Expressed	Expressed	Expressed	naquinol 7)	95
					Trimethyla	
					mine N-	
					oxide	sps RS061
	Energy				reductase	95 or
	Metabolis				(ubiquinol	sps RS013
TMAOR3e	m	Expressed	Expressed	Expressed	8)	95
					Trehalose	
	Transport,				transport to	
OMP TRE	Extracellul				periplasm	sps RS073
Н	ar	Below	Below	Below	(oprB)	70
	Alternate					
	Carbon				Trehalose	
	Metabolis				Phosphotas	
TRE6PP	m	Expressed	Expressed	Expressed	e	Gap
	Transport,				Trehalose	
	Extracellul				Transport	
TREHtex	ar	Expressed	Expressed	Expressed	vis PTS	Gap
	Alternate					
	Carbon					
	Metabolis					sps_RS272
TREH	m	Expressed	Expressed	Expressed	Trehalase	35
	Transport,					
	Extracellul				Sucrose	
SUCRPTS	ar	Expressed	Expressed	Expressed	transport	Gap

					via PTS	
					system	
FFSD	Alternate Carbon Metabolis m	Expressed	Expressed	Expressed	beta- fructofuran osidase	Gap
SUCD	Alternate Carbon Metabolis	Evoressed	Evoressed	Expressed	Sucrose phosphoryl	Gan
	Alternate Carbon Metabolis	Expressed	Expressed	Expressed	fructokinas	sps_RS181
FRUK	m	Expressed	Expressed	Expressed	e	05
OMP_SU CR	Transport, Extracellul ar	Below	Below	Below	Sucrose transport to periplasm (oprB)	sps_RS073 70
OMD CIT	Transport, Extracellul	Evenand	Evenand	Eveneousd	citrate transport to periplasm (ompF, ompC, or	sps_RS109 15 or sps_RS143 50 or sps_RS143 45 or sps_RS113 60 or sps_RS243 95 or sps_RS117 70
OMP CIT	ar	Expressed	Expressed	Expressed	oprF)	/0

Data S1 Table C: Metabolite Structural Information. Table contains metabolite names, formulas, and charges from the model. SMILES strings are provided for the metabolites along with an indication of the source of the structure. Additionally, a mapping to the TECRdb database used by the Group Contribution package is included.

						Structure
ID	Name	Kegg ID	Charge	Formula	SMILES	Source
					C1C(NC2	
					=C(N1)N=	
					C(NC2=O)	
					N)CN(C=	
					O)C3=CC	
	10-				= C(C=C3)	
	Formvltetr				C(=O)NC(
	ahvdrofola			C20H21N	$\dot{CCC(=O)}$	
cpd 10fthf	te	C00234	-2	707	O)C(=O)O	Pubchem
<u> </u>					$\overline{[H]C(=0)}$	
	1.2-Diacyl-				OCC(COP	
	sn-glycerol				(0)(0)=0)	
cpd 12dag	3-			C5H5O8P	OC([H])=	Manually
3n	phosphate	C00416	-2	R2	0	Drawn
	phosphate	000110		102	[H]C(=0)	
	1 2-				OCC(CO)	
	Diacylolyc			C5H6O5R	OC([H])=	Manually
end 12dar	erol	C00641	0	2		Drawn
epu_12ugi	3	00041	0	2	0	Diawii
	Dhospho-				C(C(C) = 0)	
	D-				OP(=0)(
	dvcerovl			C3H4O10		Manually
end 13dng	phosphate	C00236	_4	P2	(=0)(0)0	Drawn
cpu_15upg	1	00230		12	(0)(0)0	Diawii
and lan2a	1-					
cpu_1ap20	Anniopio	C05771	1	C2U10NO	CC(CNDO	Dubaham
1	pall-2-01	05771	1	CONTINU		Fubchelli
	I- Dermalina					
	Pyrroline-					
. 1 1	J-				CICC(N=	
cpd_1pyr5	carboxylat	C02012	1	CELLORO	CI)C(=0)	D 1 1
С	e	C03912	-1	C5H6NO2	0	Pubchem
					CIC=CC(
					=NCIC(=	
1 00 11 1	2,3-				O(O-	
cpd_23dhd	Dihydrodi	G00010	_])C(=O)[O	D 1 1
p	picolinate	C03340	-2	C7H5NO4	-]	Pubchem
	(R)-2,3-				CC(C)(C(
cpd_23dh	Dihydroxy				C(=O)O)O	
mb	-3-	C04272	-1	C5H9O4)O	Pubchem

	methylbuta					
	noate					
	(\mathbf{K}) -2,3-					
					CCC(C)(C)	
and 22 db	-J-				CCC(C)(C)	
cpu_25uii	methylpent	C06007	1	C6U1104	(C(-0)0)	Dubaham
mp	(S) 2 [5]	00007	-1	0111104	0,0	rubellelli
	(3)-2-[3-					
	(5 ₋				C1=NC(=	
	(J-				C(N)C2C(
	D-				C(C(02)C)	
	ribosvl)imi				OP(=O)(O	
	dazole-4-				(0)(0)(0)(0)	
	carboxami				C(=O)NC(
	do]succina			C13H15N	CC(=O)O)	
cpd 25aics	te	C04823	-4	4O12P	C(=O)O	Pubchem
_	2,5-					
	Diamino-				C(C1C(C(
	6-hydroxy-				C(O1)NC2	
	4-(5'-				=C(C(=O))	
	phosphorib				NC(=N2)N	
	osylamino))N)O)O)O	
cpd_25dhp	-			C9H14N5	P(=O)(O)	
р	pyrimidine	C01304	-2	O8P	0	Pubchem
	LL-2,6-				C(CC(C(=	
1.0.01	Diaminohe				0)0)N)CC	
cpd_26dap	ptanedioat	000000	0	C/H14N2	(C(=O)O)	D 1 1
-LL	e	C00666	0	04	N	Pubchem
	meso-2,6-				C(CC)(C) =	
and Ocdan	Diaminone			C71114N12	$(C(-\Omega)\Omega)$	
cpd_26dap	ptanedioat	C00690	0	C/H14N2	(C(=0)0)	Dubaham
-1VI	e 2	C00680	0	04	IN	Pubchem
	Δminoethy					
	Inhosphon			C2H6NO3	C(CP(=0))	
end 2aen	ate	C03557	-2	P	O(O)N	Pubchem
-pa_2aep	(S)-2-	203337	-2	1		
	Aceto-2-				CCC(C(=	
cpd 2ahbu	hydroxybu				O(C) = O(C) = O(C)	
t	tanoate	C06006	-1	C6H9O4	0)0)0	Pubchem
	2-Amino-				, ,	
	4-hydroxy-				C1C(=NC	
	6-				2=C(N1)N	
cpd_2ahh	hydroxyme			C7H8N5O	=C(NC2=	
	thyl-7.8-	C04807	-3	8P2	O)N)COP(Pubchem
	dihydropte				=O)(O)OP	
-----------	-----------------	--------	-----	----------	--	---------
	ridine				$(=\hat{O})(\hat{O})O$	
	diphosphat				()())	
	e					
	2_{-} Amino-					
	2-Ammo-					
	4-ilyuloxy-					
	0-				CIC(NC	
	nydroxyme				CIC(=NC	
1 . 1 1	thyl-7,8-				2=C(NI)N	
cpd_2ahh	dihydropte			C7H9N5O	=C(NC2=	
mp	ridine	C01300	0	2	O)N)CO	Pubchem
	L-2-					
	Amino-3-					
cpd 2aobu	oxobutano				CC(=O)C(
t	ate	C03508	0	C4H7NO3	C(=O)O)N	Pubchem
					C1=CC=C	
	1-(2-				(C(=C1)C(
	Carboxyph				=0)0)NC	
	envlamino)				C(=0)[C@]	
	1 deoxy					
	D ribulaça					
1 2	D-Houlose			C101112N		
cpd_2cpr5	J -	C01202	2	CI2HI3N	=0)(0)0)	D 1 1
p	phosphate	C01302	-3	09P	0)0	Pubchem
	2-					
	Dehydro-					
	3-deoxy-				C(C(C(C	
	D-arabino-				COP(=O)(
	heptonate				0)0)0)0)	
cpd_2dda7	7-			C7H10O1	O)C(=O)C	
р	phosphate	C04691	-3	0P	(=O)O	Pubchem
_	2-					
	Dehvdro-					
	3-deoxy-				C(C(C(CO	
	D-				P(=O)(O)	
	gluconate				0)0)0)C(
cnd 2dda6	6-				=0)C(=0)	
n	nhosnhate	C04442	. 2	COHSOOD		Pubchem
Р	2	CUTTT2	-3	0110071		
	2- Dahardara				C(-0)C(-0)C(-0)C(-0)C(-0)C(-0)C(-0)C(-0)	
1 0 11	Denydropa	000000	1	CCURCA)C(=0)C(=)	D 1 1
cpa_2dhp	ntoate	C00966	-1	С6Н9О4		Pubchem
					CC(=CCC	
					C(=CCCC(
	2-				=CCCC(=	
	Demethyl				CCCC(=C	
cpd_2dmm	menaquino			C45H62O	CCC(=CC	
q7	ne 7	NA	0	2	CC(=CCC	Pubchem

					1=CC(=O)	
					$C^{2}=CC=C$	
					$C = C^2 C^2 C^2 C^2$	
					$C = C_2 C_1 = 0$	
					O(C)C(C)	
	2-Deoxy-				CIC(C(OC	
	D-ribose 1-				10P(=0)(
cpd_2dr1p	phosphate	C00672	-2	C5H9O7P	0)0)C0)0	Pubchem
	2-Deoxy-				C1C(C(OC	
	D-ribose 5-				10)COP(=	
cpd 2dr5p	phosphate	C00673	-2	C5H9O7P	0)(0)0)0	Pubchem
· _ ·	2-					
	- Hydroxy-					
	3-					
end 2h3on	oxopropan				C(=O)C(C)	
cpu_21150p	onte	C01146	1	C3H3O4	(-0)0)0	Dubchem
Р		01140	-1	0511504	(-0)0)0	1 ubenem
	Z- I I				CC(C)C(=	
1.0	Isopropyi	000(01	2	CTUDO 1	CC(=0)0)	D 1 1
cpd_21ppm	maleate	C02631	-2	C7H8O4	C(=0)O	Pubchem
	2-keto-4-					
	methylthio				CSCCC(=	
cpd_2kmb	butyrate	C01180	-1	C5H7O3S	O(=O)O	Pubchem
					CC(C(=O))	
					C)C(=O)S	
					CCNC(=O	
)CCNC(=	
					\hat{O}	
					C)COP(=0)	
					(0)OP(=	
					(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(
					1C(C(C(U)))	
					1)N2C=N	
	2-				C3=C2N=	
	Methylacet				CN=C3N)	
cpd_2maac	oacetyl-			C26H38N	O)OP(=O)	
oa	CoA	C03344	-4	7018P3S	0(0)0)0	Pubchem
	2-Methyl-					
	4-amino-5-				CC1=NC=	
	hydroxyme				C(C(=N1)	
	thylpyrimi				N)COP(=	
	dine				Ó)([O-	
cpd 2mah	diphosphat			C6H8N3O		
mp	e	C04752	-3	7P2	0-])[0-]	Pubchem
			5		CC = C(C)C	• • •
end 2mb2	2-			C26H38N	(=0)SCCN	
	2- Mathulbut	C03245	А	7017029	C(-0)CC	Dubaham
coa	wiemyiout-	003343	-4	/01/135		rubenem

	2-enoyl-				NC(=O)C(
	CoA				C(C)(C)C	
					OP(=O)([
					\mathbf{O} -	
])OP(=O)([
					0-	
					$\Gamma(C(01)N)$	
					2C=NC3=	
					C2N=CN=	
					C3N)O)OP	
					(=O)([O-	
])[O-])O	
					CCC(C)C(
					=O)SCCN	
					C(=O)CC	
					NC(=0)C(
					OP(=O)(O)	
					O(-0)(0)	
					0)0CC1C	
					(C(C(O1)	
					N2C=NC3	
					=C2N=CN	
	2-				=C3N)O)O	
cpd_2mbc	Methylbut			C26H40N	P(=O)(O)	
oa	anoyl-CoA	C01033	-4	7017P3S	0)0	Pubchem
	· .				CC(=C(CC)	
and Image	C1S-2-				(=0)0)C(=0)	
cpd_2mcac	nitate	C04225	3	C7H5O6	0)0)0(-0)	Pubchem
11	maic	04223	-3	C/11500	CC(C(=0))	1 ubellelli
	2-				[0-	
	Hydroxybu])C(CC(=	
	tane-1,2,3-				0)[O-	
	tricarboxyl])(C(=O)[
cpd_2mcit	ate	C02225	-3	C7H7O7	O-])O	Pubchem
	2-C-					
	methyl-D-					
1.2.4	erythritol			05111107		
cpa_2me4	4-	C11/2/	า	D D	(UUP(=U))	Dubaham
Р	$2 - C_{-}$	011434	-2	Г	CC1(C(CO)	rubellelli
	2-C- methyl-D-				P(=0)(OP(
cpd 2mec	ervthritol			C5H10O9	=0)(01)(0)	
dp	2,4-	C11453	-2	P2	0)0)C0	Pubchem

	cyclodipho sphate					
cpd_2mp2	2- Methylpro p-2-enoyl-	C03460	-4	C25H36N 7017P3S	$\begin{array}{l} CC(=C)C(\\ =O)SCCN\\ C(=O)CC\\ NC(=O)C(\\ C(C)(C)C\\ OP(=O)(O\\)OP(=O)(\\ O)OCC1C\\ (C(C(O1)\\ N2C=NC3\\ =C2N=CN\\ =C3N)O)O\\ P(=O)(O)\\ O)O\end{array}$	Puhchem
	2-	000100		1011135		1 doenem
and Johut	Oxobutano	C00100	1	C4H5O3	CCC(=0)	Dubchem
cpd_20but	2- Octaprenyl -6- hydroxyph enol	C05811	0	C46H70O 2	C(-C)C = CCC = CCCC(= CCCC(= CCCC) = CCCC(= CCC) = CCC(= CC) = CCC(= CCC) = C(C) = C	Pubchem
cpd_2omb zl	2- Octaprenyl -6- methoxy- 1,4- benzoquin ol 2- Octaprenyl	C05813	0	C47H72O 3	$CC(=CCC) \\ C(=CCCC) \\ =CCCC(=C) \\ CCCC(=C) \\ CCC(=CC) \\ CC(=CCC) \\ C(=CCC) \\ =C10)OC) \\ O)C)C)C) \\ C)C)C)C) \\ C \\ CC1=C(C) \\ =C(C) \\ =C(C) \\ CC(=C1) \\ CC(=C1) \\ CCC(=C1) \\ CCC(=C1) \\ CCCCCCC \\ CCCCCCCCCCCCCCCCCCCCCCCC$	Pubchem
cpd_20mh mbl	-3-methyl- 5-hydroxy-	C05815	0	C48H74O 4)CC=C(C)	Pubchem

	6-				CCC=C(C)	
	methoxy-				CCC = C(C)	
	1.4-				CCC=C(C)	
	benzoauin				CCC = C(C)	
	ol				CCC=C(C)	
	01				CCC = C(C)	
					CCC = C(C)	
					CCC-C(C)	
					CCI=C(C(
	_				0)0C)0)C	
	2-				C=C(C)CC	
	Octaprenyl				C=C(C)CC	
	-3-methyl-				C=C(C)CC	
	6-				C = C(C)CC	
	methoxy-				C=C(C)CC	
	1,4-				C=C(C)CC	
cpd 20mm	benzoquin			C48H74O	C = C(C)CC	
bl _	ol	C05814	0	3	C = C(C)C	Pubchem
					CC(=CCC	
					C(=CCCC(
	2					
	2- O - to					
	Octaprenyi					
1.0	-6-			04711720	=C1)0C)0	
cpd_2omp	methoxyph	~~~~		C4/H/20)C)C)C)C)C)	
h	enol	C05812	0	2	C)C)C)C	Pubchem
					CC(=CCC	
					C(=CCCC(
					=CCCC(=	
					CCCC(=C	
					CCC(=CC	
					CC(=CCC	
					C(=CCC1	
					=CC=CC=	
	2-				C1O)C)C)	
	Octaprenvl				C)C)C)C)	
end 20ph	nhenol	C05810	0	C46H70O	C)C	Pubchem
-pa_2opn	2-nhosnho-	202010		2 1011/00	CC(CO)(C)	
	2 phospho-				(COP(=O))	
					(0.01(-0))	
and 2-1-2	J-			CIAUDON	(0)00000000000000000000000000000000000	
cpu_2p4c2	alphospho)	C11426	A	$C14\Pi ZZIN$		Dubation
me	-2-C-	CI1436	-4	301/P3	U(U(U(U)))	Pubchem

	methvl-D-				N2C=CC(
	ervthritol				=NC2=O)	
					N(0)O(0)	
					OP(=O)(O	
					(-0)(0)	
	D)0	
	D-					
	Glycerate				C(C(C(=0	
	2-)O)OP(=O	
cpd_2pg	phosphate	C00631	-3	C3H4O7P)(O)O)O	Pubchem
	2-				C(C(=O)O)	
cpd_2pgly	Phosphogl)OP(=O)(
c	ycolate	C00988	-3	C2H2O6P	0)0	Pubchem
	2-					
	Succinyl-					
	6-hydroxy-					
	2.4-				C1=CC(C(
	cyclohexad				C(=C1)C(
	iene-1-				=0)CCC(=	
end 2shch	carboxylat			C11H10O	0)0)C(=0	
cpa_25hen	e	C05817	_2	6		Pubchem
		000017	-2	0	$C_{1-CC}(-$	1 doenem
	3-(4-				CI = CC(=	
	Hydroxypn					
1.0.41	enyl)pyruv	C011 7 0	1	COLLECA	(=0)C(=0)	D 1 1
cpd_34hpp	ate	C011/9	-1	C9H7O4	0)0	Pubchem
	3-					
	Carboxy-					
	2-hydroxy-					
	4-				CC(C)C(C	
cpd_3c2h	methylpent				(C(=O)O)	
mp	anoate	C04411	-2	C7H10O5	O)C(=O)O	Pubchem
	3-					
	Carboxy-					
	3-hydroxy-					
	4-				CC(C)C(C	
cpd 3c3h	methylpent				C(=O)O)(
mn	anoate	C02504	-2	C7H10O5	C(=0)0)0	Pubchem
1-	3-		2		-(0)0)0	••
	Carboyy-					
	1_methyl					
					CCCCCCC	
and 2 day	2- avancetar				(-0)C(-0)	
cpu_3c4m	oxopentan	C04226	~	0711905	(=0)C(=0)	D.1 1
op	oate	C04236	-2	C/H8O5	U)U(=0)U	Pubchem
					CIC(C(C(
	3-				=O)CC1(C	
	Dehydroqu				(=O)O)O)	
cpd_3dhq	inate	C00944	-1	C7H9O6	0)0	Pubchem

	2				C1C(C(C(
	3- Debydroch				=0)0=01	
end 3dhsk	ikimate	C02637	-1	C7H7O5	C(-0)0)0	Pubchem
		02001			CC(C(C)O)C(=O)SC CNC(=O) CCNC(=O)C(C(C)(C)COP(=O)(
end 3hmb	(2S,3S)-3- Hydroxy- 2- methylbuta			C26H40N	O)OP(=O) (O)OCC1 C(C(C(O1) N2C=NC3 =C2N=CN =C3N)O)O P(=O)(O)	
coa	novl-CoA	C04405	-4	7018P3S	$\frac{1}{0}$	Pubchem
	3- Hydroxy- 2- methylpro				CC(CO)C(
cpd_3hmp	panoate	C01188	-1	C4H7O3	=O)[O-]	Pubchem
cpd_3ig3p	C'-(3- Indolyl)- glycerol 3- phosphate	C03506	-2	C11H12N O6P	C1=CC=C 2C(=C1)C(=CN2)C(C (COP(=O)(O)O)O)O	Pubchem
cpd_3mb2 coa	3- Methylbut- 2-enoyl- CoA	C03069	-4	C26H38N 7O17P3S	$\begin{array}{c} CC(=CC(=\\ O)SCCNC\\ (=O)CCN\\ C(=O)C(C\\ (C)(C)CO\\ P(=O)(O)\\ OP(=O)(O)\\ OP(=O)(O)\\ OCC1C(C\\ (C(O1)N2\\ C=NC3=C\\ 2N=CN=C\\ 3N)O)OP(\\ =O)(O)O\\ O)C\\ \end{array}$	Pubchem
cpd_3mgc	5- Methylglut aconyl-			C27H37N	O)SCCNC (=O)CCN	
oa	CoA	C03231	-5	7019P3S	C(=O)C(C)	Pubchem

					(C)(C)CO P(=O)(O) OP(=O)(O))OCC1C(C (C(O1)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O) O)CC(=O) O	
cpd 3mob	3-Methyl- 2- oxobutano ate	C00141	-1	С5Н7О3	CC(C)C(= 0)C(=0)0	Pubchem
cpd 3mop	(S)-3- Methyl-2- oxopentan oate	C00671	-1	С6Н9О3	CCC(C)C(=O)C(=O) O	Pubchem
cpd_3ophb	3- Octaprenyl -4- hydroxybe nzoate	C05809	-1	C47H69O 3	CC(=CCC)C(=CCCC(=CCCC(=C)CCCC(=CC)CCC(=CCC)C(=CCC)C(=CCC1)=C(C=CC((=CC1)C(=O))O)O)C)C)C)C)C)C)C)CCCCCCCCCCCCCCCC	Pubchem
cpd_3pg	3- Phospho- D- glycerate	C00197	-3	C3H4O7P	C(C(C(=O)O)O)OP(=O)(O)O	Pubchem
cpd_3php	3- Phosphohy droxypyru vate	C03232	-3	С3Н2О7Р	C(C(=O)C (=O)O)OP (=O)(O)O	Pubchem
cpd 3psme	5-O-(1- Carboxyvi nyl)-3- phosphoshi kimate	C01269	-4	C10H9O1 0P	C=C(C(=O)O)OC1C C(=CC(C1 O)OP(=O) (O)O)C(= O)O	Pubchem

	4-					
	Aminobuta				C(CC(=O)	
cpd_4abut	noate	C00334	0	C4H9NO2	O)CN	Pubchem
	4-				C1=CC(=	
	Aminoben				CC=C1C(
cpd_4abz	zoate	C00568	-1	C7H6NO2	=O)[O-])N	Pubchem
cpd_4adch o	4-amino-4- deoxychori smate	C11355	-1	C10H10N O5	C=C(C(=O))[O-])OC1C=C (C=CC1[N H3+])C(= O)[O-]	Pubchem
cpd_4amp	4-Amino- 2-methyl- 5- phosphom ethylpyrim idine	C04556	-2	C6H8N3O 4P	CC1=NC=C(C(=N1)) $N)COP(=O)(O)O$	Pubchem
	4-(cytidine 5'- diphospho) -2-C-				CC(CO)(C (COP(=O)(O)OP(=O) (O)OCC1 C(C(C(O1) N2C=CC(=NC2=O)	
cpd_4c2m	methyl-D-	C11425	2	C14H23N 2O14P2	N)O)O)O)	Dubaham
cpd_4fuma cac	4- Fumarylac etoacetate	C01061	-2	C8H6O6	C(C(=O)C C(=O)[O-])C(=O)C= CC(=O)[O -]	Pubchem
cpd 4hba	4- Hydroxy- benzyl alcohol	C17467	0	C7H8O2	C1=CC(= CC=C1CO)O	Pubchem
cpd_4hbco	4- Hydroxybe nzovl-CoA	C02949	-4	C28H36N 7O18P3S	CC(C)(CO P(=O)(O) OP(=O)(O))OCC1C(C (C(O1)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O) C(C(=O)N	Pubchem

					CCC(=0)	
					NCCSC(-)	
					NCCSC(=	
					0)04=00	
					=C(C=C4)	
					0)0	
	4-				C1=CC(=	
	Hydroxybe				CC=C1C(
cpd 4hbz	nzoate	C00156	-1	C7H5O3	=O)(O(O=	Pubchem
	4-					
	Imidazolon				C1=NC(C(
	e-5-			C6H7N2O	=0)N1)CC	
and dian	rononcoto	C03680	1	2	C(-0)0	Dubaham
cpu_4izp	propanoate	03080	-1	3	C(-0)O	rubellelli
					C(C(=0)C)	
	4-				C(=0)0)C	
cpd_4mlac	Maleylacet				(=O)C=CC	
ac	oacetate	C01036	-2	C8H6O6	(=O)O	Pubchem
	4-Methyl-					
	2-				CC(C)CC(
	oxopentan				=O)C(=O)	
cpd 4mop	oate	C00233	-1	C6H9O3	0	Pubchem
<u>-r</u> r	4-Methyl-					
	5 (2				CC1-C(S)	
	J-(2-				C=N1)CC	
and America				CLUNNOA	C=NTCC	
cpd_4mpet	nyı)-	004227	2	COHONU4	OP(-0)(0)	D 1 1
Z	thiazole	C04327	-2	P5		Pubchem
					C(C(C(=O	
	4-				O)N)C(=	
	Phospho-			C4H6NO7	O)OP(=O)	
cpd_4pasp	L-aspartate	C03082	-2	Р	0(0)	Pubchem
	4-				C(C(C(C(=	
	Phospho-				0)0)0)0)	
	D-				OP(=O)(O	
cpd 4per	ervthronate	C03393	-3	C4H6O8P)0	Pubchem
opa_iper		000000			CC(C)(CO)	1 do enteni
					P(-0)(0)	
	D-4'-			COLLIZIO])C(C(=0)	
	Phosphopa			C9HI5NO	NCCC(=O	
cpd_4ppan	ntothenate	C03492	-3	8P)[O-])O	Pubchem
					CC(C)(CO	
	N-((R)-4-				P(=O)(O)	
	Phosphopa				O)C(C(=O)	
	ntothenoyl)NCCC(=	
cpd 4ppcv)-L-			C12H20N	O)NC(CS)	
s	cysteine	C04352	-3	209PS	C(=O)O)O	Pubchem

	4-(1-D-				C(C(C(C(
	Ribitylami				CO(O)O(O)O	
	n_{0} -5-				NC1=C(C)	
				COLLIANIA	(-0)NC(-	
1 4 5		004722	0	C9HI0N4	(=0)NC(=	D 1 1
cpd_4r5au	1	C04/32	0	06	O)NI)N	Pubchem
	(6R)-6-(L-					
	erythro-					
	1,2-					
	Dihydroxy					
	propyl)-					
	5.6.7.8-				CC(C(C1C	
	tetrahydro-				$N=C^{2}C(N)$	
	19-				1)(C(=0)N)	
and 5679+	hudrountor			COLLANIA	$\Gamma(C(-N2)N)$	
cpu_3078t	inguloypter	C00296	0	C_{2}	C(-N2)N	Dubaham
1111	111 5 1	00380	0	03	0,0,0	rubenem
	5-amino-1-					
	(5-					
	phospho-				C1=NC(=	
	D-				C(N1C2C(
	ribosyl)imi				C(C(O2)C)	
	dazole-4-				OP(=O)(O	
	carboxylat			C9H11N3)O)O)N)	
cpd 5aizc	e	C04751	-3	O9P	C(=O)O	Pubchem
	5-Amino-					
	4-				C(CC(=O))	
	oxonentan				O(C(=O)C)	
end 5aon	oate	C00430	0	C5H9NO3	N	Pubchem
cpu_suop	oute	00450	0	051171105		1 doenem
	5 Amina				C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(
	5-Ammo-				COP(-O)(
	0-(5'-				(0)(0)(0)(0)	
	phosphorib				O)NCI=C(
cpd_5aprb	itylamino)		_	C9H15N4	C(=O)NC(
u	uracil	C04454	-2	O9P	=O)N1)N	Pubchem
					C(C1C(C(
					C(01)NC2	
	5-Amino-				=C(C(=O))	
	6-(5'-				NC(=O)N2	
	phosphorib)N)O)O)O	
	osvlamino)			C9H13N4	P(=O)(O)	
cpd 5apru	uracil	C01268	-2	O9P	0	Pubchem
-roupru	5-				$C_1 = C(N(C))$	
	nhosphorih				=N1)C2C(
	phosphorio				C(C(O2)C)	
	USYI-J-				OP(-O)(C)	
				COLL1 1312	OP(=0)(0)	
	inoimidazo		_	C9HIIN3)()()()()N	
cpd_5caiz	le	C15667	-3	O9P	C(=O)O	Pubchem

	5-Deoxy-				CC(C(C(C	
end 5drib	D-ribose	NA	0	C5H10O4	=0)0)0)0	Pubchem
epu_suns	Diffeet	1111		00111001	$C_{12} - NC(-$	1 uoenem
	5				C12-NC(-	
	3- 111			CELLANIAO	O)NCI(C(
1 71 .	Hydroxyis	G11001	0	C5H4N4O	=0)NC(=	D 1 1
cpd_5hiu	ourate	C11821	0	4	0)N2)0	Pubchem
	5-					
	Methylthio				CSCC1C(
	-5-deoxy-				C(C(O1)O)	
cpd_5mdr1	D-ribose 1-			C6H11O7	P(=O)(O)	
р	phosphate	C04188	-2	PS	O)O)O	Pubchem
-	5-					
	Methvlthio					
	-5-deoxy-				CSCC(C(C	
	D-ribulose				(=0)COP(
and 5mdru				C6H1107	=0)(0)0)	
cpu_Jindiu	nhogenhoto	C04592	2		-0)(0)0)	Dubaham
1p	phosphate	04382	-2	15	O_{0}	rubenenn
	-				C(C(01)N)	
	5-				2C=NC3=	
	Methylthio			C11H15N	C2N=CN=	
cpd_5mta	adenosine	C00170	0	503S	C3N)O)O	Pubchem
					CN1C(CN	
					C2=C1C(=	
					O)NC(=N2	
)N)CNC3=	
					CC=C(C=	
	5-				C3)C(=O)	
	Methyltetr				NC(CCC(
	ahydrofola			C20H24N	=0)0)C(=	
cpd 5mthf	te	C00440	-1	706	0)0	Pubchem
-pa_onun		200110	1	, 00	CN1C(CN	
					$C^2 = C^1 C (-$	
					$C_2 = C_1 C_1 C_1 C_1 C_1 C_1 C_1 C_1 C_1 C_1$	
					$\frac{O(1)}{O(1)}$	
)N)CNC3=	
					C3)C(=O)	
					NC(CCC(
					=O)NC(C	
	5-				CC(=O)N	
	Methyltetr				C(CCC(=	
	ahydropter				OOOC = O	
cpd 5mthg	oyltri-L-			C30H39N)O)C(=O)	
lu c	glutamate	C04489	0	9012	O(C=O)O	Pubchem

	5-				CSCC1C(
	Methylthio			C6H12O4	C(C(01)0	
cpd 5mtr	-D-ribose	C03089	0	S	$)\hat{O}\hat{O}$	Pubchem
	N1-(5-				, ,	
	Phospho-				CC1=CC2	
	alpha-D-				=C(C=C1)	
	ribosyl)-				C)N(C=N2)	
	5 6-				$C_{C}(C)$	
	dimethylbe				$O_{3}COP(=$	
end 5prdm	nzimidazol			C14H17N	O(O)O(O)	
bz	A	C04778	_2	207P	0)(0)0)0)	Pubchem
02	C	04//0	-2	2071		1 ubenem
	6				C(C(-0))	
	0- D1 1				C(C(-0)0)	
	Phospho-			C(111001	(0,0,0,0)	
1 (D-	C00245	2	COHIUUI	OP(=0)(0)	D-1.1.
cpd_6pgc	gluconate	C00345	-3	OP		Pubchem
	6-phospho-				C(C(=0))	
	D-				1)0)0)0)	
1 - 1	glucono-	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~			OP(=O)(O	
cpd_6pgl	1,5-lactone	C01236	-2	С6Н9О9Р)0	Pubchem
	(6R)-6-(L-					
	erythro-					
	1,2-					
	Dihydroxy				CC(C(C1C	
	propyl)-				N=C2C(=	
	7,8-				N1)C(=O)	
	dihydro-			C9H12N4	NC(=N2)N	
cpd_78dhp	6H-pterin	C00268	0	02)O)O	Pubchem
					C1=CC2=	
					C(C(=C1))	
	7-Chloro-				Cl)NC=C2	
	L-			C11H10N	CC(C(=O))	
cpd_7cltrp	tryptophan	C19687	-1	2O2C1	O)N	Pubchem
	8-Amino-					
	7-				CC(C(=O))	
	oxononano			C9H17NO	CCCCCC(
cpd_8aonn	ate	C01092	0	3	=O)[O-])N	Pubchem
					CC(=O)C	
					C(=O)SCC	
					NC(=O)C	
					CNC(=O)	
					C(C(C)(Ć)	
					$\dot{COP}(=O)($	
	Acetoacetv			C25H36N	O)OP(=O)	
cpd aacoa	l-CoA	C00332	-4	7018P3S	(Ó)0CC1	Pubchem

					C(C(C(01)	
					$N_{2}C = N_{1}C_{2}$	
					112C-11CS	
					=C2N=CN	
					=C3N(0)O	
					P(=O)(O)	
					0)0	
					CC(=O)[O	
cpd_ac	Acetate	C00033	-1	C2H3O2	-]	Pubchem
	Acetoaceta				CC(=O)C	
cpd acac	te	C00164	-1	C4H5O3	C(=O)[O-]	Pubchem
	Acetaldehv					
cpd acald	de	C00084	0	C2H4O	CC=O	Pubchem
opu_uouiu				021110	CC(=0)SC	
					CNC(-0)	
					CONC(-0)	
					CCNC(-0)	
) C(C(C)) C	
)COP(=O)(
					O)OP(=O)	
					(O)OCC1	
					C(C(C(O1)))	
					N2C=NC3	
					=C2N=CN	
					=C3N)O)O	
	Acetyl-			C23H34N	P(=O)(O)	
cpd accoa	CoA	C00024	-4	7017P3S	$\dot{0}0$	Pubchem
1_					CC(=O)N	
	N-Acetyl-				C(CCC) =	
	I -olutamyl				O(OP(=O))	
	5_			C7H9NO8	(0)0)C(=	
and aca5n	J- phosphate	C04133	3	D	(0)0)C(-	Dubchem
cpu_acg5p	N A patril	04133	-3	1	0,0	1 ubenem
	N-Acetyl-					
	L-					
	glutamate					
	5-				CC(=O)N	
cpd_acg5s	semialdehy			C7H10NO	C(CCC=O	
а	de	C01250	-1	4)C(=O)O	Pubchem
	N-Acetyl-				CC(=O)N	
	D-				C1C(C(C(
	glucosami			C8H15NO	OC1O)CO	
cpd_acgam	ne	C00140	0	6)O)O	Pubchem
	N-Acetyl-				CC(=O)N	
	D-				C1C(CÍCÍ	
	glucosami				OC1OP(=	
cnd acoam	ne 1-			C8H14NO	O(O)O(C)	
In	nhosnhate	C04256	?	9P	0)0)0	Pubchem
14	Phosphare	201230	-7	11	5,5,5	1 400110111

	N-Acetvl-				CC(=O)N	
	D-				C1C(C(C(
	glucosami				OC1O)CO	
cnd acoam	ne 6-			C8H14NO	P(=0)(0)	
6pa_aegain	nhosnhate	C00357	-2	9P	$\frac{1}{1000}$	Pubchem
ор	phosphate	000007		71	C(-0)N	1 doenem
	N Acotyl				C(CCC) = C(CCC)	
	IN-ACCLYI-				C(CCC(-	
and acalu	L-	C00624	2	C7H0NO5	0)0)0(-0)	Dubaham
cpu_acgiu	giutamate	C00024	-2	C/119NO3	$\int O$	rubenenn
					CC(C(=0))	
1	N-Acetyl-			C111110N		
cpd_acma	D-	000710	1	CHHIN	O(O)O)N	D 1 1
m	muramoate	C02713	-1	08	C(=O)C	Pubchem
					CC(C(=0))	
					U)NC(=O)	
	N-Acetyl-				C(C)OC1C	
	D-				(C(OC(C1	
cpd_acma	muramoyl-			C14H23N	0)C0)0)N	
ma	L-alanine	C02999	-1	209	C(=O)C	Pubchem
	N-Acetyl-				CC(=O)N	
	D-				C1C(C(C(
cpd_acman	mannosam			C8H15NO	OC1O)CO	
a	ine	C00645	0	6)O)O	Pubchem
					CC(=O)N	
					C1C(CC(O	
	N-				C1C(C(CO	
	Acetylneur			C11H18N)O)O)(C(=	
cpd acnam	aminate	C00270	-1	09	0)0)0)0	Pubchem
					CC(=O)N	
	N2-Acetyl-			C7H14N2	C(CCCN)	
cpd acorn	L-ornithine	C00437	0	03	C(=O)O	Pubchem
· -					CC(=0)0	
	O-Acetvl-				CC(C(=0))	
cpd acser	L-serine	C00979	0	C5H9NO4	O)N	Pubchem
	Acetvl				CC(=O)OP	
cpd actn	phosphate	C00227	-2.	C2H3O5P	(=0)(0)(0)	Pubchem
-FF	FF				CC1=C2C(
					C(C(IN-	
					12)C3(C(C))	
					(C(=N3)C(
					=C4C(C(C))	
					=C4C(C(C))	
	Adenosyl				=C4C(C(C (=N4)C=C 5C(C(C1=	
cnd adcob	Adenosyl			С58Н84Са	=C4C(C(C (=N4)C=C 5C(C(C1= N5)CCC(=	
cpd_adcob	Adenosyl cobinamid	C06508	1	C58H84Co	=C4C(C(C)) (=N4)C=C 5C(C(C)= N5)CCC(= O(N)(C)C)	Puhchem

					CCC(=0)	
					N)(C)CC(
					=O(N)CC	
					CC(=0)N	
					(C)CC(-0)	
					(C)	
)N)C)CC(
					=O)N)(C)	
					CCC(=O)	
					NCC(C)O.	
					ICH2-	
					OI)N2C=	
					NC3=C2N	
					=CN=C3N	
)O)O.[Co]	
					CC1=C2C(
					C(C(IN-	
					$J^{2}C^{2}C^{2}C^{2}C^{2}C^{2}C^{2}C^{2}C$	
					(C(-N3)C(
					=C4C(C(C))	
					(=N4)C=C	
					5C(C(C1=	
					N5)CCC(=	
					O(N)(C)C)	
					CCC(=0)	
					=0)N(C)C	
					CC(=O)N)	
					(C)CC(=O	
)N)C)CC(
					=O)N)(C)	
					CCC(=0)	
					NCC(C)O	
					P(=O)(O)	
					O.[CH2-	
]C1C(C(C(
	Adenosyl				O1)N2C=	
	cobinamid				NC3=C2N	
cpd adcob	e			C58H83Co	=CN=C3N	
an	nhosnhate	C06509	_1	N16014P	1000 [Co]	Pubchem
чр	Phosphate		-1		CC1 - C2C(
					CCI=C2C(
					C(C([N-	
					J2)C3(C(C	
	Adenosyl				(C(=N3)C(
cpd_adcob	cobyrinate			C55H68Co	=C4C(C(C))	
dam	diamide	C06506	-4	N11015	(=N4)C=C	Pubchem

					5C(C(C)) =	
					JC(C(C)) =	
					N5)CCC(=	
					O(O)(C)C)	
					CCC(=O)	
					O)(C)CC(
					=O)N)C)C	
					CC(=0)0)	
					(C)CC(=0	
					(0)00(0)	
					-0)0)(C)	
					-0)0)(C)	
					O.[CH2-	
]C1C(C(C(
					O1)N2C=	
					NC3=C2N	
					=CN=C3N	
)O)O.[Co+	
					3]	
					CC1=C2C(
					C(C([1] - 12))	
					$\frac{12}{5}C_{3}(C(C))$	
					(C(=N3)C(
					=C4C(C(C))	
					(=N4)C=C	
					5C(C(C1=	
					N5)CCC(=	
					O(N)(C)C)	
					CCC(=O)	
					N(C)CC(
					=0)N)C)C	
					CC(-O)N	
					CC(-O)N	
					(C)CC(=0)	
)N)C)CC(
					=O(N)(C)	
					CCC(=O)	
					O.[CH2-	
]C1C(C(C(
					O1)N2C=	
	adenosvl-				NC3=C2N	
cnd adcob	cobvric			C55H76Co	=CN=C3N	
hex	acid	C06507	0	N15011	$(0) \cap [C_0]$	Pubchem
пол	autu	00007	0		C1 - NC2 -	
					CI = NC2 = C(N1)C(
		G001 (-	_		C(NI)C(=	D 1 1
cpd_ade	Adenine	C00147	0	C5H5N5	NC=N2)N	Pubchem
cpd_adgco	Adenosine			C68H95Co	CC1=C2C(
ba	-GDP-	C06510	-1	N21O21P2	C(C([N-	Pubchem

	cobinamid]2)C3(C(C	
	e				(C(=N3)C(
					=C4C(C(C)	
					(=N4)C=C	
					5C(C(C) = 100)	
					N5)CCC(=	
					O(N)(C)C)	
					CCC(-0)	
					N(C)CC(
					-0)N(C)C	
					CC(=O)N	
					(C)CC(=0	
)N)C)CC(
					=O(N)(C)	
					CCC(=O)	
					NCC(C)O	
					P(=O)(O)	
					OP(=O)(O	
)OCC6C(C	
					(C(O6)N7	
					C=NC8=C	
					7N=C(NC	
					8=0)N)O)	
					O.[CH2-	
					O1)N2C=	
					NC3=C2N	
					=CN=C3N	
					(0) = (0) = (0)	
					C1 = NC2 =	
					C(C(=N1))	
					C(C(-N))	
					$C_2 C(C(C))$	
				C101112N	$C_{C}(C)(C)$	
and adm	Adamasina	C00212	0	C10H15IN	03)00)0)	Dubaham
cpd_adn	Adenosine	C00212	0	304		Publichem
					CI=NC2=	
					C(C(=NI))	
					N)N=CN2	
					C3C(C(C(
					O3)COP(=	
					O)(O)OP(
				C10H12N	=O)(O)O)	
cpd_adp	ADP	C00008	-3	5O10P2	O)O	Pubchem
					C1=NC2=	
cpd_adpgl	ADPgluco			C16H23N	C(C(=N1)	
c	se	C00498	-2	5015P2	N)N=CN2	Pubchem

					C3C(C(C(
					$O_{3}^{(0)}(O_{1}^{(0)}) = 0$	
					O(O)OP(
					=0)(0)00	
					4C(C(C(C	
					O4)CO)O)	
					O)O)O)O	
					C1=NC2=	
					C(C(=N1))	
					N)N=CN2	
					C3C(C(C)	
					$O_{3}^{(0)} O_{2}^{(0)} =$	
					O(0)OP(
					=0)(0)00	
	ADP-D-				40(0(0(0	
	glycero-D-				O4)C(CO)	
cpd_adphe	manno-			C17H25N	0)0)0)0)	
p-DD	heptose	C06397	-2	5O16P2	O)O	Pubchem
					C1=NC2=	
					C(C(=N1))	
					N)N=CN2	
					C3C(C(C))	
					$O_{3}^{(0)}(C)P(-$	
					$O_{J}(O)OD($	
					U)(U)UP(
					=0)(0)00	
					C(C(C(C=	
	ADP			C15H21N	0)0)0)0)	
cpd_adprib	Ribose	C00301	-2	5O14P2	0)0	Pubchem
					C(CCN=C	
cpd_agm	Agmatine	C00179	2	C5H16N4	(N)N)CN	Pubchem
					[H]C(=O)	
	acvl-					
	glyceropho				HI(O)COP	
	sphoethano			C6H13NO	(0)(=0)0	
and agna	Ispino	C04438	1	700	(0)(0)0	Dubaham
cpu_agpc	lainine	04438	-1	/1 K		1 ubenem
					CI=NC2=	
	~				C(C(=NI))	
	S-				N)N=CN2	
	Adenosyl-				C3C(C(C(
	L-				O3)CSCC	
	homocyste			C14H20N	C(C(=O)O)	
cpd ahcys	ine	C00021	0	6O5S)N)O)O	Pubchem
	2-Amino-				C1C(=NC	
	4-hydroxy-				2=C(N1)N	
	6-(ervthro-			C9H12N5	=C(NC)=	
and about	1 2 2	C04805	1	O12D2	ONDC(C)	Dubaham
cpa_anat	1,2,3-	004893	-4	013P3	O(N)C(C)	rubcnem

	trihydroxy propyl)dih ydropteridi ne triphosphat e				COP(=O)(O)OP(=O) (O)OP(=O))(O)O)O)O	
cpd_aicar	5-Amino- 1-(5- Phospho- D- ribosyl)imi dazole-4- carboxami de	C04677	-2	C9H13N4 O8P	C1=NC(= C(N1C2C(C(C(O2)C OP(=O)(O)O)O)O)N) C(=O)N	Pubchem
cpd air	5-amino-1- (5- phospho- D- ribosyl)imi dazole	C03373	-2	C8H12N3 07P	C1=C(N(C =N1)C2C(C(C(O2)C OP(=O)(O)O)O)O)N	Pubchem
cpd_akg	2- Oxoglutara te	C00026	-2	С5Н4О5	C(CC(=O) O)C(=O)C (=O)O	Pubchem
cpd_ala-B	beta- Alanine	C00099	0	C3H7NO2	C(CN)C(= O)O	Pubchem
cpd_ala-D	D-Alanine	C00133	0	C3H7NO2	$\frac{CC(C(=O))}{O)N}$	Pubchem
cpd_ala-L	L-Alanine	C00041	0	C3H7NO2	CC(C(=0) O)N	Pubchem
cpd_alaala	D-Alanyl- D-alanine	C00993	0	C6H12N2 O3	CC(C(=O) NC(C)C(= O)O)N	Pubchem
cpd_alac-S	(S)-2- Acetolactat e	C06010	-1	С5Н7О4	CC(=O)C(C)(C(=O) O)O	Pubchem
cpd_alltn- R	R- Allantoin	C02348	0	C4H6N4O 3	C1(C(=O) NC(=O)N1)NC(=O)N	Pubchem
cpd_alltn- S	S- Allantoin	C02350	0	C4H6N4O 3	C1(C(=O) NC(=O)N1)NC(=O)N	Pubchem
cpd alltt	Allantoate	C00499	0	C4H8N4O 4	C(C(=O)[O-])(NC(=O) N)NC(=O) N	Pubchem

					C[S+](CC	
					C(C(=0))	
					O_{-}	
	S					
	S-				C(C(01)N)	
	Adenosyl-			G1 51 200 1	2C=NC3=	
	L-	~~~~		CI5H23N	C2N=CN=	
cpd_amet	methionine	C00019	<u> </u>	605S	C3N)O)O	Pubchem
					C[S+](CC	
					CN)CC1C(
	S-				C(C(O1)N)	
	Adenosyl				2C=NC3=	
cpd_ameta	methionina			C14H24N	C2N=CN=	
m	mine	C01137	2	6O3S	C3N)O)O	Pubchem
	S-				C[S+](CC	
	Adenosyl-				C(=O)C(=	
	4-				$\dot{O}O\dot{O}\dot{C}\dot{C}\dot{I}$	
	methylthio				C(C(C(O1)))	
	-2-				N2C=NC3	
	oxobutano			C15H19N	=C2N=CN	
cnd amob	ate	C04425	0	5065	=C3N)O)O	Pubchem
epa_amoo		001123		2005	C1=NC2=	1 uoonom
					C(C(=N1))	
					C(C(-N))	
					N) N - C N 2	
					C3C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C	
				C101101	O3)COP(=	
				CI0HI2N	0)(0)0)0)	
cpd_amp	AMP	C00020	-2	507P	0	Pubchem
					C1=CC=C	
	Anthranilat				(C(=C1)C(
cpd_anth	e	C00108	-1	C7H6NO2	=O)O)N	Pubchem
					C1=NC2=	
					C(C(=N1))	
					N)N=CN2	
					C3C(C(C(
					O3)COP(=	
					O(O)OP(
					=0)(0)OP	
					(=0)(0)0	
					P(=0)(0)	
	D1 D4				C(04)N5C	
	1,1,1+-					
	DIS(J - dom corr1)					
	auchosyl)			C201124N		
	tetrapnosp	C012(0	4	C20H24N		D1-1
cpd_ap4a	nate	C01260	-4	10019P4	U	Pubchem

					C1=NC2=	
					C(C(=N1))	
					$NN=CN^2$	
					C3C(C(C(
					$O_{3}COP(=$	
					O(O)OP(
					=0)(0)0P	
					(=0)(0)0	
					P(=0)(0)	
					OP(=O)(O)	
					O(C)	
	P1 P5-				(C(04)N5)	
	Bis(5'-				C=NC6=C	
	adenosvl)				5N=CN=C	
	nentanhosn			C20H24N	6N(0)O(0)O(0)O(0)O(0)O(0)O(0)O(0)O(0)O(0)O	
end an5a	hate	C04058	-5	10022P5	$\frac{1}{10}$	Pubchem
cpu_ap5a	nate	04030	-5	1002213	C1 = NC2 =	1 ubenem
					$C_1 = NC_2 = C(C(=N1))$	
					NN=CN2	
					C3C(C(C))	
	Adenosine				$O_{3}^{(0)}(C) = 0$	
	S'_				O(0)OS(
	J-			C10H12N	-0)(-0)0	
and and	fata	C00224	2	5010PS	-0)(-0)0	Dubaham
cpu_aps	D	00224	-2	501015		1 ubenem
	D- Arabinose				C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(
	S_				O(OP(=0))	
end ara5n	J- nhosnhate	C01112	_2	C5H9O8P	(0)01(-0)	Pubchem
cpu_ara5p	phosphate	01112	-2	03119081	(0)0	1 ubenem
and arah	т				C(01)0)0	
	L-	C00250	0	C5U10O5	C(01)0)0	Dubaham
	Alabillose	C00239	0	CJIII005	$\int O \int O$	rubenenn
				CGUISNA	C(CC(C) = 0)	
and and I	I Argining	C00062	1	$C0\Pi I SN4$	-C(N)N	Dubaham
cpu_arg-L	L-Arginne	C00002	1	02	-C(N)N	Fubchem
	N(amaga)				C(CC(C) = 0)	
	N(omega)-					
	(L-				=C(N)NC(
	Arginino)s	C0240C	1	CIUHI/N	CC(=0)0)	D-1.1.
cpd_argsuc	uccinate	C03406	-1	406	C(=0)0	Pubchem
1		001470	2	4 1104	O[As](=O)	D 1 1
cpd_arsna	Arsenate	C014/8	-2	ASHO4	(0)0	Pubchem
1	•		<u>^</u>		J[As]([O-	D 1 1
cpd_arsni2	arsenite	C06697	0	AsH3O3])[O-]	Pubchem

					C(C(C(=O	
	т			C4H8N2O	O(0) = O(0) = O(0)	
and san T		C00152	0	2	(0)	Darkaham
cpd_asn-L	Asparagine	C00152	0	3		Pubchem
	_				C(C(C(=O	
	L-				O(N) C(=	
cpd_asp-L	Aspartate	C00049	-1	C4H6NO4	0)0	Pubchem
	L-					
	Aspartate					
	4-				C(C=O)C(
	semialdehv				C(=O)[O-	
cpd aspsa	de	C00441	0	C4H7NO3	1)[NH3+1	Pubchem
opu_uopou		000111			C1 = NC2 =	
					C(C(-N1))	
					C(C(-N))	
					N) N - $CN2$	
					$O_3)COP(=$	
					O)(O)OP(
					=O)(O)OP	
				C10H12N	(=O)(O)O)	
cpd_atp	ATP	C00002	-4	5013P3	O)O	Pubchem
	Betaine				C[N+](C)(
cpd betald	aldehyde	C00576	1	C5H12NO	C)CC=O	Pubchem
• <u> </u>					C(C1C(C(
					$\dot{c}(\dot{c}(\dot{o}))\dot{o}$	
					czcioćic	
					$(C^{2}O)O)O$	
				С12H220	(020)0)0	
and hal	cellobiose	C00185	0	11	$\sum_{i=1}^{n} (i) (i) (i) (i) (i) (i) (i) (i) (i) (i)$	Dubchem
cpu_ogi	centoutose	00185	0	11	CCCC(-0)	1 ubenenn
)SCCNC(=	
					O)CCNC(
					=O)C(C(C)	
)(C)COP(=	
					O)(O)OP(
					=O)(O)OC	
					C1C(C(C(
					O1)N2C=	
					NC3=C2N	
					=CN=C3N	
	Butanovl-			C25H38N)O)OP(=O	
cnd btcoa	CoA	C00136	_4	7017P3S		Pubchem
-pa_oteou		200120	T	, 01,130	C1C2C(C)	
				CIOUISN	C(-0)	
		C00120	1		C(-0)0)N	D11
cpd_btn	Biotin	C00120	-1	2038	C(=0)N2	Pubchem

					CCCC(=O	
cpd_but	Butyrate	C00246	-1	C4H7O2)0	Pubchem
cpd_ca2	Calcium	C00076	2	Ca	[Ca]	Pubchem
cpd camp	сАМР	C00575	-1	C10H11N 506P	C1C2C(C(C(O2)N3C =NC4=C3 N=CN=C4 N)O)OP(= O)(O1)O	Pubchem
cpd cbasp	N- Carbamoyl -L- aspartate	C00438	-2	C5H6N2O 5	C(C(C(=O)O)NC(=O)N)C(=O) O	Pubchem
end_chi	Cobinamid	C05774	0	C48H72Co N1108	CC1=C2C(C(C([N-]2)C3(C(C)(C(=N3)C()=C4C(C(C)(=N4)C=C)5C(C(C1=)N5)CCC(=)N5)CCC(=)N)(C)CC(=)	Pubchem
cpd_cbi	e Cob(I)ala min	C05774	0	C62H88Co N13O14P	$[Co+3] \\ CC1=CC2 \\ =C(C=C1) \\ C)N(C=N2) \\ CCC(C(C) \\ C)CO(C) \\ (C)CNC(C) \\ =O)CCC4(C)CCC(C) \\ C(C)CCC(C) \\ C(C)CCC(C) \\ C(C)CCC(C) \\ C(C)CCC(C) \\ C(C)CCCC(C) \\ C(C)CCCCCC \\ C(C)CCCCCC \\ C(C)CCCCCC \\ C(C)CCCCCCC \\ C(C)CCCCCCC \\ C(C)CCCCCCC \\ C(C)CCCCCCCC \\ C(C)CCCCCCCC \\ C(C)CCCCCCCC \\ C(C)CCCCCCCC \\ C(C)CCCCCCCCC \\ C(C)CCCCCCCCCC$	Pubchem

					CAIN	
					C4[N-	
]5)C)CCC(
					=O)N)(C)	
					C)CCC(=	
					O(N)(C)C	
					C(-0)NO	
					C(-0)N)C	
)CCC(=O)	
					N)(C)CC(
					=O)N)C)C	
					C(=O)N)C	
					$O[C_0]$	
					C(-O)(N)	
	a 1 1				C(=O)(N)	
	Carbamoyl				OP(=O)(O	
cpd_cbp	phosphate	C00169	-2	CH2NO5P)0	Pubchem
					C1=CN(C(
					=0)N=C1	
					N)C2C(C(
					C(O)COP	
					C(02)COP	
					(=O)(O)O	
				C9H12N3	P(=O)(O)	
cpd cdp	CDP	C00112	-3	O11P2	O)O)O	Pubchem
					CC1C(=0)	
					C(C(C(0)))	
					C(C(C(OI)))	
					OP(=0)(0	
)OP(=O)(
					O)OCC2C	
					(C(C(O2)))	
	CDP-4-				N3C=CC(
	dehydro-6-				=NC3=O)	
and admid	denyulo o			CISU2IN	\mathbf{N}	
cpu_cup4u	deoxy-D-	001010				D 1 1
6dg	glucose	C01219	-2	3015P2	0	Pubchem
					[H]C(=O)	
					OC[C@H]	
					(COP(O)) =	
					\hat{O}	
					@H]([C@	
					H](O)[C@	
					(<i>a</i>)H]1O)N	
					1C = CC(N)	
					=NC1=O	
and admits	CDDdiam1			C14117N	$\Omega C(\Pi) =$	
cpu_cupua		C002(0	~	$C14\Pi1/IN$		D.1. 1.
g	glycerol	00269	-2	3015P2R2	U	Pubchem
	CDP-			C15H23N	C1=CN(C(
cpd_cdpg	glucose	C00501	-2	3O16P2	=O)N=C1	Pubchem

					N)C2C(C(
					C(O2)COP	
					(-0)(0)0	
					(-0)(0)0	
					P(=0)(0)	
					0030(0(0	
					(C(O3)CO)	
					()	
					0	
	Methanethi					
cpd_ch4s	ol	C00409	0	CH4S	CS	Pubchem
					CC(=O)N	
					C1C(C(C(
					OC1O)CO	
					OC2C(C(
					C(C(O2)C)	
				C16H28N	0)0)0NC	
end chitch	Chitobiose	C01674	0	2011	(=0)C)O	Pubchem
epu_enitoo	Cintobiose	010/4	0	2011	(-0)C)C	1 ubenem
and abal	ahalina	C00114	1	C5U14NO	C[N+](C)(Duhaham
cpu_cnoi	chonne	C00114	1	CJH14NO		Fubchem
					C=C(C(=O	
)O)OCIC=	
	Chorismat				C(C=CC1	
cpd_chor	e	C00251	-2	C10H8O6	O(C=O)O	Pubchem
					C1=CC=C	
	trans-				(C=C1)C=	
cpd_cinnm	Cinnamate	C00423	-1	C9H7O2	CC(=O)O	Pubchem
					C(C(=O)O)	
					$)\hat{C}(\hat{C}C(=O)$	
					(O)(C(=O))	
end cit	Citrate	C00158	-3	C6H5O7	0)0	Pubchem
		000100		0011007	C(CC)(C) =	
	т			C6U12N2	C(CC(C) = 0)	
and alter T	L- Citmallin a	C00227	0	CONTSINS	C(-0)N	Dark als area
cpd_chr-L	Citruinne	C00327	0	03	C(-0)N	Publichem
					OCI(C(=0)	
)O)OP(=O	
)(O)OCC2	
	CMP-3-				C(C(C(O2))	
	deoxy-D-				N3C=CC(
	manno-				=NC3=O)	
	octulosona			C17H24N	N)O)O)C(
cpd ckdo	te	C04121	-2	3O15P	0(0(00)	Pubchem
	CMP-8-				C1C(C(C(
	amino-3.8-				OC1(C(=0))	
cpd ckdo8	dideoxy-			C17H26N)[O-	
n	D-manno-	C21334	_1	4014P	1)OP(=O)([Pubchem
			1			- 40 0110111

	oct-2-				O-	
	ulosonic				1)OCC2C(
	acid				$\hat{C}(C(O2)N)$	
	aera				3C = CC(=	
					NC3-O(N)	
					(0)	
					NH3+JO)	
					0)0	
cpd_cl	Chloride	C00698	-1	Cl	[Cl-]	Pubchem
					C1=CC(=	
					CC=C1C(
					C(CO)NC(
					$=$ $\hat{O})C(C1)\hat{C}$	
	Chloramph			C11H12C1	1)0)[N+1(=	
end em	enicol	C00918	0	2N2O5	0)[0-]	Pubchem
epu_em	emeen	000710	0	211205	CC(=0)0	1 uoonom
					CC(C(C1-	
					CC(C(C)) = C(C)	
	C1 1 1				CI)[N+](=	
	Chloramph				0)[0-	
_	enicol 3-		_	CI3HI4CI])O)NC(=	
cpd_cmac	acetate	C03601	0	2N2O6	O)C(CI)CI	Pubchem
					C1=CN(C(
					=O)N=C1	
					N)C2C(C(
					C(O2)COP	
				C9H12N3	(=O)(O)O)	
cpd cmp	CMP	C00055	-2	O8P	0)0	Pubchem
cpd co2	CO2	C00011	0	CO2	C(=O)=O	Pubchem
- F					CC(C)(CO)	
					P(=0)(0)	
					OP(=O)(O)	
) 0 C C 1 C C C	
					C(01)N2	
					C = NC2 C	
					C=INC3=C	
					3N)O)OP(
					=O)(O)O)	
					C(C(=O)N)	
	Coenzyme			C21H32N	CCC(=O)	
cpd_coa	А	C00010	-4	7016P3S	NCCS)O	Pubchem
cpd_cobalt						
2	Co2+	C00175	2	Co	[Co+2]	Pubchem
cpd cobalt						
3	Co3+	C19171	3	Co	[Co+3]	Pubchem

					CC1=CC2	
					=C(C=C1)	
					C)N(C=N2)	
					$O_3)CO)OP$	
					(=0)([0])	
					(-0)(0-	
					$\int \int $	
					NC(-0)C	
					=N6)C(=C	
					/C(C(C(=	
					N7)C=C8	
					C(C(C(=N	
					8)C(=C4[
					N-	
]5)C)CCC(
					=O)N)(C)	
					C)CCC(=	
					O)N)(C)C	
					C(=O)N)C	
)CCC(=O)	
					N)(C)CC(
					=O)N)C)C	
					C(=O)N)C	
					$O_{\rm ICH2}$	
					01)N2C=	
					NC3=C2N	
					=CN=C3N	
and coha	Cohamida			C72H100C)0)0[Co+	
cpu_coba	Cobalilité	C00104	0	c/211100C	21	Dubaham
IIICOa	coenzyme	C00194	0	01100171	S	rubenem
1 61	G ¹ C 11			C1011100		
cpd_contal	Coniferald	G02(()	0	CIUHIOO	1)C=CC=	D 1 1
d	ehyde	C02666	0	3	0)0	Pubchem
					CC1=C2C	
					C3=C(C(=	
					C(N3)CC4	
					=C(C(=C(
					N4)CC5=	
					C(C(=C(N	
					5)CC(=C1	
	Coproporp				CCC(=O)	
cpd_cpppg	hyrinogen			C36H40N	O)N2)C)C	
3	III	C03263	-4	408	CC(=O)O)	Pubchem

					C)CCC(=	
					0)0)CCC(
					=0)0)C	
					[O-	
					[Cr](=0)(
end cro4	chromate	NA	-2	CrO4	=0)[0-]	Pubchem
epa_erer	emonate	1111		0101	<u>оло</u>	1 ubenenn
end CrOH].[OH-	
	$C_r(OH)$	NA	0	CrO3H3	$\int Cr + 3$	Dubchem
5			0	005115	$\frac{J}{C} = \frac{C}{C} = \frac{C}$	1 ubenem
					-0)N-C1	
and acn	Cutasina	C00380	0	CAUSN2O	-0) $N-01$	Dubaham
cpu_csn	Cytosine	00380	0	C4HJN3U	\mathbf{N}	Fubclielli
					CI = CIN(C(
					=0)N=C1	
					N)C2C(C(
					C(02)COP	
					(=0)(0)0	
				COLLIANIA	P(=O)(O)	
1 /	CTD	00000	4	C9H12N3	OP(=O)(O)	D 1 1
cpd_ctp	CIP	C00063	-4	014P3)0)0)0	Pubchem
cpd_cu2	Cu2+	C00070	2	Cu	[Cu+2]	Pubchem
cpd_cyan	cyanide	C01326	0	HCN	C#N	Pubchem
					C(C(C(=O	
cpd_cys-	Cystyl-			C5H10N2)NCC(=O)	
gly	Glycine	C01419	0	O3S	O)N)S	Pubchem
				C3H7NO2	C(C(C(=O	
cpd_cys-L	L-Cysteine	C00097	0	S)O)N)S	Pubchem
					C(CSCC(C	
	L-				(=O)O)N)	
cpd_cysth-	Cystathion			C7H14N2	C(C(=O)O)	
L	ine	C02291	0	O4S)N	Pubchem
					C1=CN(C(
					=O)N=C1	
					N)C2C(C(
				C9H13N3	C(O2)CO)	
cpd_cytd	Cytidine	C00475	0	05	O)O	Pubchem
					C1C(C(OC	
					1N2C=NC	
					3=C2N=C	
	Deoxyaden			C10H13N	N=C3N)C	
cpd_dad-2	osine	C00559	0	503	0)0	Pubchem
	5'-				CC1C(C(C	
	Deoxyaden			C10H13N	(O1)N2C=	
cpd_dad-5	osine	C05198	0	503	NC3=C2N	Pubchem

)0)0 C1C(C(OC 1N2C=NC	
					C1C(C(OC 1N2C=NC	
					1N2C=NC	
					3=C2N=C	
					N=C3N)C	
					OP(=O)(O	
				C10H12N) $OP(=O)($	
cpd dadp	dADP	C00206	-3	509P2	0)0)0	Pubchem
-F F					C1C(C(OC	
					1N2C=NC	
					3=C2N=C	
					N=C3NC	
				C10H12N	OP(=O)(O	
cpd damp	damp	C00360	-2	506P	(0)(0)(0)	Pubchem
	7 8-	00000		0001		1 uoenenii
	Diaminono			C9H21N2	CCCC(=0	
cnd dann	nanoate	C01037	1	0^{2}		Pubchem
	nunoute	01057	1	02	C1C(C(OC))	1 ubenem
					1N2C=NC	
					3=C2N=C	
					N=C3NC	
					OP(=O)(O	
					OP(=0)(0)	
				C10H12N	O(OP(=0))	
end datn	datp	C00131	-4	5012P3	(0)0)0	Pubchem
	3 4-	000101	•	001210		
	dihydroxy-					
	2-butanone				CC(=0)C(
2	2 outanone 4-				COP(=O)(
cpd_db4n_t	nhosnhate	C15556	-2	С4Н7О6Р	$\frac{1}{2}$	Pubchem
epa_ao-ip j	phosphate	015550	<u>L</u>	0.117001	$C_{1=NC_{2=}}$	1 doenem
					C(C(=N1))	
					NC(CC(=NT))	
					(0))(0)(=0)	
					(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(
	$N6_{-}(1.2_{-})$				$C_{3}C(C(C))$	
	Dicarboxy				$O_3)COP(=$	
end deam	ethvl)_			C14H14N	O(O)O(O)	
n pa_acani	AMP	C03794	_4	5011P	0	Pubchem
P 2	4 71411		+	50111		
					1N2C=CC	
					(=NC2-0)	
				COH12N2	NCOP(=	
end dedn	dCDP	C00705	_3	O10P?	O(O)OP(Pubchem
end dedn	dCDP	C00705	_2	C9H12N3	1N2C=CC (=NC2=O) N)COP(= O)(O)OP(Puhchem

					=O)(O)O)	
					0	
					C1C(C(OC	
					1N2C=CC	
					(=NC2=O)	
				C9H12N3	N)COP(=	
cpd dcmp	dCMP	C00239	-2	O7P	0)(0)0)0	Pubchem
					C1C(C(OC	
					1N2C=CC	
					(=NC2=O)	
					N)COP(=)	
					O(O)OP(
					=O)(O)OP	
				C9H12N3	(=0)(0)(0)(0)	
end detn	dCTP	C00458	-4	O13P3	$\left(\begin{array}{c} 0 \\ 0 \end{array} \right)$	Pubchem
opa_aoop	uem		· · ·	01010	C1C(C(OC))	
					1N2C=CC	
	Deoxycyti			C9H13N3	(=NC2=0)	
end devt	dine	C00881	0	04	N(1(02)0)	Pubchem
epa_acyr	unie	000001				1 doenem
					1N2C=NC	
					3-C2N-C(
					3-0.210-0(
					COP(=O)(
				C10U12N	COT(-0)(-0)	
and dadn	AGDB	C00261	2	5010P2	(0)0P(-0)	Dubaham
cpu_ugup	uoDi	000301	-3	301012	(0)0)0	1 ubenem
					1N2C=NC	
					3=C2N=C(
				CIALLAN	NC3=O(N)	
1 1	1010	G002 (2		CI0HI2N	COP(=O)(D 1 1
cpd_dgmp	dGMP	C00362	-2	507P	0)0)0	Pubchem
					IN2C=NC	
	_				3=C2N=C(
	Deoxygua		_	C10H13N	NC3=O)N)	
cpd_dgsn	nosine	C00330	0	504	CO)O	Pubchem
					C1C(C(OC	
					1N2C=NC	
					3=C2N=C(
					NC3=O)N)	
					COP(=O)(
					O)OP(=O)	
				C10H12N	(O)OP(=O	
cpd dgtp	dGTP	C00286	-4	5O13P3)(O)O)O	Pubchem

	Dihydroxy				C(C(=O)C)	
	acetone				OP(=O)(O	
cpd_dhap	phosphate	C00111	-2	C3H5O6P)O)O	Pubchem
					CC(C(C1C	
					N=C2C(=	
	6,7-				N1)C(=O)	
	Dihydrobi			C9H13N5	NC(=N2)N	
cpd_dhbpt	opterin	C00268	0	O3)O)O	Pubchem
					C1C(=NC	
					2=C(N1)N	
					=C(NC2=	
					O)N)CNC	
					3=CC=C(
					C=C3)C(=	
	7,8-				O)NC(CC	
	Dihydrofol			C19H19N	C(=O)O)C	
cpd_dhf	ate	C00415	-2	706	(=O)O	Pubchem
					C1C(=NC	
					2=C(N1)N	
					=C(NC2=	
					O)N)C(C(
	Dihydrom				COP(=O)(
	onapterin-				O)OP(=O)	
cpd_dhmpt	triphosphat			C9H12N5	(O)OP(=O	
p	e	C21094	-4	O13P3)(0)0)0)0	Pubchem
					C1=CC=C	
	1,4-				2C(=C1)C(
	Dihydroxy				=CC(=C2	
	-2-			64 4 77 6 4	O(C(=O)O)	
cpd_dhna	naphthoate	C03657	-1	C11H7O4)0	Pubchem
	2-Amino-					
	4-hydroxy-					
	6-(D-					
	erythro-					
	1,2,3-					
	trihydroxy				CIC(=NC	
	propyl)-				2=C(NI)N	
	/,8-			001110315	=C(NC2=	
1 11 .	dihydropte	GO 107 1	0	C9H13N5	O(N)C(C(D 1 1
cpd_dhnpt	ridine	C04874	0	04	CU)U)U	Pubchem
1 11	(S)-				CIC(NC(=	
cpd_dhor-	Dihydroor	G00225		C5H5N2O	U)NCI=O)	D 1 1
S	otate	C00337	-1	4	C(=0)0	Pubchem
1 11	D'1 1			001110015	CIC(=NC	
cpd_dhpm	Dihydrone	G0.502.5	-	C9H12N5	2=C(NI)N	D 1 1
p	opterin	C05925	-2	07/P	=C(NC2=	Pubchem

	monophos				O)N)C(C(
	phate				CO)OP(=	
	1				O(O)OOO	
					C1C(=NC)	
					2 = C(N1)N	
					=C(NC)=	
					O(1)CNC	
					2 - CC - C(
	Dibudranta			C14H12N	5-CC-C(
and dhut	Dillydropte	C00021	1	$C14\Pi15N$	C=CS(C)	Darkaham
cpd_dnpt	roate	C00921	-1	003	0)0	Publichem
	4,5-					
	dihydroxy-					
	2,3-				CC(=O)C(
	pentanedio				=O)C(CO)	
cpd_dhptd	ne	C11838	0	C5H8O4	0	Pubchem
					C1(C(=O))	
	Dialuric			C4H4N2O	NC(=O)N	
cpd dialu	Acid	NA	0	4	C1=O)Ó	Pubchem
· -					C1C(C(OC	
					1N2C=NC	
					3=C2N=C	
					NC3=0)C	
				C10H11N	OP(-O)(O	
and dimn		C06106	r	407D	0f(-0)(0)	Dubaham
cpu_ump	unvir	C00190	-2	4071	$\int O \int O$	Fubchenn
					IN2C-NC	
	_ .				3=C2N=C	
	Deoxyinos			C10H12N	3=C2N=C NC3=O)C	
cpd_din	Deoxyinos ine	C05512	0	C10H12N 4O4	3=C2N=C NC3=O)C O)O	Pubchem
cpd_din	Deoxyinos ine	C05512	0	C10H12N 4O4	3=C2N=C NC3=O)C O)O C1C(C(OC	Pubchem
cpd_din	Deoxyinos ine	C05512	0	C10H12N 4O4	3=C2N=C NC3=O)C O)O C1C(C(OC 1N2C=NC	Pubchem
cpd_din	Deoxyinos ine	C05512	0	C10H12N 4O4	3=C2N=C NC3=O)C O)O C1C(C(OC 1N2C=NC 3=C2N=C	Pubchem
cpd_din	Deoxyinos ine	C05512	0	C10H12N 4O4	1N2C-NC 3=C2N=C NC3=O)C O)O C1C(C(OC 1N2C=NC 3=C2N=C NC3=O)C	Pubchem
cpd_din	Deoxyinos ine	C05512	0	C10H12N 4O4	3=C2N=C NC3=O)C O)O C1C(C(OC 1N2C=NC 3=C2N=C NC3=O)C OP(=O)(O	Pubchem
cpd_din	Deoxyinos ine	C05512	0	C10H12N 4O4	3=C2N=C NC3=O)C O)O C1C(C(OC 1N2C=NC 3=C2N=C NC3=O)C OP(=O)(O)OP(=O)(Pubchem
cpd_din	Deoxyinos ine	C05512	0	C10H12N 4O4 C10H11N	1N2C-NC 3=C2N=C NC3=O)C O)O C1C(C(OC 1N2C=NC 3=C2N=C NC3=O)C OP(=O)(O)OP(=O)(O)OP(=O)	Pubchem
cpd_din	Deoxyinos ine dITP	C05512 C01345	0	C10H12N 4O4 C10H11N 4O13P3	1N2C-NC 3=C2N=C NC3=O)C O)O C1C(C(OC 1N2C=NC 3=C2N=C NC3=O)C OP(=O)(O)OP(=O)(O)OP(=O) (O)O)O	Pubchem
cpd_din cpd_ditp	Deoxyinos ine dITP 2.3-	C05512 C01345	0	C10H12N 4O4 C10H11N 4O13P3	1N2C-NC 3=C2N=C NC3=O)C O)O C1C(C(OC 1N2C=NC 3=C2N=C NC3=O)C OP(=O)(O)OP(=O)(O)OP(=O)(O)OP(=O) (O)OP(=O)	Pubchem
cpd_din cpd_ditp	Deoxyinos ine dITP 2,3- diketo5-	C05512 C01345	0	C10H12N 4O4 C10H11N 4O13P3	1N2C-NC 3=C2N=C NC3=O)C O)O C1C(C(OC 1N2C=NC 3=C2N=C NC3=O)C OP(=O)(O)OP(=O)(O)OP(=O) (O)OP(=O)	Pubchem
cpd_din cpd_ditp	Deoxyinos ine dITP 2,3- diketo5- methylthio	C05512 C01345	0	C10H12N 4O4 C10H11N 4O13P3	IN2C-NC 3=C2N=C NC3=O)C O)O C1C(C(OC 1N2C=NC 3=C2N=C NC3=O)C OP(=O)(O)OP(=O)(O (O)OP(=O) (O)O)O	Pubchem
cpd_din cpd_ditp	Deoxyinos ine dITP 2,3- diketo5- methylthio	C05512 C01345	0	C10H12N 4O4 C10H11N 4O13P3	$\frac{1}{3} = \frac{2}{2} = \frac{2}{3} = \frac{2}{2} = \frac{2}{3} = \frac{2}$	Pubchem
cpd_din cpd_ditp	Deoxyinos ine dITP 2,3- diketo5- methylthio -1-	C05512 C01345	0	C10H12N 4O4 C10H11N 4O13P3	$\frac{1}{2} = \frac{1}{2} = \frac{1}$	Pubchem
cpd_din cpd_ditp cpd_dkmp	Deoxyinos ine dITP 2,3- diketo5- methylthio -1- phosphope	C05512 C01345	0	C10H12N 4O4 C10H11N 4O13P3 C6H9O6P	$\frac{1}{3} = \frac{2}{2} = \frac{2}{3} = \frac{2}$	Pubchem Pubchem
cpd_din cpd_ditp cpd_dkmp p	Deoxyinos ine dITP 2,3- diketo5- methylthio -1- phosphope ntane	C05512 C01345 C15650	0	C10H12N 4O4 C10H11N 4O13P3 C6H9O6P S	$\frac{1}{3} = \frac{2}{2} = \frac{2}{3} = \frac{2}$	Pubchem Pubchem
cpd_din cpd_ditp cpd_dkmp p	Deoxyinos ine dITP 2,3- diketo5- methylthio -1- phosphope ntane	C05512 C01345 C15650		C10H12N 4O4 C10H11N 4O13P3 C6H9O6P S	$\frac{1}{3} = \frac{2}{2} = \frac{2}{3} = \frac{2}$	Pubchem Pubchem
cpd_din cpd_ditp cpd_dkmp p cpd_dmbzi	Deoxyinos ine dITP 2,3- diketo5- methylthio -1- phosphope ntane 5,6-	C05512 C01345 C15650	0 	C10H12N 4O4 C10H11N 4O13P3 C6H9O6P S	$\frac{1}{2} = \frac{1}{2} = \frac{1}$	Pubchem Pubchem Pubchem

	enzimidaz ole					
cpd_dmlz	6,7- Dimethyl- 8-(1-D- ribityl)lum azine	C04332	0	C13H18N 4O6	CC1=C(N(C2=NC(= O)NC(=O) C2=N1)C C(C(C(CO)O)O)O)C	Pubchem
cpd dmpp	Dimethylal lyl diphosphat e	C00235	-3	C5H9O7P 2	CC(=CCO P(=O)(O) OP(=O)(O)O)C	Pubchem
- <u>F</u> FF	Dimethyl)-)-	
cpd_dms	sulfide Dimothyl	C00580	0	C2H6S	CSC	Pubchem
cpd_dmso	sulfoxide	C11143	0	C2H6OS	CS(=O)C	Pubchem
cpd_dnad	Deamino- NAD+	C00857	-2	C21H24N 6O15P2	C1=CC(= C[N+](=C 1)C2C(C(C(O2)COP (=O)(O) P(=O)(O) OCC3C(C(C(O3)N4C =NC5=C4 N=CN=C5 N)O)O)O O)C(=O)O	Pubchem
and doda	Dodecanoi	C02679	1	C12H23O	CCCCCC CCCCCC(Dubchem
cpd_dodca n	Dodecanoi c acid (neutral)	C02679	-1	2 C12H24O 2	-0)[0-] CCCCCCC CCCCCC(=0)0	Pubchem
cpd_dpcoa	Dephospho -CoA	C00882	-2	C21H33N 7O13P2S	CC(C)(CO P(=O)(O) OP(=O)(O))OCC1C(C (C(O1)N2 C=NC3=C 2N=CN=C 3N)O)O)C (C(=O)NC CC(=O)N CCS)O	Pubchem

	Deoxyribo				C(C=O)C(
cpd_drib	se	C01801	0	C5H10O4	C(CO)O)O	Pubchem
					CC1C(NC(
					=O)N1)CC	
	Dethiobioti			C10H17N	CCCC(=O	
cpd_dtbt	n	C01909	-1	203)O	Pubchem
					CC1=CN(
					C(=O)NC1	
					=O)C2CC(
					C(O2)COP	
					(=O)(O)O	
	1775 5	~~~~		C10H13N	P(=O)(O)	- 1 1
cpd_dtdp	dTDP	C00363	-3	2011P2	0)0	Pubchem
					CC1C(C(C	
					(C(O1)OP(
					=O)(O)OP	
	dTDP-3-				(=O)(O)O	
	amino-3,6-					
	dideoxy-				$O_2)N_3C \equiv$	
	alpha-D-			CICULTEN	C(C(=0)N)	
cpa_atap3	galactopyr	C10047	2	C16H25N	C3=0)CO	D11
adgalp	anose	C1994/	-2	3014P2	(0)NO	Pubchem
					CCIC(C(=	
					O(C(C))	
					O(-0)(-0)(-0)	
	ATDD 2				(0)0P(-0)	
	dehydro 6				C(CC(02))	
	deoxy-				N3C=C(C(
	alpha-D-				= 0)NC3 =	
end dtdn3	galactopyr			C16H22N	O(C)O(O)	
ddgaln	anose	C19960	-2	2015P2	0	Pubchem
uuguip	unose	017700		201012	CC1C(C(C))	
					(C(01)OP(
					=0)(0)OP	
					(=0)(0)(0)	
					CC2C(CC(
					O2)N3C=	
	dTDP-6-				C(C(=O)N)	
cpd dtdp6	deoxy-L-			C16H24N	$\dot{C3=O}CO$	
dm	mannose	C03319	-2	2O15P2)0)0)0	Pubchem
					CC1C(=0)	
	dTDP-4-				C(C(C(O1)))	
	dehydro-6-				OP(=O)(O	
cpd_dtdpd	deoxy-D-			C16H22N)OP(=O)(
dg	glucose	C11907	-2	2O15P2	O)OCC2C	Pubchem

					(CC(O2)N)	
					(CC(O2))	
					3C-C(C(-	
					ONC3= O	
					C)O)O)O	
					CC1C(=O)	
					C(C(C(O1)))	
					OP(=O)(O	
)OP(=O)(
					O)OCC2C	
	dTDP-4-				(CC(02)N	
	dehvdro-6-				3C = C(C(=	
end dtdnd	deoxy-L-			C16H22N	ONC3=O)	
dm	mannose	C00688	_2	2015P2	C(0)	Pubchem
um	mannose	000000	-2	201312	C(0)(0)(0)(0)	1 ubenenn
					=0)02000	
					C(O2)COP	
					(=O)(O)O	
					P(=O)(O)	
					OC3C(C(C	
cpd_dtdpgl	dTDPgluc			C16H24N	(C(O3)CO	
c	ose	C00842	-2	2O16P2)0)0)0)0	Pubchem
					CC1=CN(
					C(=O)NC1	
					$=$ $\hat{O})\hat{C^2CC}$	
					C(O2)COP	
				C10H13N	(=0)(0)0)	
and dtmn	ATMP	C00364	2	208P	(0)(0)0)	Pubchem
cpa_amp	uIIVIF	C00304	-2	2001	O	rubeneni
					C(=0)NCI	
					=0)C2CC(
					C(O2)COP	
					(=O)(O)O	
					P(=O)(O)	
				C10H13N	OP(=O)(O	
cpd_dttp	dTTP	C00459	-4	2O14P3)O)O	Pubchem
					C1C(C(OC	
					1N2C=CC	
					(=0)NC2=	
					O)COP(=	
					O(O)OP(
				C9H11N2	=0)(0)01	
and dudn	AUDP	C01246	2	011D2		Dubaham
cpa_auap	uUDP	01340	-3	01172		rubenem
				001111212		
		G00065	-	C9H1IN2	IN2C=CC	D 1 1
cpd_dump	dUMP	C00365	-2	O8P	(=O)NC2=	Pubchem
					O)COP(=	
-----------	-------------	--------	----------	-----------	--	--------------
					O(O)O)O	
					C1C(C(OC	
					1N2C=CC	
	Deoxyuridi			C9H12N2	(=O)NC2=	
cpd_duri	ne	C00526	0	05	O)CO)O	Pubchem
					C1C(C(OC	
					1N2C=CC	
					(=O)NC2=	
					O)COP(=	
					O)(O)OP(
				COLL11110	=O(O)OP	
		C004(0	4	C9HTIN2	(=0)(0)0)	D-1.1.
cpd_dutp		C00460	-4	014P3	0	Pubchem
	D vululoso				CC(-O)C(
and dyv15	D-xylulose				C(COP(-O))	
n	nhosnhate	C11437	_2	С5Н9О7Р	C(COI(=0))	Pubchem
P	D-	011457		0,11,0,11)(0)0)0)0	1 ubenem
	Ervthrose				C(C(C(C=	
	4-				O)O)O)OP	
cpd e4p	phosphate	C00279	-2	C4H7O7P	(=0)(0)0	Pubchem
	D-erythro-					
	1-					
	(Imidazol-					
	4-				C1=C(NC	
	yl)glycerol				=N1)C(C(
	3-			C6H9N2O	COP(=O)(
cpd_eig3p	phosphate	C04666	-2	6P	0)0)0)0	Pubchem
	Ethanolam	G00100		COLUNIO	C(CO)N	D 1 1
cpd_etha	ıne	C00189	<u> </u>	C2H8NO	C(CO)N	Pubchem
cpd_etoh	Ethanol	C00469	0	C2H6O	CCO	Pubchem
					C(C1C(C(
	DD				C(O1)(CO	
	D-Fructose			0(111100	(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(
and for	0-	C00085	2	C6H11O9	P(=O)(O)	Durb als and
cpd_16p	pnospnate	C00085	-2	P	0	Pubchem
	Fatty agid					
	I ally actu			C1/H270	CCC(-0)	
end fal	C14.0	C06424	_1	2	0	Pubchem
-pa_iai	C11.0j	C0012T	-1		\tilde{C}	
	Fatty acid				CCCCCC	
	(Iso-			C17H33O	CCCCCCC	
cpd_fa11	C17:0)	C16995	-1	2	=0)0	Pubchem

						CC(C)CC	
					C13H25O	CCCCCC	
cnd fa	a13	Iso-C13:0	NA	-1	2	CC(=O)O	Pubchem
- <u>r</u>							
		9F-					
and fo	171	Hontadaga			C17H21O		
	a1/1	Tieptadece	C16526	1	2		Darkaham
nð		noic acid	C10330	-1	2	0)0	Pubchem
						CCCCCCC	
						C=CCCCC	
cpd_fa	a181	C18:1ome			C18H33O	CCCCCC(
n7		ga7	NA	-1	2	=O)O	Pubchem
						CC(C)CC	
		Fatty acid				CCCCCC	
		(Iso-			C15H29O	CCCC(=O	
cnd fa	a3	C15:0)	C16537	-1	2	$\mathbf{\hat{0}}$	Pubchem
- <u>-</u>	-					CC(C)CC	
		Fatty acid					
		fatty actu			C16U210		
1.0	((1SO-	000240	1	21011310		D 1 1
cpd_fa	a6	C16:0)	C00249	-1	2		Pubchem
						CC1=CC2	
						=C(C=C1)	
						C)N(C3=N	
						C(=O)NC(
						=O)C3=N2	
)CC(C(C(
						COP(=O)(
						O)OP(=O)	
						(0)0000	
						(0)0004	
						C(C(C(04)))	
						NSC=NC6	
						=C5N=CN	
					C27H31N	=C6N)O)O	
cpd_fa	ad	FAD	C00016	-2	9O15P2)0)0)0	Pubchem
						CC1=CC2	
						=C(C=C1)	
						C)N(C3=C	
						(N2)C(=0)	
						NC(=0)N3	
						COP(-O)	
						$\frac{(-0)}{(-0)}$	
						(0)OP(=0)	
						C(C(C(O4)	
					C27H33N	N5C=NC6	
cpd fa	adh2	FADH2	C01352	-2	9015P2	=C5N=CN	Pubchem

					=C6N)O)O	
)0)0)0	
	Formaldeh					
cpd_fald	yde	C00067	0	CH2O	C=O	Pubchem
cpd_fdp	D-Fructose 1,6- bisphospha te	C00354	-4	C6H10O1 2P2	C(C1C(C(C(O1)(CO P(=O)(O) O)O)O)O) OP(=O)(O)O	Pubchem
cpd_fe2	Fe2+	C14818	2	Fe	[Fe+2]	Pubchem
cpd fe3	Fe3+	C14819	3	Fe	[Fe+3]	Pubchem
cpd fgam	N2- Formyl- N1-(5- phospho- D- ribosyl)gly cinamide	C04376	-2	C8H13N2 O9P	C(C1C(C(C(O1)NC(=O)CNC= O)O)O)OP (=O)(O)O	Pubchem
					C(CC(=O)	
cpd_fglut- S	S- Formylglut athione	C01031	-1	C11H16N 307S	NC(CSC= O)C(=O)N CC(=O)O) C(C(=O)O)N	Pubchem
cpd_ficytc c	Ferricytoc hrome c	C00125	3	C42H50Fe N8O6S2	CC1=C(C2 =CC3=NC (=CC4=N C(=CC5= C(C(=C([N-]5)C=C1[N-]2)C)CCC(=O)O)C(= C4C)CCC(=O)O)C(= C3C=C)C) C.[Fe+5]	Pubchem
cpd fmn	flavin mononucle otide	C00061	-2	C17H19N 4O9P	CC1=CC2 =C(C=C1 C)N(C3=N C(=O)NC(=O)C3=N2)CC(C(C(COP(=O)(Pubchem

					0)0)0)0)	
					0	
					CC1=CC2	
					=C(C=C1)	
					C)N(C3=C	
					(N2)C(=O)	
					NC(=O)N3	
	flavin)CC(C(C(
	mononucle				COP(=O)([
cpd_fmnR	otide			C17H21N	O-])[O-	
D	reduced	C01847	-2	409P])0)0)0	Pubchem
					CC1=C(C2	
					=NCI=CC	
					3=C(C(=C	
					([N-	
]3)C=C4C(
					=C(C)=N4	
					$C(C(-C_2))$	
					C(C(-C2))	
					15C = CC	
					(10) C C C (=	
					0)0)CCC(
end focyte	Ferrocytoc			C42H50Fe	=0)0)C)C	
c	hrome c	C00126	2	N806S2	.[Fe+2]	Pubchem
cpd for	Formate	C00058	-1	CH1O2	C(=O)[O-]	Pubchem
-p	N-	200020				
	Formimido				C(CC(=O))	
	vl-L-			C6H9N2O	O)C(C(=O)	
cpd forglu	glutamate	C00439	-1	4)Ó)N=CN	Pubchem
	2-				, ,	
	(Formamid					
	o)-N1-(5-				C(C1C(C(
	phospho-				C(O1)N=C	
	D-				(CNC=O)	
	ribosyl)ace			C8H14N3	N)O)OP	
cpd_fpram	tamidine	C04640	-2	O8P	(=O)(O)O	Pubchem
	5-					
	Formamid					
	0-1-(5-				Cl=NC(=	
	phospho-				C(NIC2C(
	D-				C(C(O2)C)	
	ribosyl)imi				OP(=0)(0)	
	uazoie-4-			C10112N	(U)U(U)N	
and fait	carboxami	C04724	2	LIUHI3N	U=U)U(=U)	Dubahaw
cpu iprica	ue	UU4/34	-2	409P	JIN	rubchem

					CC(=CCC	
					C(=CCCC(
					=CCOP(=	
	Farnesvl				O(O)OP(
	dinhosnhat			C15H25O	=0)(0)01(
and frdn	aipiiospiiat	C00448	2	702	-0)(0)0)	Dubaham
cpu_nup		C00440	-3	/12	C)C)C	1 ubenem
1.01	D 1.	G01404		G1011004	1)C=CC(=	D 1 1
cpd_frlt	Ferulate	C01494	-1	C10H9O4	0)0)0	Pubchem
1.0.1	Formamid	~~~				
cpd_frmd	e	C00488	0	CH3NO	C(=O)N	Pubchem
					C(=CC(=O	
)[O-	
])C(=O)[O	
cpd_fum	Fumarate	C00122	-2	C4H2O4	-]	Pubchem
					C(C1C(C(
					C(C(O1)O	
	D-Glucose				P(=O)(O)	
	1-			C6H11O9	0)0)0)0)	
cpd_g1p	phosphate	C00103	-2	Р	0	Pubchem
	Glyceralde				C(C(C=O))	
	hyde 3-				O)OP(=O)	
cpd g3p	phosphate	C00661	-2	C3H5O6P	(Ó)O	Pubchem
	sn-					
	Glycero-3-					
	phosphoet				C(COP(=O	
	hanolamin			C5H14NO)(0)OCC(
cpd g3pe	e	C01233	0	6P	$\hat{CO}ON$	Pubchem
<u>8-1-</u>					C(C(COP(
	Glyceroph				=0)(0)0C	
	osphoglyce			C6H14O8	C(CO)OOO	
end g3ng	rol	C03274	-1	P)0	Pubchem
<u>epa_65p6</u>	101	005271	1	1		1 ubenem
	D-Glucose				C(C=0)0)	
	6			C6H11O0	O(O)O(O)	
and abn	0- nhosnhoto	C00002	2	D	(-0)(0)0	Dubaham
cpu_gop	phosphate	C00092	-2	Γ	(-0)(0)0	rubenem
	р					
	D- Calastana	C00124	0	C(1112O(C(C(01))	Dubaham
cpu_gai	Galaciose	C00124	0	0011200		rubenem
	-1-1- D					
	alpha-D-					
	Galactose			GUILLOG	P(=O)(O)	
	1-	G00445	-	C6H11O9	0)0)0)0)	D 1 1
cpd_gal1p	phosphate	C00446	-2	Р	O	Pubchem

					C(C1C(C))	
					C(C(01))	
					020(00(0	
					(C2O)O)O	
cpd_galact				C12H22O)CO)O)O)	
an	Galactan	C05796	0	11	O)O	Pubchem
					C(C1C(C(
	D-				$\dot{c}(\dot{c}(\dot{o}))\dot{o}$	
	Glucosami				P(=0)(0)	
and com1	no 1			C6H12NO	$\frac{1}{0}$	
cpu_gann		00(15(1	OIIISNO		D-1.1.
p	phosphate	C06156	-1	8P	O	Pubchem
					C(C1C(C(
	D-				C(C(O1)O)	
	Glucosami)N)O)O)O	
cpd gam6	ne 6-			C6H13NO	P(=O)(O)	
n	phosphate	C00352	-1	8P	\mathbf{O}	Pubchem
Р	N1 (5	000352	1	01	C(C1C(C))	1 doenem
	Dh a 11					
	Phospho-				C(01)NC(
	D-				=O(CN)O)	
	ribosyl)gly			C7H14N2	O)OP(=O)	
cpd_gar	cinamide	C03838	-1	O8P	(O)O	Pubchem
	Glycolalde					
end geald	hvde	C00266	0	C2H4O2	C(C=O)O	Pubchem
opu_gouiu		000200		0211102	C1 = NC2 =	1 uo entenn
					C1-NC2-	
					C(C(O3)C)	
					OP(=O)(O	
)OP(=O)(
					O(O(O(O(O(O(O(O(O(O(O(O(O(O(O(O(O(O(O(
				C10H12N	N=C(NC2	
end odn	GDP	C00035	-3	5011P2	=0)N	Pubchem
epu_gup	GDI	000055		501112	C1-NC2-	1 doenem
					C1-NC2-	
					C(NIC3C(
					C(C(O3)C)	
					OP(=O)(O	
)OP(=O)(
					O)O)OP(=	
	Guanosine				O(O)OP(
	3' 5'-				=0)(0)0)	
	bis(diphos			C10H11N	ON-COV	
	ois(uipilos	C01229		5017D4	C_{2}	Dark also
cpa_gapap	pnate)	CU1228	-6	JU1/P4	$C_2=U)N$	rubchem
					CI=NC2=	
					C(N1C3C(
					C(C(O3)C)	
cpd gdpm	GDP-			C16H23N	OP(=O)(O	
ann	mannose	C00096	-2	5O16P2)OP(=O)(Pubchem

					O)OC4C(
					C(C(C(O4)))	
					(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(
					(NC2=O)N	
					C1=NC2=	
					C(N1C3C(
					C(C(O3)C)	
					OP(=O)(O	
)OP(=O)(
	Guanosine				O)OP(=O)	
	3'-				(0)0)0P(
	dinhosnhat				=0)(0)0P	
	alphosphat				(-0)(0)01	
	trinhognhot			C10H11N	(-0)(0)0)	
and adute	uipilospilat	C04404	7	5020D5	C_{2}	Dark als area
cpa_gaptp	e	C04494	- /	5020P5	C2=0)N	Pubchem
					CC(=CCC	
					C(=CCCC(
					=CCCC(=	
	Geranylger				CCOP(=O)	
	anyl				(O)OP(=O	
	diphosphat			C20H33O)(O)O)C)C	
cpd ggdp	e	C00353	-3	7P2)C)C	Pubchem
cpd_gglua	gammaglut amyl- gamma- aminobuty raldehyde	C15700	0	C9H16N2 04	C(CC=O) CNC(=O) CCC(C(= O)O)N	Pubchem
	gammaglut	010700	0		0)0)11	1 uo enteni
cpd_gglua bt	amyl- gamma- aminobuty rate	C15767	-1	C9H15N2 O5	C(CC(=O) O)CNC(= O)CCC(C(=O)O)N	Pubchem
					C(CCNC(
	gammaglut				=O)CCC(
cpd gglupt	amyl			C9H20N3	C(=0)O)N	
rc	putrescine	C15699	1	03	DCN	Pubchem
	r es ente		1		C(C1C(C)	• • •
					C(C(01))	
and als D	D Clusses	C00021	^	C6U1206		Dubcharr
cpu_gic-D	D-Glucose	C00031	0	C0H12U0		rubchem
	-				C(CC(=0))	
	L-			C5H10N2	N)C(C(=O)	
cpd_gln-L	Glutamine	C00064	0	03)O)N	Pubchem
	glutamyl-				C(CC(=O)	
cpd_glu-	L-aspartic			C9H12N2	O)C(C(=O	
asp-L	acid	NA	-2	07)NC(CC(=	Pubchem

					O)O)C(=O	
)O)N	
					C(CC(=O)	
	D-				O)C(C(=O)	
cpd_glu-D	Glutamate	C00217	-1	C5H8NO4)O)N	Pubchem
					C(CC(=O)	
	L-				O)C(C(=O	
cpd_glu-L	Glutamate	C00025	-1	C5H8NO4)O)N	Pubchem
	L-					
	Glutamate					
	1-				C(CC(=O)	
1 1 1	semialdehy	002741	0	CELIONICO	O)C(C=O)	D 1 1
cpd_glu1sa	de	C03741	0	C5H9NO3	N	Pubchem
	L-				C(CC(=0))	
	Glutamate			C5119NO7	OP(=O)(O)	
and alu5n	J-	C02287	2	CJHONO/	(0)	Dubaham
cpu_giusp	T	C03287	-2	ſ	0)0)N	rubenem
	L- Glutamate					
	5-				C(CC(C) =	
	semialdehv				O(O)(O)(O)(O)(O)(O)(O)(O)(O)(O)(O)(O)(O)	
cpd glu5sa	de	C01165	0	C5H9NO3	0	Pubchem
					C(CC(=O)	
	gamma-L-				NC(CS)C(
	Glutamyl-			C8H13N2	=O)O)C(C	
cpd_glucys	L-cysteine	C00669	-1	O5S	(=O)O)N	Pubchem
					C(=O)C(=	
cpd_glx	Glyoxylate	C00048	-1	C2H1O3	O)O	Pubchem
					C(C(=O)O)	
cpd_gly	Glycine	C00037	0	C2H5NO2)N	Pubchem
					C(C(C(=O	
	glycyl-L-)O)NC(=O	
cpd_gly-	aspartic			C6H9N2O)CN)C(=O	D 1 1
asp-L	acid	NA	-1	5)0	Pubchem
	- 1 1 T				C(CC(=0))	
and also	glycyl-L-			C7U11N2	O)C(C(=0))	
cpd_gry-	giutanne	NIA	1	$C/\Pi I I N 2$)0)NC(-0)	Dubaham
giu-L	aciu	INA	-1	05	$\int C N + I(C) ($	Fubchem
	Glycine			C5H11NO	C(C) = 0	
end olvh	betaine	C00719	Λ	2	[0-]	Pubchem
-p~_5190	Jeunie	200/17	0		C(C(CO)O)	
cpd glvc	Glycerol	C00116	0	C3H8O3)0	Pubchem
cpd glvc-	(R)-		•		C(C(C(=O)))	
R	Glycerate	C00258	-1	C3H5O4	$\dot{0}$	Pubchem

	sn-				C(C(COP(
cpd glyc3	Glycerol 3-				=O)(O)O)	
p	phosphate	C00093	-2	C3H7O6P	0)0	Pubchem
1	1 1				C(C(=O)O)	
cpd glyclt	Glycolate	C00160	-1	C2H3O3)0	Pubchem
	5				, C(C1C(C(
					C(C(01))	
					(C(02))	
					3C(0C(C(
					(30)000	
					CO(O)O(O)O(O)O(O)O(O)O(O)O(O)O(O)O(O)O(O	
					C4C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C	
					C(04)C(0)	
end glyco				C24H42O	(0,0)(0,0)(0)	
gen	glycogen	C00182	0	21	0)0)0	Pubchem
gen	D-	000102	0	21	0)0)0	1 ubenem
	Glycero-				C(C(C)C)	
	D-manno-				C(C(C(01)))	
	hentose				OP(=O)(O	
	1 7-				$\frac{1}{10000000000000000000000000000000000$	
end gmh1	hisphospha			C7H12O1	(0)OP(=0)	
7bn	te	C19879	_4	3P2	(0)01(0)	Pubchem
/op	D_	019079		512	C(C(C)C)	1 doenem
	D- Glucoro				C(C(C(C)))	
	D manno				OP(-O)(O	
and amh1	D-IIIdillio-			C7H13O1	(-0)(0)	
cpu_giiiii	nepiose 1-	C07838	2	0P	(0,0,0,0,0)	Dubchem
Р		07838	-2	01	C(C(C)C)	Tubenenn
	D- Glucoro				C(C(C(C)))	
	D manna				C(C(C(01)))	
and amh7	D-manno-			C7U12O1	O(0)O(0)O(0)	
cpu_giiii/	nepiose /-	C10992	2	OD	(0)0F(-0)	Dubaham
p	phosphate	C19002	-2	UP	(0)0	Fubchem
					C1 = NC2 = C(N1C2C)	
					C(R1C3C)	
					C(C(O3)C)	
					OP(-O)(O)	
				C101112N	-C(NC)	
	CMD	C00144	2	CIUHI2N	=C(NC2=	Dubaham
epa_gmp	UMP	C00144	-2	200P	C1-NC2	rubenem
	ח 1 ח				CI=NC2=	
	P1,P4-				C(NIC3C(
	B18(5'-				C(C(03)C)	
	guanosyl)			CONTOAN	OP(=O)(O)	
1 4	tetraphosp	0012(1		C20H24N	OP(=0)(D 1 1
cpd_gp4g	hate	C01261	-4	10021P4	O=OOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOOO	Pubchem

					(O)OP(=O	
)(0)0CC4	
					C(C(C(04))	
					C(C(C(O4)))	
					=C5N=C(
					NC6=O(N)	
					0)0)0)0)	
					N=C(NC2	
					=O)N	
					CC(=CCC	
					C(=CCOP(
	Geranvl				$= \hat{O} (O) OP$	
	diphosphat			C10H17O	(=0)(0)(0)	
end ordn	e	C00341	-3	7P2	(0)	Pubchem
epu_grup		000041	5	/12	$C_{1-NC_{2-}}$	1 doenem
					CN1C2C	
					$C(\Omega(\Omega))$	
					C(C(O3)C)	
				~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~	O(0)O(0)N=	
				CI0HI3N	C(NC2=O)	
cpd_gsn	Guanosine	C00387	0	505	Ν	Pubchem
					C(CC(=O)	
					NC(CSSC	
					C(C(=O)N)	
					CC(=O)O)	
					NC(=O)C	
					CC(C(=0))	
					O(0) = O(0) = O(0)	
					NCC(-0)	
	Ovidized			C201120N)NCC(-0)	
1 /1	Oxidized	000127	2	C20H30N	O(C(C) - O)	D 1 1
cpd_gthox	glutathione	C00127	-2	601282)U)N	Pubchem
					C(CC(=O))	
					NC(CS)C(
					=O)NCC(=	
	Reduced			C10H16N	0)0)C(C(
cpd_gthrd	glutathione	C00051	-1	306S	=O)O)N	Pubchem
					C1=NC2=	
					C(N1C3C(
					C(C(O3)C)	
					OP(=O)(O	
					OP(=0)(0)	
					$\frac{1}{2} \frac{1}{2} \frac{1}$	
					(0)0r(-0)	
				CIDITION		
1.	OTT	000044		CIUHI2N	N=C(NC2	D 1 1
cpd_gtp	GTP	C00044	-4	5014P3	=0)N	Pubchem
					C1=NC2=	
cpd_gua	Guanine	C00242	0	C5H5N5O	C(N1)C(=	Pubchem

				O)NC(=N2	
)Ń	
H+	C00080	1	Н	[H]	Pubchem
H2	C00282	0	H2	[HH]	Pubchem
1-hydroxy- 2-methyl- 2-(E)- butenyl 4-			C511009D	CC(=CCO P(=O)([O-])OP(=O)([
dipnosphat	C11011	2	C3H9U8P	0-j)[0-	Dubaham
e	C11811	-3	2])00	Publichem
H2O	C00001	0	H2O	0	Pubchem
Hydrogen peroxide	C00027	0	H2O2	00	Pubchem
Hydrogen sulfide	C00283	-1	HS	S	Pubchem
Bicarbonat e	C00288	-1	CHO3	C(=O)(O)[O-]	Pubchem
L- Homocyste ine	C00155	0	C4H9NO2 S	C(CS)C(C(=O)O)N	Pubchem
hexadecan oate (n- C16:0)	C00249	-1	C16H31O 2	CCCCCC CCCCCC CCCC(=O)O	Pubchem
hexadecan oate (n- C16:0) (neutral)	C00249	0	C16H32O 2	CCCCCC CCCCCC CCCCC(=O)O	Pubchem
hexadecen oate (n- C16:1)	C08362	-1	C16H29O 2	CCCCCC C=CCCCC CCCC(=0)0	Pubchem
Heme Ω	C15672	_2	C49H56Fe N4O5	CC1=C(C2 =CC3=NC (=CC4=C(C(=C([N-]4)C=C5C(=C(C(=N5)C=C1[N-]2)C=C)C) C(CCC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)C)C) C(=C3CC	Puhchem
	H+ H2 I-hydroxy- 2-methyl- 2-(E)- butenyl 4- diphosphat e H2O Hydrogen peroxide Hydrogen sulfide Bicarbonat e L- Homocyste ine hexadecan oate (n- C16:0) hexadecan oate (n- C16:0) (neutral) hexadecen oate (n- C16:1)	Image: H+C00080H2C002821-hydroxy- 2-methyl- 2-(E)- butenyl 4- diphosphat eC11811H2OC00001Hydrogen peroxideC00027Hydrogen sulfideC00283Bicarbonat eC00288L- Homocyste ineC00155hexadecan oate (n- C16:0) (neutral)C00249hexadecean oate (n- C16:1)C00249hexadecean oate (n- C16:1)C00249	H+ C00080 1 H2 C00282 0 1-hydroxy- 2-methyl- 2-(E)- - - butenyl 4- - - diphosphat - - e C11811 -3 H2O C00001 0 Hydrogen - - peroxide C00277 0 Hydrogen - - sulfide C00283 -1 Bicarbonat - - e C00155 0 hexadecan - - oate (n- C00249 -1 hexadecan - - oate (n- C00249 0 hexadecen - - oate (n- C08362 -1 C16:1) C08362 -1	H+ C00080 1 H H2 C00282 0 H2 1-hydroxy- 2-methyl- 2-(E)- K K K butenyl 4- diphosphat C5H908P C5H908P e C11811 -3 2 H2O C00001 0 H2O Hydrogen peroxide C00277 0 H2O2 Hydrogen sulfide C00283 -1 HS Bicarbonat e C00288 -1 CHO3 L- Homocyste ine C00155 0 S hexadecan oate (n- C16:0) C00249 -1 2 hexadecan oate (n- C16:1) C00249 0 2 hexadecen oate (n- C16:1) C08362 -1 2 hexadecen oate (n- C16:1) C08362 -1 2 hexadecen oate (n- C16:1) C08362 -1 2 Heme Q C15672 -2 N4O5	Image: matrix

$ \begin{array}{ c c c c c } \hline \\ c c c c c c c c c c c c c c c c c c c$
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$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$
all-trans- Heptapren yl diphosphatCO4216CO35H570CC(=CCO P(=O)(O) OP(=O)(O) OP(=O)(O) OD(CCC)Pubchemcpd_hepdpeC04216-37P2C)C)C<
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$
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all-trans- Hexapreny 1 diphosphatc01230c3CC(=CCC CCC(=C CCCC(=C CCCC(=C CCCC(=C CCCC(=C CCCC(=C CCCC(=C OP(=O)(O) OP(=O)(OP(=O)(C OP(=O)(CPubchemcpd_hexdpeC01230-37P2COCC)CPubchemmercury (charged cpd_hg2+2)C007032Hg[Hg+2]Pubchemcpd_hg2+2)C007032HgC1=CC(= C(C=C1O) CC(=C1O) CC(=O)O)Pubchemcpd_hgenti sHomogenti sateC00544-1C8H7O4OPubchemclasseC00544-1C8H7O4OPubchem
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1 diphosphat cpd_hexdp1 diphosphat eC01230-3OP(=O)(C30H49O O)O)C)C)OP(=O)(O)O)C)C)Mercury (charged cpd_hg2Mercury (charged chargedHg[Hg+2]Pubchemcpd_hg2+2)C007032HgC1=CC(= C(C=C1O) OC1=CC(= C(C=C1O) OC1=CC(= C(C=C1O) OPubchemcpd_hgenti sHomogenti sateC00544-1C8H7O4OPubchemCpd_hgenti sHomogenti sateC00544-1C8H7O4OPubchem
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Mercury (charged +2)C007032Hg[Hg+2]Pubchemcpd_hg2+2)C007032HgC1=CC(= C(C=C10) CC(=O)C)Pubchemcpd_hgenti sHomogenti sateC00544-1C8H7O4OPubchemClassC00544-1C8H7O4OPubchemCC(CO)C(C(C)CC NC(=O)CC NC(=O)C(C(C)C)C(OP(=O)(O)CC(O)C(C(C)C)C OP(=O)(O)CC(O)C(C(C)C)C
$\begin{array}{c c c c c c c c c c c c c c c c c c c $
cpd_hg2+2)C007032Hg[Hg+2]Pubchemcpd_hgentiHomogenti $C1=CC(= C(C=C10) CC(=O0)$ CC(=0)O)CC(=0)O)CC(=O)C(=O)CCsateC00544-1C8H7O4OPubchemPubchemCC(CO)C(=O)SCCNCC(=O)CCCC(=O)CCCC(=O)CCNC(=O)CCNC(=O)C(C(C)C)CNC(=O)C(OP(=O)(O)NC(=O)C(
cpd_hgentiHomogentiC00544-1C8H7O4 $C1=CC(= C(C=C10) C(C=C10) C(C=O)O)$ sateC00544-1C8H7O4OPubchemCC(CO)C(CC(CO)C(C) C(C=O)CC)CC(CO)C(C=O)CC)CC(CO)C(C=O)CC)CC(CO)C(C=O)CC)NC(=O)CCNC(=O)CCNC(=O)C(C)OP(=O)(O)CC(C)C)
cpd_hgenti sHomogenti sateC00544-1C8H7O4C(C=C1O) CC(=O)O)PubchemSC00544-1C8H7O4OPubchemCC(CO)C(=O)SCCN C(=O)CC NC(=O)C(C(C)C)C OP(=O)(O)CC(CO)C(=O)SCCN C(=O)CC NC(=O)C(OP(=O)(O)
cpd_hgentiHomogentiCO0544-1C8H7O4CC(=O)O)PubchemsateC00544-1C8H7O4OPubchemCC(CO)C(=O)SCCN C(=O)CCCC(CO)C(=O)SCCN C(=O)CCCC(CO)C(NC(=O)CC OP(=O)(O
s sate $C00544$ -1 $C8H/O4$ O Pubchem CC(CO)C(=O)SCCN C(=O)CC NC(=O)C(C(C)(C)C OP(=O)(O
CC(CO)C($=O)SCCN$ $C(=O)CC$ $NC(=O)C($ $C(C)(C)C$ $OP(=O)(O$
=O)SCCN C(=O)CC NC(=O)C(C(C)(C)C OP(=O)(O
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= C2N - CN
cpd hibeo obutyryl- $C25H39N$ $P(=0)(0)$
a C_0A C_04047 -3 $7018P3S$ O_0O Pubehem

					C1=C(NC)	
	L-				=N1)CC(C	
	Histidinol			C6H11N3	OP(=O)(O	
end hisn	nhosnhate	C01100	_1	O/P	O(0)	Pubchem
cpu_msp	phosphate	01100	-1	041	C1 = C(NC)	Tubenem
	т			COLLIANIA		
1 1 * 4 1	L-	C000(0	1	CoHI2N3	=NI)CC(C	D 1 1
cpd_histd	Histidinol	C00860	I	0		Pubchem
					C1=C(C(=	
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	TT1			GANTANT		
	HVdroxVm			C40H38N	((((((((((((((((((((((((((((((((((((
end hmhil	Hydroxym	C01024	-8	C40H38N 4O17	CCC(=0)	Pubchem
cpd_hmbil	ethylbilane	C01024	-8	C40H38N 4O17	CCC(=0) 0 $CC(C)(CO)$	Pubchem
cpd_hmbil	ethylbilane	C01024	-8	C40H38N 4O17	CCC(=0) O $CC(C)(CO$ $P(=O)(O)$	Pubchem
cpd_hmbil	ethylbilane	C01024	-8	C40H38N 4O17	CCC(=0) O $CC(C)(CO$ $P(=O)(O)$ $OP(=O)(O)$	Pubchem
cpd_hmbil	ethylbilane	C01024	-8	4017	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O	Pubchem
cpd_hmbil	ethylbilane	C01024	-8	C40H38N 4O17	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O)OCC1C(C	Pubchem
cpd_hmbil	ethylbilane	C01024	-8	4017	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O)OCC1C(C (C(O1)N2 C_NC2_C	Pubchem
cpd_hmbil	ethylbilane	C01024	-8	4017	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O)OCC1C(C (C(O1)N2 C=NC3=C	Pubchem
cpd_hmbil	ethylbilane	C01024	-8	4017	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O) OCC1C(C (C(O1)N2 C=NC3=C 2N=CN=C	Pubchem
cpd_hmbil	ethylbilane	C01024	8	4017	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O) OCC1C(C (C(O1)N2 C=NC3=C 2N=CN=C 3N)O)OP(Pubchem
cpd_hmbil	ethylbilane	C01024	-8	4017	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O))OCC1C(C (C(O1)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O)	Pubchem
cpd_hmbil	ethylbilane	C01024	-8	4017	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O))OCC1C(C (C(01)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O) C(C(=O)N	Pubchem
cpd_hmbil	ethylbilane	C01024	8	4017	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O))OCC1C(C (C(O1)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O) C(C(=O)N CCC(=O)	Pubchem
cpd_hmbil	ethylbilane	C01024	8	4017	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O))OCC1C(C (C(O1)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O) C(C(=O)N CCC(=O) NCCSC(=	Pubchem
cpd_hmbil	Hydroxym ethylbilane Hydroxym	C01024	-8	4017	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O))OCC1C(C (C(01)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O) C(C(=O)N CCC(=O) NCCSC(= O)CC(C)(Pubchem
cpd_hmbil cpd_hmgc	Hydroxym ethylbilane Hydroxym ethylglutar	C01024	-8	C40H38N 4O17 C27H39N	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O) OCC1C(C (C(01)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O) C(C(=O)N CCC(=O) NCCSC(= O)CC(C)(CC(=O)O)	Pubchem
cpd_hmbil cpd_hmgc oa	Hydroxym ethylbilane Hydroxym ethylglutar yl-CoA	C01024 C00356	8	C40H38N 4O17 C27H39N 7O20P3S	$\begin{array}{c} CCC(=0) \\ O \\ CC(C)(CO \\ P(=O)(O) \\ OP(=O)(O) \\ OP(=O)(O) \\ OCC1C(C \\ (C(O1)N2 \\ C=NC3=C \\ 2N=CN=C \\ 3N)O)OP(\\ =O)(O)O \\ CO(C(=O)N \\ CCC(=O) \\ NCCSC(= \\ O)CC(C)(\\ CC(=O)O) \\ O)O \end{array}$	Pubchem
cpd_hmbil cpd_hmgc oa	Hydroxym ethylbilane Hydroxym ethylglutar yl-CoA	C01024 C00356	8	C40H38N 4O17 C27H39N 7O20P3S	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O) OCC1C(C (C(01)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O) C(C(=O)N CCC(=O) NCCSC(= O)CC(C)(CC(=O)O) O)O C(CC(=O)	Pubchem
cpd_hmbil cpd_hmgc oa	Hydroxym ethylbilane Hydroxym ethylglutar yl-CoA	C01024 C00356	8	C40H38N 4O17 C27H39N 7O20P3S	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O) OP(=O)(O) OCC1C(C (C(01)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O) C(C(=O)N CCC(=O) NCCSC(= O)CC(C)(CC(=O)O) O)O C(CC(=O) NC(CSCO	Pubchem
cpd_hmbil cpd_hmgc oa	Hydroxym ethylbilane Hydroxym ethylglutar yl-CoA	C01024 C00356	8	C40H38N 4O17 C27H39N 7O20P3S	CCC(=O) O CC(C)(CO P(=O)(O) OP(=O)(O) OCC1C(C (C(01)N2 C=NC3=C 2N=CN=C 3N)O)OP(=O)(O)O) C(C(=O)N CCC(=O) NCCSC(= O)CC(C)(CC(=O)O) O)O C(CC(=O) NC(CSCO)C(=O)NC	Pubchem
cpd_hmbil cpd_hmgc oa	Hydroxym ethylbilane Hydroxym ethylglutar yl-CoA S- (Hydroxy	C01024 C00356	8	C40H38N 4O17 C27H39N 7O20P3S	$\begin{array}{c} CCC(=0) \\ O \\ CC(C)(CO \\ P(=O)(O) \\ OP(=O)(O) \\ OP(=O)(O) \\ OCC1C(C \\ (C(O1)N2 \\ C=NC3=C \\ 2N=CN=C \\ 3N)O)OP(\\ =O)(O)O) \\ C(C(=O)N \\ CCC(=O) \\ NCCSC(= \\ O)CC(C)(\\ CC(=O)O) \\ O)O \\ C(CC(=O) \\ O)O \\ C(CC(=O) \\ NC(CSCO \\)C(=O)NC \\ C(=O)OC $	Pubchem
cpd_hmbil cpd_hmgc oa	Hydroxym ethylbilane Hydroxym ethylglutar yl-CoA S- (Hydroxy methyl)glu	C01024 C00356		C40H38N 4O17 C27H39N 7O20P3S C11H18N	$\begin{array}{c} CCC(=0) \\ O \\ CC(C)(CO \\ P(=O)(O) \\ OP(=O)(O) \\ OP(=O)(O) \\ OCC1C(C \\ (C(01)N2 \\ C=NC3=C \\ 2N=CN=C \\ 3N)O)OP(\\ =O)(O)O) \\ C(C(=O)N \\ C(C(=O)N \\ CCC(=O) \\ NCCSC(= \\ O)CC(C)(\\ CC(=O)O) \\ O)O \\ C(CC(=O) \\ O)C \\ C(=O)NC \\ C(=O)O) \\ C(=O)O) \\ C(C(=O)O) \\ C(=O)O) \\ C(C(=O)O) \\ C(=O)O) \\ C(=O)O \\ C(=O)O) \\ C(=O)O \\ $	Pubchem

	L-					
cpd_hom-	Homoserin	0000(0	0	GALLONIOS	C(CO)C(C)	D 1 1
L	e	C00263	0	C4H9NO3	(=0)0)N	Pubchem
	1 / 1				CCCCCC	
	neptadecan			01711220		
	oate (n-	C1(005	1	CI/H330		D-1.1.
cpd_npdca	C17:0)	C16993	-1	2		Publichem
	hantadagan					
	neptadecen			C17H21O		
and hnde	$C17\cdot1)$	ΝΔ	_1	2	$0[0_{-}]$	Pubchem
cpu_npuc	Hydroxypy		-1	2	C(C(=0)C)	1 ubenenn
end hnyr	ruvate	C00168	-1	C3H3O4	(=0)0)0	Pubchem
epa_npyr	Tuvute	000100	1	0511501	C1 = NC2 =	1 doenem
	Hypoxanth				C(N1)C(=	
end hxan	ine	C00262	0	C5H4N4O	ONC=N2	Pubchem
opu_intuit		000202			C(C(=N)C)	
	Iminoaspar				(=0)0)C(=	
cpd iasp	tate	C05840	-2	C4H3NO4	0)0	Pubchem
					CC(C)C(=	
					O)SCCNC	
					(=O)CCN	
					C(=O)C(C)	
					(C)(C)CO	
					P(=O)(O)	
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)OCC1C(C	
					(C(O1)N2	
					C=NC3=C	
					2N=CN=C	
					3N)O)OP(
	Isobutyryl-			C25H38N	=O)(O)O)	
cpd_ibcoa	CoA	C00630	-4	7017P3S	0	Pubchem
					C=C(C(=O	
)O)OCIC=	
1 • 1	Isochorism	G0000 F	2	CLARAC	CC=C(CI	D 1 1
cpd_1chor	ate	C00885	-2	C10H8O6	O)C(=O)O	Pubchem
					C(C(C(C(C(=	
					(0)(0)(0)(0)(0)	
and ist	Incaitert	C00211	2	CALLOT	=0)0)0(=	Dubatan
cpa_1cit	isocitrate	C00311	-3	C0H3U/		ruocnem
					CI=NCZ=	
					U(U(=U)N)	
				C10H11N	$\frac{1}{C^3C(C)C}$	
end idn	ПР	C00104	.2	4011P2	$O_3)COP(-$	Pubchem
epa_iap			-3	101114		1 uoononi

					O)(O)OP(
					=0)(0)01(
					0)0	
	т			C6H13NO	CCC(C)C(
and its I	L- Isolouoino	C00407	0	2	C(-0)0N	Dubaham
cpu_ne-L	Isoleucille	C00407	0	2	C(-0)0)N	rubeneni
					CI=NC2=	
					C(C(=0)N)	
					I)N=CN2	
					C3C(C(C(
					O3)COP(=	
				C10H11N	0)(0)0)0)	
cpd_imp	IMP	C00130	-2	408P	0	Pubchem
					C1=CC=C	
					2C(=C1)C	
cpd_indole	Indole	C00463	0	C8H7N	=CN2	Pubchem
					C1(C(C(C	
					C(C1OP(=	
					0)(0)0)0	
					P(=O)(O)	
					O)OP(=O)	
					(Ó)O)OP(
	mvo-				=O)(O)O)	
	Inositol				OP(=O)(O	
cpd inosh	hexakispho			C6H6O24	O(0) OP(=0)	
n	sphate	C01204	-12	P6)(0)0	Pubchem
P	spinate	01201	12	10	$C_1(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C($	1 uoviteini
					C(C1OP(=	
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	$1D_{-}mv_{O_{-}}$				(0)OP(=0)	
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	1 2 4 5 6				(0)0)0F(
and incom	1,3,4,3,0-			C(117O21	-0)(0)0)	
cpd_mosp	pentakisph	C01294	10	CON/021	OP(-0)(0)	Dubaban
<u>p1</u>	osphate	C01284	-10	P3		Pubenem
	myo-	G00105	0	GUUDOC	C(CIO)O)	D 1 1
cpd_inost	Inositol	C00137	0	C6H12O6	0)0)0)0	Pubchem
					CI=NC2=	
					C(C(=O)N)	
					I)N=CN2	
					C3C(C(C(
				C10H12N	O3)CO)O)	
cpd_ins	Inosine	C00294	0	405	0	Pubchem
	Isopenteny			C5H9O7P	CC(=C)CC	
end indn	1	C00129	-3	2	OP(=O)(O	Pubchem

dip	hosphat)OP(=O)(
e	-				O)O	
					C1=NC2=	
					C(C(=O)N)	
					1)N=CN2	
					C3C(C(C(
					O3)COP(=	
					O)(O)OP(
					=O)(O)OP	
				C10H11N	(=O)(O)O)	
cpd_itp ITF	C	200081	-4	4O14P3	O)O	Pubchem
					CC(C)CC(
					=O)SCCN	
					C(=O)CC	
					NC(=O)C(
					C(C)(C)C	
					OP(=O)(O	
)OP(=O)(
					O)OCCIC	
					(C(C(OI)))	
					N2C=NC3	
					=C2N=CN	
т	1 1			COCILIAN	=C3N(0)0	
	valeryl-	202020	4	C26H40N	P(=O)(O)	Dubaham
cpd_ivcoa Co.	A C	.02939	-4	/01/P35	0)0	Pubchem
cpd_k K+	C	200238	1	K	[K+]	Pubchem
3-L	Deoxy-				avarada	
D-r	nanno-				C(C(C(C(
2-	1				C(CO)O)O	
oct	ulosona	2010(2	1	00111200	(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(D 1 1
cpd_kdo te		21063	-1	C8H13O8	O(C(=0))	Pubchem
3-L	Deoxy-					
D-t	nanno-				C(COP(=O))	
				C9111201	(0)0)000	
and kdolen nho	o- Anto C	01179	2	1D	(0)(0)(0)(0)(0) = 0	Dubaham
cpu_kuoop piic	spilate C	204470	-3	11	O(C(-0))	Publieni
and log D D I	actoto C	200256	1	C2U5O2	CC(C(-0))	Dubaham
cpu_iac-D D-I		.00230	-1	0311303	CC(C(-0))	
end lac I I I	actate C	00186	1	C3H5O3	CC(C(-0))	Dubchem
		200100	-1	0311303	റ്റ്രല	
					H(O C(a))	
					H](O[C@ H]2[C@H]	
				C24H42O	H](O[C@ H]2[C@H] (O)[C@@	

						C@@H1(
						O)O[Ca)	
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						OOO[C@H]	
						H_{140}	
						@H130)[C	
						@H120)	
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						HJIO	
					C6H13NO	CC(C)CC(
cpd_	leu-L	L-Leucine	C00123	0	2	C(=O)O)N	Pubchem
						CC(C(=O))	
						SCC(C(=O	
)NCC(=O)	
		(R)-S-				O)NC(=O)	
		Lactoylglu			C13H20N	CCC(C(=)	
cpd	lgt-S	tathione	C03451	-1	308S	0)0)N)0	Pubchem
	_ U					CCCCCC	
						CCCCCC(
						CC(=0)N	
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		2.2 Dis(2)					
		2,3-DIS $(3$ -				C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(
		nyuroxytet				$U_{j}UP(=U)$	
		radecanoy				(0)0)NC(
)-D-					
		glucosamı				CCCCCCC	
		nyl-1,6-				CCCC)O)	
		beta-D-				OC(=O)C	
		2,3-bis(3-				C(CCCCC	
		hydroxytet				CCCCCC)	
		radecanoyl				O)O)CO)O	
)-beta-D-)OC(=O)C	
		glucosami				C(CCCCC	
		nyl 1-			C68H126	CCCCCC)	
cpd	lipidA	phosphate	C04919	-4	N2O23P2	0)0	Pubchem

					CCCCCC	
					CC(=O)N	
					C1C(C(C(
					OC1OCC2	
					C(C(C(C)))	
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					02)OP(-0)	
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					=O)CC(C	
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cnd linidA	Disacchari			C68H127	(2)	
de	de	C04032	2	N2020P	00	Dubchem
us	ue	C04932	-2	N2020F		rubenem
					CCCCCC	
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					CC(=O)N	
	2.3-Bis(3-				C1C(C(C(
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	radoonovi					
) hata D				O(0)O(0)C	
)-beta-D-				0)0)0C(=	
	glucosamı				O)CC(CC	
	nyl 1-			C34H64N	CCCCCC	
cpd lipidX	phosphate	C04824	-2	O12P	O(O(333)	Pubchem
	1 1				C(CCN)C	
				C6H15N2	C(C(-0))	
11 т	тт ·	000047	1	COIII J N 2	C(C(-0))	D 1 1
cpd_lys-L	L-Lysine	C00047	I	02)N	Pubchem
					C(C(C(=O	
)O)O)C(=	
cpd mal-L	L-Malate	C00149	-2	C4H4O5	0)0	Pubchem
1_					CC(C)(CO)	
					P(-0)(0)	
					$\frac{\Gamma(-U)(U)}{\Omega V(C)}$	
					0P(=0)(0	
)OCC1C(C	
					(C(O1)N2	
					C=NC3=C	
					2N=CN=C	
					2NOOD	
					=0)(0)0)	
cpd_malco	Malonyl-			C24H33N	C(C(=O)N)	
a	CoA	C00083	-5	7019P3S	CCC(=O)	Pubchem

					NCCSC(=	
					O)CC(=O)	
					$\dot{0}0$	
					C(C1C(C))	
					C(C(01))	
					$C^{2}C(OC(C))$	
					$(C^2O)OOO$	
				C12U22O	$(C_2O)OOO$	
and malt	Maltaga	C00208	0	C12H22O	(0,0,0)	Dubaham
cpu_man	Manose	C00208	0	11		Fubchem
					$C_2C(0C(C$	
					(C20)0)0	
					C3C(OC(C	
					(C3O)O)O	
					C4C(OC(C	
					(C4O)O)O	
					C5C(OC(C	
					(C50)0)0	
					C6C(OC(C	
					(C6O)O)O	
					C7C(OC(C	
					(C7O)O)O	
)CO)CO)C	
					O)CO)CO)	
cpd malth	Maltohepta			C42H72O	CO)O)O)O	
p	ose	C06216	0	36)0	Pubchem
-					C(C1C(C(
					C(C(O1)O)	
					C2C(OC(C	
					(C2O)O)O	
					(C30)0)0	
					C4C(OC(C	
					(C40)0)0	
					$C_{10}(0)$	
					(C50)000	
					(C(0))	
and malth	Maltahar			C26U620		
cpd_maith	wianonexa	C01026	Δ	C30H02U		Dul al
X	ose	C01936	0	31	0)0)0)0	Pubchem
				CONTRAC		
	Maltopenta		-	C30H52O	C2C(OC(C	
cpd_maltpt	ose	NA	0	26	(C2O)O)O	Pubchem

					$C^{2}C(OC(C$	
					(C30)0)0	
					C4C(OC(C	
					(C40)0)0	
					C5C(OC(C	
					(C50)0)0	
					$\hat{\mathbf{D}}$	
					O(CO)O(O)	
					C(C(OI)O	
					C2C(OC(C	
					(C2O)O)O	
					C3C(OC(C	
					(C30)0)0	
	Maltotrios			C18H32O	ົ້າດູ່ມີດູ້	
end malttr	A	C01835	0	16		Pubchem
epu_manu		01055	0	10		1 ubenem
					C(C(01)0)	
					C2C(OC(C	
					(C2O)O)O	
					C3C(OC(C	
					(C3O)O)O	
					C4C(OC(C	
					(C40)0)0	
					(C+O)CO)C	
	N f = 14 = 4 = 4 = -			C2411420		
cpd_mailu	Manoteira	G00050	0	C24H42O	0)0)0)0)	D 1 1
r	ose	C02052	0	21	0	Pubchem
					C(C1C(C(
	D-				C(C(O1)O)	
	Mannose				P(=O)(O)	
cpd man1	1-			C6H11O9	OOOOO	
n n	phosphate	C00636	-2	Р	0^{\prime}	Pubchem
P	phophic	200020		-	C(C)C(C)	
	П				C(C(01))	
	D- Manuara					
1 (Mannose			0(111100)0)0)0)0	
cpd_man6	6-			C6H11O9	P(=O)(O)	
p	phosphate	C00275	-2	Р	0	Pubchem
cpd_mercp	Mercaptop				C(C(=O)C)	
pyr	yruvate	C00957	-1	C3H3O3S	(=O)O)S	Pubchem
	L-				. , ,	
	Methionin			C5H11NO	CSCCCCC	
end mat I		C00073	Δ	28		Pubchem
epu_met-L	C	00073	0	20	$\frac{1}{1}$	
	5.10			020112031	CICZUN(
	5,10-			C20H20N	C = [N+]2C	
cpd_methf	Methenylte	C00445	-1	706	3=C(N1)N	Pubchem

	trahydrofol				=C(NC3=	
	ate				O(N)C4=C	
					C=C(C=C	
					4C(=0)N	
					C(CCC) =	
					0)0)C(=0	
					0)0)0(0)	
and ma?	Μα	C00305	2	Μα	JΟ [Mα+2]	Dubchem
cpu_mg2	Ivig	000303		Ivig	$\begin{bmatrix} w_1g + 2 \end{bmatrix}$	1 ubenem
	1D muo				C(C(1))	
	ID-IIIy0-			C(111100	C(C10)0)	
cpa_m1p-	Inositol 1-	001177	2	CohiiO9	OP(=O)(O	D 1 1
D	phosphate	C011//	-2	Р)0)0)0)0	Pubchem
					CC(C(CC(
					=O)[O-	
])C(=O)[O	
					-	
	Methylisoc])(C(=O)[
cpd_micit	itrate	C04593	-3	C7H7O7	O-])O	Pubchem
					C1C2CN(
					CN2C3=C	
					(N1)N=C(
					NC3=O(N)	
					C4=CC=C	
	5 10-				(C = CA)C(
	J,10- Mathylanat				(C, C+)C(
	atrobudrof			C20H21N	-0) $RC(C)$	
and mithf	ellata	C00142	2	C2011211N	C(-0)0)	Dubaham
cpu_mm		C00145	-2	/00	C(-0)0	Fubchem
	(S)-					
	Methylmai					
	onate					
cpd_mmal	semialdehy				CC(C=O)	
sa	de	C06002	-1	C4H5O3	C(=O)O	Pubchem
					CC1=CC=	
					CC2=C1C(
					=O)C(=C(
					C2=O)CC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)CCC	
cpd mmal	methymen			C47H68O	=C(C)CCC	
7	aquinol 7	NA	0	2	=C(C)C)C	Pubchem
,	"Yumor /	1121	0		CC1=CC=	i dochem
and mman	methylmen			C47H660	CC2=C1CC	
cpu_mmqn	aquir are 7	NIA	•	24/11000	-0)C(-C(Dubcharr
1	aquinone /	INA	0	2	-U)U(=U(rubenem

					C2=O)CC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)C)C	
cpd mn2	Mn2+	C19610	2	Mn	[Mn+2]	Pubchem
1_	Manganese				O = [Mn] =	
cpd mn40	(IV) oxide	C21744	0	MnO2	0	Pubchem
<u>-p</u>					[O -	
					$1[M_0](=0)$	
cnd mobd	Molybdate	C06232	-2	M_0O4	(=0)[0-]	Pubchem
epa_mooa	Worybudde	000252			CC1=C(C2)	1 doonom
					=CC=CC=	
					$C^{2}C(=C1C)$	
					C=C(C)CC	
					C = C(C)CC	
					C=C(C)CC	
					C=C(C)CC	
					C = C(C)CC	
					C = C(C)CC	
	Menaquino			C46H66O	C = C(C)C	
epd_mal7	17	NA	0	2	0)0	Pubchem
- <u>r</u> <u>r</u>					CC1=C(C(
					=O)C2=C	
					C=CC=C2	
					C1=O)CC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)CCC	
					=C(C)CCC	
	Menaquino			C46H64O	=C(C)CCC	
cpd mqn7	ne 7	NA	0	2	=C(C)C	Pubchem
cpd mthex	Methvlglv				CC(=O)C=	
1 0	oxal	C00546	0	C3H4O2	0	Pubchem
cpd_na1	Sodium	C01330	1	Na	[Na]	Pubchem
					C1=CC(=	
					CN=C1)C(
cpd_nac	Nicotinate	C00253	-1	C6H4NO2	=O)[O-]	Pubchem
	Nicotinami				C1=CC(=	
	de adenine				C[N+](=C	
	dinucleotid			C21H26N	1)C2C(C(
cpd_nad	e	C00003	-1	7O14P2	C(O2)COP	Pubchem

					(=O)([O-])OP(=O)(O)OCC3C (C(C(O3) N4C=NC5 =C4N=CN =C5N)O)O)O)O)C(= O)N	
cpd_nadh	Nicotinami de adenine dinucleotid e - reduced	C00004	-2	C21H27N 7O14P2	C1C=CN(C=C1C(= O)N)C2C(C(C(O2)C OP(=O)(O)OP(=O)(O)OCC3C (C(C(O3) N4C=NC5 =C4N=CN =C5N)O)O)O)O	Pubchem
cpd nadp	Nicotinami de adenine dinucleotid e phosphate	C00006	-3	C21H25N 7017P3	C1=CC(= C[N+](=C C[N+](=C C[N+](=C C(C C(O2)COP C=O)(O)O)O)O)O)O)O)O)O)OOOOOOOOOOOOOOOOO	Pubchem
cpd_nadph	Nicotinami de adenine dinucleotid e phosphate - reduced	C00005	-4	C21H26N 7O17P3	C1C=CN(C=C1C(= O)N)C2C(C(C(O2)C OP(=O)(O)OP(=O)(O)OCC3C (C(C(O3) N4C=NC5 =C4N=CN =C5N)OP(Pubchem

					=O)(O)O)	
					O)O)O	
	Ammoniu					
cpd_nh4	m	C00014	1	H4N	Ν	Pubchem
cpd_ni2	Ni2+	C19609	2	Ni	[Ni+2]	Pubchem
					C1=CC(=	
					C[N+](=C	
					1)C2C(C(
	Nicotinate				C(O2)COP	
	D-			C1111101	(=0)(0)0)	
and alarmat	ribonucleot	C01195	2	CIIHI2N	O(0) =	Duhaham
cpa_nicrnt	lde	C01185	-2	09P)0	Pubchem
					CI = CC(=	
					1)C2C(C(
					$C(O_2)COP$	
					O(0)(0)(0=)	
					-	
				C11H14N])O)O)C(=	
cpd_nmn	NMN	C00455	-1	208P	O)N	Pubchem
	Nitric					
cpd_no	oxide	C00533	0	NO	[N]=O	Pubchem
cpd_no2	Nitrite	C00088	-1	NO2	N(=O)[O-]	Pubchem
					[N+](=O)([
cpd_no3	Nitrate	C00244	-1	NO3	O-])[O-]	Pubchem
cpd_o2	O2	C00007	0	O2	0=0	Pubchem
cpd_o2-	Superoxide	C00704	-1	O2	[O-][O]	Pubchem
					C(C(=O)C)	
	Oxaloaceta		_		(=O)O)C(=	
cpd_oaa	te	C00036	-2	C4H2O5	0)0	Pubchem
	. 1				CCCCCC	
	octadecano			C1011250		
and acdae	ale $(n - C_1 \cdot R \cdot \Omega)$	NA	1	2		Dubaham
cpu_ocuca	C10.0)	INA	-1	Ζ		Fubclielli
	ate (n-					
end ocdea	C18.0			C18H36O		
n	neutral	NA	0	2	=0)0	Pubchem
			•		CCCCCC	
	octadeceno				CCC=CCC	
cpd_ocdce	ate (n-			C18H33O	CCCCCC(
a	C18:1)	C00712	-1	2	=O)[O-]	Pubchem
					CC(=CCC	
	all-trans-			C40H65O	C(=CCCC(
cpd_octdp	Octaprenyl	C04146	-3	7P2	=CCCC(=	Pubchem

	diphosphat				CCCC(=C	
	e				CCC(=CC	
	-				CC(=CCC)	
					C = C C O P (
					C(-CCOF(
					=0)(0)0P	
					(=0)(0)0)	
					(C)C)C)C)	
					C)C)C)C	
	5- Hydroxy- 2-oxo-4- ureido-2,5- dihydro- 1H-					
	imidazole-				C1(=NC(=	
	5-				O)NC1(C(
	carboxylat			C5H6N4O	=O)O)O)N	
cpd ohcu	e	C12248	0	5	C(=O)N	Pubchem
	2-Oxo-3-	_			C(C(C(=0	
	hvdroxy-4-				C(=0)0	
	nhosnhobu				O(OP(=0))	
and shah	phosphoou	C06054	2	CALLACORD	(0)01(-0)	Dubaham
cpd_onpb	tanoate	C00034	-3	С4П4О8Р		Publichem
1 т	L-	000077	1	C5H13N2	C(CC)(C) =	D 1 1
cpd_orn-L	Ornithine	C000//	1	02	0)0)N)CN	Pubchem
					C1=C(NC(
					=O)NC1=	
				C5H3N2O	O)C(=O)[
cpd_orot	Orotate	C00295	-1	4	O-]	Pubchem
cpd_orot5p	Orotidine 5'- phosphate	C01103	-3	C10H10N 2O11P	C1=C(N(C (=0)NC1= O)C2C(C(C(O2)COP (=O)(O)O) O)O)C(=O)O	Pubchem
· _ 1					CC(C)(CO	
	Pantethein e 4'-	001124	2	C11H21N	P(=O)(O) O)C(C(=O))NCCC(= O)NCCS)	Delaham
cpd_pan4p	pnosphate	C01134	-2	2078	U	rubcnem
cpd_panos	Danaga	000712	0	C18H32O	C(C1C(C(C(C(01)0 CC2C(C(C (C(02)0C	Dubaham
e	Panose	C00/13	0	10	(U(UU)U)	Pubchem

					C(C(C=O)	
					0)0)0)0)	
					0)0)0)0)	
					0	
1 /						
cpd_pant-	(K)-	C00522	1	COULTOA	C(C(=0))	D 1 1
K	Pantoate	C00522	-1	C6H1104	0-j)0	Pubchem
					CI = NC2 = C(C(NI1))	
					C(C(=NI))	
					(n) = C + C + C + C + C + C + C + C + C + C	
	Adamasina				$C_{3}COP(-$	
	Auenosine				O(0)O(0)O(0)O(0)O(0)O(0)O(0)O(0)O(0)O(0)	
	bisnhosnha			C10H11N	P(=0)(0)	
end nan	te	C00054	_4	5010P2	$\frac{1}{0}$	Pubchem
opu_pup		000051	· · ·	501012	C1=NC2=	1 doenem
					C(C(=N1))	
					NN=CN2	
					C3C(C(C(
					O3)COP(=	
	3'-				0)(0)0S(
	Phosphoad				=O)(=O)O	
	enylyl			C10H11N)OP(=O)(
cpd_paps	sulfate	C00053	-4	5013P2S	0)0)0	Pubchem
					CCCCCC	
	pentadecen				CCCCCC	
	oate (n-			C15H27O	C=CC(=O)	
cpd_pde	C15:1)	C17676	-1	2	0	Pubchem
					CC1=NC=	
	Pyridoxine				C(C(=C1O))	
	5'-			C8H10NO)CO)COP(
cpd_pdx5p	phosphate	C00627	-2	6P	=O)(O)O	Pubchem
					[H]C(=O)	
					OCC(COP	
	Phosphatid				(O)(=O)O	
_	ylethanola	~~~~~		C7H12NO	CCN)OC([
cpd_pe	mine	C00350	0	8PR2	HJ)=O	Pubchem
					CC(=CCC	
	a11 Ano 11 m					
	all-trans-				COP(-O)	
	rentapreny				O(OP(=0))	
	1 dinhoanhat			C25U41O	(0)0Y(=0)	
and nande	aipnospnat	C04217	2	C23H41U 7D2	(U)U)U(U)	Dubaham
epu penup		0421/	-3	114		

					C=C(C(=O)	
	Phosphoen				OOOP(=O)	
cpd pep	olpyruvate	C00074	-3	C3H2O6P)(Ó)O	Pubchem
	12				[H]C(=O)	
					OCIC@H1	
					(COP(O)) =	
					000000000000000000000000000000000000	
	Phosphatid			C8H12O1	OOC([H])	
end nolv	vlølvcerol	C00344	-1	OPR2	=0	Pubchem
opa_porj	<i>J</i> 1 <u>5</u> 1 <u>J</u> 00101			01102	[H]C(=0)	
					(COP(O)) =	
					(0) 100)	
	Phosphatid				OP(O)(O)	
	vlalvcerop			C8H11O1	=0.00(0)	
end nalvn	hosphate	C03892	_3	3P2P2	-0)00([II	Pubchem
cpu_pgryp	nospilate	003072	-5	JI 2K2	$\int -0$	1 ubenem
	T_				$C_1 = C_2 = C_1$	
	L- Dhenvlalan			COHIINO	(C - C1)CC	
and nha I	ino	C00070	0	2	(C(-0)0)	Dubaham
cpu_piic-L	IIIC	00079	0	2	CC1-C(C2)	1 ubenem
					-CC3-C(
					$-CC_{3}-C($	
					C(-C([N-1])) = CAC([N-1])	
					-C(C) - C + C(C)	
					-C(C(-1)+	
					C(C(-N5))	
					C = C = C = N	
					C = C I [IN = I]	
					JZ = C = C = C = C	
					C = C (C) (C)	
					CCC(-0)	
and also				C241121E-	O)CCC(-	
cpd_pnem	Ductolicano	C00022	1	C34H31Fe	0)0.[Fe+2]	Dutation
e	Protoneme	C00032	-1	IN404	J	Pubenem
	pnospnona	C0(701	2		OD(O)O	D-1.1.
cpd_phn	te	C06/01	-2	НОЗР	OP(0)0	Pubchem
	Phosphono					
cpd_phnac	acetaldehy	G001 (7	2	CALLAC AD	C(C=O)P(D 1 1
ald	de	C03167	-2	C2H3O4P	=0)(0)0	Pubchem
	U-					
	Phospho-					
	L-			a 41703	C(COP(=O	
	homoserin			C4H8NO6)(U)U)C(C	
cpd_phom	e	C01102	-2	P	(=O)O)N	Pubchem

					C1=CC=C	
					(C=C1)CC	
	Phenylnyr				(=0)C(=0)	
and phow	1 henyipyi	C00166	1	C0H7O3		Dubaham
cpu_phpyi	uvale	C00100	-1	C9H/O5	0	Fubchem
	0-				alala	
	Phospho-				C(C(C(C(C(=	
	4-hydroxy-				O)O)N)O)	
	L-			C4H8NO7	OP(=O)(O	
cpd_phthr	threonine	C06055	-2	Р)O	Pubchem
					[O-	
]P(=O)([O-	
cpd pi	Phosphate	C00009	-2	HO4P	1)[O-1	Pubchem
- FF	F				CC(C)(CO)	
					P(=0)(0)	
					DP(-D)(0)	
					OF(-0)(0)	
					(C(01)N2)	
					C=NC3=C	
					2N=CN=C	
					3N)O)OP(
					=O)(O)O)	
					C(C(=O)N)	
					CCC(=O)	
					NCCSC(=	
cpd pmco	Pimelovl-			C28H41N	O(CCCCCC)	
a	CoA	C01063	-5	7019P3S	C(=0)0)0	Pubchem
u		01005		7017155	C(C)(C)	1 uoenem
	(D)				C(C(-0))	
and mate	(IX)- Dontothono			COLLIANO	C(C(-0))	
cpa_pnto-	Pantotnena	C009(4	1	C9HIONO		D-1.1.
K	te	C00864	-1	3)0)0	Pubchem
					CCC(=O)[
cpd_ppa	Propionate	C00163	-1	C3H5O2	O-]	Pubchem
					C1=C(C(=	
					C(N1)CN)	
					CC(=O)O)	
	Porphobili			C10H13N	CCC(=O)	
cpd ppbng	nogen	C00931	-1	204	0	Pubchem
- <u>-</u>	8				CCC(=0)S	
					CCNC(=0)	
					CCNC(-	
					C) C C C C C C C C C C C C C C C C C C	
					C)COP(=0)	
)(O)OP(=	
					U)(U)OCC	
	Propanoyl-			C24H36N	1C(C(O))	
cpd_ppcoa	CoA	C00100	-4	7017P3S	1)N2C=N	Pubchem

					C3=C2N=	
					$C_{1} = C_{2}$	
					CN = C3N	
					O)OP(=O)	
					(0)0)0	
					C1=CC(C	
					=CC1O)(C	
					C(=O)C(=	
					$\dot{OOOC} = O$	
cpd pphn	Prephenate	C00254	-2	C10H8O6)0	Pubchem
opa_ppini	Trephenate	000251		01011000)0 [0	1 uo en en
					10^{-1}	
	D' 1 1				$\frac{J}{U} = \frac{J}{U} = \frac{J}$	
	Dipnospna	G00010	2])OP(=O)([D 1 1
cpd_pp1	te	C00013	-3	HO7P2	0-])[0-]	Pubchem
					CC1=C(C2)	
					=CC3=C(
					C(=C(N3))	
					C=C4C(=	
					C(C(=N4))	
					C=C5C(=	
					C(C(=N5))	
					$C = C (N_2)$	
					$C = C \ln 2$	
	_				0)0)000000	
	Protoporph			C34H32N	=O(O(C))	
cpd_ppp9	yrin	C02191	-2	404	=C)C)C=C	Pubchem
					CC1=C2C	
					C3=C(C(=	
					C(N3)CC4	
					=C(C(=C(
					N4)CC5=	
					C(C(-C(N)))	
					C(C(-C(N + C)))	
					S)CC(-C)	
					CCC(=0)	
					O(N2)CC	
	Protoporph				C(=O)O)C	
	yrinogen			C34H38N)C=C)C)C	
cpd_pppg9	IX	C01079	-2	404	=C)C	Pubchem
	5-					
	Phospho-				C(C1C(C(
	beta-D-					
	ribosylami			C5H11NO	(0,1)(0,1)(0,1)(0,1)(0,1)(0,1)(0,1)(0,1)	
end pram	ne	C03090	1	7D)(0)0	Pubchem
cpu_prain	ne	03090	-1	/ [$\int_{C} (0) 0$	
	NI (5					
	IN-()-			G101103	(C(=CI)C(
	Phospho-			C12H13N	=O)O)NC2	
cpd_pran	D-	C04302	-3	O9P	C(C(O2))	Pubchem

	ribosyl)ant				COP(=O)(
	hranilate				0)0)0)0	
					C1=NC2=	
					C(N1C3C(
					C(C(O3)C)	
					OP(=O)(O	
)0)0)0)N	
					=CN(C2=	
					N)C4C(C(
	1-(5-				C(O4)COP	
cpd prbam	Phosphorib			C15H19N	(=O)(O)O)	
p	osyl)-AMP	C02741	-4	5014P2	0)0	Pubchem
1	,				C1=NC2=	
					C(N1C3C(
					C(C(O3)C)	
					OP(=O)(O	
) $OP(=O)($	
					O)OP(=O)	
					(0)0)0)0)	
					N=CN(C2	
					=N)C4C(C	
	1-(5-				(C(O4)CO	
	Phosphorib			C15H19N	P(=O)(O)	
cpd prbatp	osyl)-ATP	C02739	-6	5O20P4	$\dot{O}O\dot{O}$	Pubchem
	1-(5-					
	Phosphorib				C1=NC(=	
	osyl)-5-				C(N1C2C(
	[(5-				C(C(O2)C)	
	phosphorib				OP(=O)(O	
	osylamino))O)O)N	
	methyliden				C=NC3C(
	eamino]im				$C(C(O3)\hat{C})$	
	idazole-4-				OP(=O)(O	
	carboxami			C15H22N)0)0)0)0)0(
cpd prfp	de	C04896	-3	5015P2	=O)N	Pubchem
· _ ·	5-[(5-					
	phospho-1-				C1=NC(=	
	deoxyribul				C(N1C2C(
	os-1-				C(C(O2)C)	
	ylamino)m				OP(=O)(O	
	ethylidene)O)O)O)N	
	amino]-1-				C=NCC(=	
	(5-				$O)C(C(\dot{C}O)$	
	phosphorib				P(=O)(O)	
	osyl)imida			C15H22N	$\dot{0}$ $\dot{0}$ $\dot{0}$ $\dot{0}$ $\dot{0}$ $\dot{0}$ $\dot{0}$	
cpd_prlp	zole-4-	C04916	-3	5015P2	=O)N	Pubchem

	carboxami de					
cpd_pro- gly	Proly- glycine	NA	0	C7H12N2 O3	C1CC(NC 1)C(=O)N CC(=O)O	Pubchem
cpd_pro-L	L-Proline	C00148	0	C5H9NO2	C1CC(NC 1)C(=O)O	Pubchem
cpd_prpp	5- Phospho- alpha-D- ribose 1- diphosphat e	C00119	-5	C5H8O14 P3	C(C1C(C(C(O1)OP(=O)(O)OP (=O)(O)O) O)O)OP(= O)(O)O	Pubchem
cpd_ps	Phosphatid ylserine	C02737	-1	C8H11NO 10PR2	[H]C(=O) OCC(COP (O)(=O)O C[C@H](N)C(O)=O)OC([H])= O	Pubchem
cpd psd5p	Pseudourid ine 5'- phosphate	C01168	-2	C9H11N2 O9P	C1=C(C(= O)NC(=O) N1)C2C(C (C(O2)CO P(=O)(O) O)O)O	Pubchem
cpd pser-L	O- Phospho- L-serine	C01005	-2	C3H6NO6 P	C(C(C(=O)O)N)OP(=O)(O)O	Pubchem
cpd_ptdca	pentadecan oate (n- C15:0)	NA	-1	C15H29O 2	CCCCCC CCCCCC CCC(=O)[O-]	Pubchem
cpd_ptrc	Putrescine	C00134	2	C4H14N2	C(CCN)C N	Pubchem
cpd_pyam 5p	Pyridoxam ine 5'- phosphate	C00647	-2	C8H11N2 O5P	CC1=NC= C(C(=C1O)CN)COP(=O)(O)O	Pubchem
cpd_pydx5 p	Pyridoxal 5'- phosphate	C00018	-3	C8H7NO6 P	CC1=NC= C(C(=C1O)C=O)COP (=O)(O)O	Pubchem
cpd_pyr	Pyruvate	C00022	-1	C3H3O3	CC(=O)C(=O)[O-]	Pubchem

					C1=CC(=	
					C(N=C1)C	
	Quinclinat				(-0)0)C(-	
and av1.	Quinoiniat	C02722	2	CTU2NO4	(-0)0)C(-0)0)	Dark als and
cpa_quin	e	C03722	-2	C/H3NO4	0)0	Pubchem
					C(CIC(C(
	alpha-D-				C(O1)OP(
	Ribose 1-				=O)(O)O)	
cpd_r1p	phosphate	C00620	-2	C5H9O8P	O)O)O	Pubchem
					C(C1C(C(
	alpha-D-				C(O1)O)O	
	Ribose 5-				OOOP(=O)	
cpd r5p	phosphate	C03736	-2	C5H9O8P)(O)O	Pubchem
-1 - 1	D-				C(C(C(C(=	
	Ribulose				O)COP(=	
	1 5-				O(O)O(O)	
end rh15h	hisnhosnha			C5H8O11	O(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(0)(
cpu_10150	to	C01182	1	D2	(0)01(0)	Dubchem
Р	$\frac{1}{1}$	C01162		ΓΔ	(0)0	rubenenn
	NI-(alpha-					
	D-ribosyl)-					
	5,6-				C)N(C=N2	
	dimethylbe)C3C(C(C(
cpd_rdmbz	nzimidazol			C14H18N	O3)CO)O)	
i	e	C05775	0	204	0	Pubchem
	S-Ribosyl-				C(CSCC1	
	L-				C(C(C(O1)))	
	homocyste			C9H17NO	O)O)O)C(
cpd rhcys	ine	C03539	0	6S	C(=O)O)N	Pubchem
					C1C(C(C(
					C(OI)OO	
epd_rib-d	D-Ribose	C00121	0	C5H10O5)0)0	Pubchem
	Difficult	000121	0	00111000	CC1=CC2	1 uoenem
					-C(C-C)	
					-C(C-C)	
					C) N (C) $-N$	
					C(=0)NC(
				G1711001	=0)C3=N2	
	~ .			CT/H20N)CC(C(C(
cpd_ribflv	Riboflavin	C00255	0	406	CO)O)O)O	Pubchem
	D-				C(C(C(C(=	
	Ribulose				O)CO)O)O	
cpd_ru5p-	5-)OP(=O)(
D	phosphate	C00199	-2	C5H9O8P	O)O	Pubchem
					C(C(C(C	
					C(C(=O)C)	
	Sedoheptul				$\dot{0}\dot{0}\dot{0}\dot{0}$	
	ose 7-			C7H13O1	O)OP(=O)	
cpd s7p	phosphate	C05382	-2	0P	(0)	Pubchem
F	L 1		_	1		

					CC(C)(CO P(=O)([O-])OP(=O)([O-])OCC1C(C(C(O1)N 2C=NC3= C2N=CN= C3N)O)OP (=O)([O-	
cpd_sbzco a	O- Succinylbe nzoyl-CoA	C03160	-5	C32H39N 7O20P3S])[O-])C(C(=O) NCCC(=O) NCCSC(= O)CCC(= O)C4=CC =CC=C4C (=O)[O-])O	Pubchem
cpd_seln	Selenide	C01528	-1	HSe	[SeH2]	Pubchem
	Selenopho	~~~~~			OP(=[Se])(
cpd_selnp	sphate	C05172	-1	H2O3PSe	0)0	Pubchem
cpd_ser-D	D-Serine	C00740	0	C3H7NO3	C(C(C(=0))0)N)0	Pubchem
cpd_ser-L	L-Serine	C00065	0	C3H7NO3	C(C(C(=0))0)N)0	Pubchem
cpd_shcl	dihydrosir ohydrochlo rin	C02463	-8	C42H40N 4O16	$\begin{array}{l} \text{CC1}(\text{C}(\text{C2} \\ = \text{CC3} = \text{NC} \\ (= \text{CC4} = \text{C}(\\ \text{C}(= \text{C}(\text{N4}) \\ \text{CC5} = \text{C}(\text{C}(\\ = \text{C}(\text{N5})\text{C} = \\ \text{C1N2})\text{CC}(\\ = \text{O})\text{O})\text{CC} \\ \text{C}(= \text{O})\text{O})\text{C} \\ \text{C}(= \text{O})\text{O})\text{C} \\ \text{CC}(= \text{O})\text{O}) \\ \text{CC}(= \text{O})\text{O} \\ \text{CC}(= \text{O})\text{O} \\ \text{CC}(= \text{O})\text{O} \\ \text{CCC}(= \text{O}) \\ \text{O})\text{CC}(= \text{O}) \\ \text{O} \end{array}$	Pubchem
cpd_sheme	Siroheme	C00748	-8	C42H36Fe N4O16	CC1(C(C2 =CC3=NC (=CC4=C(Pubchem

					C(=C([N-	
]4)C=C5C(
					C(C(=N5))	
					C=C1IN-	
					12)CCC(=	
					$\frac{12}{2}$	
					C(-0)0)(C)C	
					C(-0)0)C	
					C(-0)0)C	
					CC(=0)0)	
					C(=C3CC(
					=0)0)00	
					C(=O)O)C	
					CC(=O)O)	
					CC(=O)O.	
					[Fe+2]	
					C1C(C(C(
					C=C1C(=	
					O)O)O)O)	
cpd skm	Shikimate	C00493	-1	C7H9O5	0	Pubchem
					C1C(C(C(
					C=C1C(=)	
	Shikimate				O(O)OP(=	
end_skm5	5-				0)(0)0)0)	
n	nhosnhate	C03175	-3	C7H8O8P	0	Pubchem
Р	N_	000170	-5	C/110001	0	1 ubenem
	Succinv1				C(CC(C) -	
	Succiniyi-				C(CC)(C) = 0	
	LL-2,0-				$(C(-\Omega)\Omega)$	
	diaminone			CITITION	(C(-0)0)	
1 10(1	planedioal	C04421	2	CITHION 207	NC(=0)C	D 1 1
cpd_s126da	e	C04421	-2	207	0(0=)	Pubchem
	N-					
	Succinyl-				C(CC(C(=	
	2-L-				O)O)NC(=	
	amino-6-				O)CCC(=	
	oxoheptan			C11H12N	O)O)CC(=	
cpd_sl2a60	edioate	C04462	-3	08	O(=O)O	Pubchem
					C(C(C(=O	
	S-Sulfo-L-			C3H6NO5)O)N)SS(=	
cpd slcys	cysteine	C05824	-1	S2	O(=O)O	Pubchem
					[O -	
cpd so3	Sulfite	C00094	-2	O3S	IS(=0)[O-]	Pubchem
1				_	[O-	
					1S(=0)(=0)	
cpd so4	Sulfate	C00059	_2	045	10^{-1}	Pubchem
-pu_30T	Sparmidin		-2		$\Gamma(CCNCC)$	
	spermum	C00215	2	CTUDDND		Dubaham
		11 111111	· 1	\mathbf{U} / \mathbf{H} / \mathbf{N})		rupenem

					C(CCNCC	
1		G00550		C10H30N	CN)CNCC	D 1 1
cpd_sprm	Spermine	C00750	4	4	CN	Pubchem
					CCI(C(C2	
					=NCI=CC	
					3=NC(=C	
					C4=C(C(=	
					C(N4)C=C	
					SC(=C(C(
					=C2)N5)C	
					C(=0)0)C	
					CC(=0)0)	
					CCC(=O)	
					O)CC(=O)	
					0)0(0300	
					C(=O)O)(
					C)CC(=O)	
					O)CCC(=	
	sırohydroc	~~~~~		C42H38N	O)O)CC(=	
cpd_srch	hlorin	C05778	-8	4016	0)0	Pubchem
					CC1=C(S	
					C(=[N+]]	
					CC2=CN=	
					C(N=C2N)	
	Succinate				C)C(CCC(
	semialdehy				=O(O(O(O(O(O(O(O(O(O(O(O(O(O(O(O(O(O(O(
	de-thiamin				COP(=O)(
cpd_ssaltp	diphosphat			C16H22N	O)OP(=O)	
p	e anion	C05381	-2	4O10P2S	(0)0	Pubchem
					C(CC(C(=	
					O)O)NC(=	
	N2-				O)CCC(=	
	Succinyl-			C10H17N	O)O)CN=	
cpd_sucarg	L-arginine	C03296	-1	405	C(N)N	Pubchem
					C1=CC=C	
					(C(=C1)C(
	0-				=O)CCC(=	
	Succinylbe				O)O)C(=O	
cpd_sucbz	nzoate	C02730	-2	C11H8O5)0	Pubchem
					C(CC(=O))	
					[O-	
])C(=O)[O	
cpd_succ	Succinate	C00042	-2	C4H4O4	-]	Pubchem
					CC(C)(CO	
cpd_succo	Succinyl-			C25H35N	P(=O)(O)	
a	CoA	C00091	-5	7019P3S	OP(=O)(O	Pubchem

)	
					(C(O1)N2)	
					C=NC3=C	
					2N=CN=C	
					3NOOP(
					$\frac{31}{0}$	
					=0)(0)0)	
					C(C(=O)N)	
					CCC(=O)	
					NCCSC(=	
					0) $CCC(-$	
					0)0)0	
					C(CC(=O))	
	N2-				O)C(C(=0)	
	Succinvl				ONC(-0)	
	Jucchiyi-			COLLIANO)0)10(-0)	
	L-		_	C9HIUNO)CCC(=0)	
cpd_sucglu	glutamate	C05931	-3	7	0	Pubchem
	N2-					
	Succinyl-					
	L-					
	alutamate				C(CC(C) -	
	5-				O(O) O(O) NC(=	
cpd_sucgs	semialdehy			C9H11NO	O)CCC(=	
a	de	C05932	-2	6	O)O)C=O	Pubchem
	O-					
	Sussinul				C(COC) =	
	Succinyi-					
	L-				O)CCC(=	
cpd suchm	homoserin			C8H12NO	O)O)C(C(
s	e	C01118	-1	6	=O)O)N	Pubchem
					C(CC(C) =	
	N2				O(O)NC(-	
1	IN2-			COLLIZIO		
cpd_sucor	Succinyl-			C9HI5N2	0)000(=	
n	L-ornithine	C03415	-1	05	O)O)CN	Pubchem
	Succinic					
	semialdehv				C(CC(=O))	
cnd succel	de	C00232	_1	C4H5O3	O)C=O	Pubchem
-pu_suesai	This areas	00232	-1	5711303	5,0 0	
1	Thocyanat	001755		CNIC		D 1 1
cpd_tcynt	e	C01755	-1	CNS	C(#N)[S-]	Pubchem
					CC(C(C1C	
					NC2=C(N	
					1)C(=0)N	
	Tatual			COLLISNE		
	Tetranydro			CAHIONO	C(=N2)N)	
cpd_thbpt	biopterin	C00272	0	03	0)0	Pubchem
	2,3,4,5-				C1CC(N=	
	Tetrahydro				$C(C1)\dot{C}(=$	
	dinicolinat				0)0)C(-0)	
	aipicolillat	002072	~	071173104		D-1 1
cpd thdp	e	C03972	-2	C/H/NO4)0	Pubchem
					C1C(NC2	
-----------	----------------------	--------	----	-----------	--	-------------
					=C(N1)N=	
					C(NC2=0)	
					N)CNC2-	
					CC = C(C = C)	
					CC = C(C = C)	
					C3)C(=0)	
	5,6,7,8-				NC(CCC(
	Tetrahydro			C19H21N	=O)O)C(=	
cpd_thf	folate	C00101	-2	706	0)0	Pubchem
					C1C(NC2	
					=C(N1)N=	
					C(NC2=O)	
					N)CNC3=	
					CC = C(C =	
					C3)C(=O)	
					NCCCCC	
					=0)NC(C)	
					CC(=0)N	
	Tetrahydro				C(CCC) =	
	nterovltri-				0)0)C(=0	
				C20H37N	(0)(0)(-0)(-0)(-0)(-0)(-0)(-0)(-0)(-0)(-	
and thalu	alutamata	C04144	0	0012	(-0)	Dubaham
cpu_ingiu	giutamate	C04144	0	9012	CC1 = C(S)	1 ubclicili
					C = D + 11C	
					C = [N +]IC	
				C101117N	C2-CN-C	
1.1		000270	1	CI2HI/N	(N=C2N)C	D 1 1
cpd_thm	Thiamin	C00378	1	408		Pubchem
					CCI=C(S	
					C = [N+]1C	
					C2=CN=C	
	Thiamin				(N=C2N)C	
cpd_thmm	monophos			C12H16N)CCOP(=O	
p	phate	C01081	-1	4O4PS)(O)O	Pubchem
					CC1=C(S	
					C = [N+]1C	
					C2=CN=C	
					(N=C2N)C	
	Thiamine)CCOP(=O	
	diphosphat			C12H16N	(O)OP(=	
cpd thmpp	e	C00068	-2	407P2S	O(O)O	Pubchem
-rmpp	Т				CC(C(C) =	
cnd thr-I	Threonine	C00188	Ο	C4H9NO3		Pubchem
end the	$I = \Lambda 11_{O}$	200100	0	01171005	CC(C(C) -	
	L-Allo-	C05510	Δ	CALIONO2		Dubaham
LA	uneomne	000019	0	C4119INU3	UJUJNJU	rubenem

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$						CC1=CNC	
cpd_thymThymineC0017802OPubchem cpd_thymd ThymidineC0021402050Pubchem cpd_tma Trimethyla02050Pubchem cpd_tma mineC005651C3H10NCN(C)CPubchem cpd_tma mineC001040C3H9NOC[N+](C)(C)[O-]Pubchem cpd_tma coxideC011040C3H9NOC](O-]Pubchem cpd_tma coxideC011040C3H9NOC](O-]Pubchem cpd_tma coxideC011040C3H9NOC](O-]Pubchem cpd_tma coxideC011040C3H9NOC](O-]Pubchem cpd_tma coxideC011040C3H9NOC](O-]Pubchem cpd_tma coxideC011040C3H9NOC](O-]Pubchem cpd_trp-L nC0007802O2C[O+](C)(C(=O)ONPubchem cpd_ttsul ThiosulfateC00320-2O3S2)[O-]Pubchem cpd_ttdcan cocidecocidecocidecocidecocidecocide cpd_ttttnt cC02084-2O6S4=O](O-]SSS(=O)(SSS(=O)(pubchem cpd_ttrp-L L-TyrosineC0008203NOPubchem					C5H6N2O	(=O)NC1=	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	cpd_thym	Thymine	C00178	0	2	Ō	Pubchem
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$						CC1=CN(
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $						C(=O)NC1	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $						=O)C2CC(
cpd_thymdThymidineC0021402050PubchemTrimethyla mineC005651C3H10NCN(C)CPubchemTrimethyla mine N- oxideC011040C3H9NO $C[N+](C)(C][O-]$ Pubchemcpd_tmaooxideC011040C3H9NO $C[N+](C)(C][O-]$ Pubchemcpd_tmaooxideC011040C3H9NO $C[N+](C)(C][O-]$ Pubchemcpd_tmaooxideC011040C3H9NO $C[N+](C)(C][O-]$ Pubchemcpd_trp-LL- Tryptopha nC000780202 $C(=0)ON$ Pubchemcpd_tsulThiosulfateC00320-2O3S2 $][O-]$ Pubchemcpd_tsulThiosulfateC00320-2O3S2 $][O-]$ Pubchemcpd_ttdan(neutral)C0642402CCCCCC CC(=O)OPubchemcpd_tttnteC02084-2O6S4 $=O](O-]$ Pubchemcpd_ttrptL-TyrosineC0008200N)OPubchem					C10H14N	C(O2)CO)	
rimethyla mineC005651C3H10NCN(C)CPubchemTrimethyla mine N- oxideC011040C3H9NO $CI(N+](C)(C)[O-]$ Pubchemcpd_tmaocxideC011040C3H9NO $CI=CC=C$ 2C(=C1)C(=CN2)CC(C(=O)O)NPubchemcpd_trp-LnC000780202 $C(=O)O)N$ Pubchemcpd_trp-LnC000780202 $C(=O)O)N$ Pubchemcpd_trp-LnC00320-2O3S2 $J[O-]$ Pubchemcpd_tsulThiosulfateC00320-2O3S2 $J[O-]$ Pubchemtetradecan oate (C14:0)C0642402CCCCCCC CC(=O)OPubchemtetrathionat cpd_ttmtC02084-2 $O6S4$ $O[O-]$ Pubchemcpd_ttmtC02084-2 $O6S4$ $O[O-]$ Pubchemcpd_ttyr-LL-TyrosineC000820 O O Pubchem	cpd_thymd	Thymidine	C00214	0	205	0	Pubchem
cpd_tmamineC005651C3H10NCN(C)CPubchemTrimethyla mine N- oxideC011040C3H9NO $C[N+](C)(C)[O-]$ PubchemL- TryptophaC1=CC=C 2C(=C1)C(TryptophaC1=CC=C 2C(=C1)C(C11H12NC1=CC=C 2C(=C1)C(C11H12Ncpd_trp-LnC000780202C(=O)O)Npd_trp-LnC000780202C(=O)O)Npd_tsulThiosulfateC00320-2O3S2)[O-]tetradecan oate (C14:0)C0642402CCCCCC CC(=O)Opd_ttdcan(neutral)C0642402CCCCCC CC(=O)Ocpd_tttnteC02084-2O6S4=O)[O-]pd_ttrp-LL-TyrosineC0008203NO		Trimethyla					
rrimethyla mine N- oxideC011040C3H9NO $C[N+](C)$ $C)[O-]PubchemL-TryptophaL-TryptophaC000780C11H12N2O2C1=CC=C2C(=C1)C(C(=O)O)NPubchemcpd_trp-LnC0007802O2C(=O)ON(C=O)ONPubchemcpd_trg-LnC00320-2O3S2)[O-]Pubchemcpd_tsulThiosulfateC00320-2O3S2)[O-]Pubchemtetradecanoate(C14:0)C0642402CCCCCCCC(=O)OPubchemcpd_ttdcan(neutral)C0642402C14H280CCCCCCCC(=O)OPubchemcpd_ttdcancoutral(C14:0)C0642402C14H280CCCCCCCCC(=O)OPubchemcpd_ttdcanfetrathionattetrathionatC02084-2O6S4=0][O-]Pubchemcpd_ttruttetrathionatcC02084-2O6S4=0][O-]Pubchemcpd_ttruttetrathionatcC0208203NOPubchem$	cpd_tma	mine	C00565	1	C3H10N	CN(C)C	Pubchem
$\begin{array}{c c} \mbox{mine N-} \\ \mbox{oxide} & C01104 & 0 & C3H9NO & C[N+](C)(\\ C)[O-] & Pubchem \\ \mbox{C1=CC=C} \\ 2C(=C1)C(\\ =CN2)CC(\\ C11H112N & 2C2(=C1)C(\\ =CN2)CC(\\ C(=O)O)N & Pubchem \\ \mbox{Pubchem} \\ \mb$		Trimethyla					
cpd_tmaooxideC011040C3H9NOC)[O-]PubchemL- TryptophaL- TryptophaC1=CC=C 2C(=C1)C((C11H12N)C1=CC=C 2C(=C1)C((C=O)O)NPubchemcpd_trp-LnC000780202C(=O)O)NPubchemcpd_tsulThiosulfateC00320-2O3S2)[O-]Pubchemtetradecan oate (C14:0)tetradecal 0ateCCCCCCC CC(=O)OPubchemcpd_ttuteC0642402CCCCCCC CC(=O)OPubchemcpd_ttuteC02084-2O6S4=O][O-]Pubchemcpd_ttuttC008203N)OPubchem		mine N-				C[N+](C)(
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	cpd_tmao	oxide	C01104	0	C3H9NO	C)[O-]	Pubchem
$\begin{array}{c c c c c c c c c c c c c c c c c c c $						C1=CC=C	
$\begin{array}{c cccc} Tryptopha \\ cpd_trp-L & n & C00078 & 0 & 2O2 & C(2)C(2) \\ C(=0)O)N & Pubchem \\ \hline \\ cpd_tsul & Thiosulfate & C00320 & -2 & O3S2 &)[O-] & Pubchem \\ \hline \\ cpd_tsul & Thiosulfate & C00320 & -2 & O3S2 &)[O-] & Pubchem \\ \hline \\ tetradecan \\ oate \\ (C14:0) & C06424 & 0 & 2 & CCCCCC \\ cpd_ttdcan & (neutral) & C06424 & 0 & 2 & CCCCCC \\ cpd_ttdcan & (neutral) & C06424 & 0 & 2 & CCCCCC \\ cpd_ttdcan & (neutral) & C06424 & 0 & 2 & CCCCCC \\ cpd_ttdcan & (neutral) & C06424 & -2 & O6S4 & O[O-] \\ \hline \\ cpd_ttnt & e & C02084 & -2 & O6S4 & O[O-] & Pubchem \\ \hline \\ cpd_tyr-L & L-Tyrosine & C00082 & 0 & 3 & N)O & Pubchem \\ \hline \end{array}$		L-				2C(=C1)C(
cpd_trp-LnC0007802O2C(=O)O)NPubchem $[O-]$ $[S(=O)(=S)$ $[O-]$ $[S(=O)(=S)$ $[S(=O)(=S)$ $[O-]$ $[cpd_tsul]$ ThiosulfateC00320-2O3S2 $[O-]$ Pubchemtetradecan oate (C14:0)tetradecalCCCCCCC C14H280CCCCCCCcpd_ttdcan(neutral)C0642402CC(=O)OPubchemcpd_ttdcan(neutral)C0642402CC(=O)OPubchemcpd_tttnteC02084-2O6S4 $=O)[O-]$ Pubchemcpd_ttrnttetrathionat eC02084-2O6S4 $=O)[O-]$ Pubchemcpd_ttrnttetrathionat eC0208203N)OPubchem		Tryptopha			C11H12N	=CN2)CC(
cpd_tsulThiosulfateC00320 -2 $O3S2$ $[O-]_{S(=O)(=S})$ Pubchemtetradecan oate (C14:0)tetradecan oate (C14:0)C14H280CCCCCC CC(=O)OCCCCCC Pubchemcpd_ttdcan(neutral)C0642402CCCCCC CC(=O)OPubchemcpd_ttdtantetrathionat eC02084 -2 O6S4 $[O-]_{S(=O)(=O)}$ SSS(=O)(=O)[O-]Pubchemcpd_ttmteC02084 -2 O6S4 $=O)[O-]$ Pubchemcpd_ttrnttC0008203N)OPubchem	cpd_trp-L	n	C00078	0	202	C(=O)O)N	Pubchem
cpd_tsulThiosulfateC00320 -2 O3S2 $]S(=O)(=S)$ Pubchemtetradecan oate (C14:0)tetradecan oate (C14:0)CCCCCCC C14H280CCCCCCC CC(=O)OPubchemcpd_ttdcan(neutral)C0642402CCCCCCC CC(=O)OPubchemcpd_ttdttetrathionat eC02084 -2 O6S4 $=O][O-]$ Pubchemcpd_tttnteC02084 -2 O6S4 $=O][O-]$ Pubchemcpd_ttrnttetrathionat eC02082 0 N)OPubchem						[O-	
cpd_tsulThiosulfateC00320 -2 O3S2)[O-]Pubchemtetradecan oate (C14:0)tetradecal (C14:0)C14H280CCCCCC CC(=O)OCCCCCC Pubchemcpd_ttdcan(neutral)C0642402CC(=O)OPubchemcpd_ttdcantetrathionat eC02084 -2 O6S4 $=O)[O-]$ Pubchemcpd_tttnteC02084 -2 O6S4 $=O)[O-]$ Pubchemcpd_tttnteC0208203N)OPubchem]S(=O)(=S	
tetradecan oate (C14:0)tetradecan oate (C14:0)CO6424C14H280CCCCCC CC(=O)OPubchemcpd_ttdcan(neutral)C0642402CC(=O)OPubchemtetrathionat tetrathionatC02084-2O6S4=O)[O-]Pubchemcpd_tttnteC02084-2O6S4=O)[O-]Pubchemcpd_tttntL-TyrosineC0008203N)OPubchem	cpd_tsul	Thiosulfate	C00320	-2	O3S2)[O-]	Pubchem
oate (C14:0) cpd_ttdcancoate (C14:0) (neutral)C06424C14H280 CCCCCCC CC(=O)OPubchemcpd_ttdcancoate (neutral)coate (C0642402[O-]S(=O)(=O))SSS(=O)((SSS)(=O)(Pubchemcpd_tttnteC02084-2O6S4=O)[O-]Pubchemcpd_tttnteC02084-2O6S4=O)[O-]Pubchemcpd_ttrt.L-TyrosineC0008203N)OPubchem		tetradecan					
$\begin{array}{c cccc} (C14:0) & C14H280 & CCCCCC \\ (neutral) & C06424 & 0 & 2 & CC(=O)O & Pubchem \\ \hline cpd_ttdcan & tetrathionat \\ cpd_ttnt & e & C02084 & -2 & O6S4 & =O)[O-] & Pubchem \\ \hline cpd_tyr-L & L-Tyrosine & C00082 & 0 & 3 & N)O & Pubchem \\ \hline \end{array}$		oate				CCCCCC	
cpd_ttdcan(neutral)C0642402CC(=O)OPubchem cpd_ttmt tetrathionat $[O-]S(=O)(=O)$ $SSS(=O)($ $SSS(=O)($ $SSS(=O)($ cpd_ttmt eC02084-2O6S4 $=O)[O-]$ Pubchem cpd_ttrt L-TyrosineC0008203N)OPubchem		(C14:0)			C14H28O	CCCCCC	
cpd_tttnttetrathionat eC02084-2O6S4 $\begin{bmatrix} O - \\]S(=O)(=O) \\ SSS(=O)() \\ =O)[O-] \end{bmatrix}$ Pubchemcpd_ttr-LL-TyrosineC0008203 NO Pubchem	cpd_ttdcan	(neutral)	C06424	0	2	CC(=O)O	Pubchem
cpd_tttnttetrathionat e $C02084$ -2 $O6S4$ $[S(=O)(=O)$ $)SSS(=O)()=O)[O-]Pubchemcpd_ttr-LL-TyrosineC0008203N)OPubchem$						[O-	
tetrathionat cpd_tttntC02084-2O6S4SSS(=O)(=O)[O-]Pubchemcpd_ttr-LL-TyrosineC0008203C1=CC(= CC=C1CCC2=C1CCcpd_tyr-LL-TyrosineC0008203N)OPubchem]S(=O)(=O	
cpd_tttnteC02084-2O6S4 $=O[O-]$ Pubchemcpd_tyr-LL-TyrosineC0008203C1=CC(= CC=C1CC (C(=O)O) N)OPubchem		tetrathionat	~~~		0.694)SSS(=O)(
cpd_tyr-L L-Tyrosine C00082 0 3 C1=CC(= C2=C1CC (C(=O)O) N)O Pubchem	cpd_tttnt	e	C02084	-2	0684	=O)[O-]	Pubchem
cpd_tyr-LL-TyrosineC000820CC=C1CCCOCCCC03N)OPubchem						Cl=CC(=	
cpd_tyr-L L-Tyrosine C00082 0 3 N)O Pubchem					00111110	CC=CICC	
cpd_tyr-L L-Tyrosine C00082 0 3 N)O Pubchem	1 / T		G00000	0	C9HIINO	(C(=O)O)	D 1 1
	cpd_tyr-L	L-Tyrosine	C00082	0	3	N)O	Pubchem
						CCCCCC	
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OUTOP(=)						OUIUP(=	
						-0)(0)0P(
						-0)(0)00	
						$O_2 O_1 O_1 O_2 O_2 O_2 O_2 O_2 O_2 O_2 O_2 O_2 O_2$	
$\frac{ODF-2,5}{bis(3)}$		DDr-2,3-				CC(-O)N	
budrovytet $C2-O)O$		bydrovytet				$C_{2} = 0 0 0$	
redecenovl		radecapovi				$\frac{C_{3}-C_{3}}{C_{3}}$	
) $glucosami$ C43H75N (=0)CC(C		Jolucosami			C43H75N	(=0)CC(C)	
cpd u23ga ne C04652 -2 3020P2 CCCCCC Pubchem	cpd u23ga	ne	C04652	-2	3O20P2	CCCCCC	Pubchem

					CCCC)O)	
					0	
					CCCCCC	
					CCCCCC(
					CC(=O)O	
					cicicoc	
					(C10)C0)	
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					1)OP(=O)([
	UDP-3-O-				0-	
	(3-				1) OCC2C(
	hydroxytet				$\Gamma(C(02)N)$	
	radecanovl				3C = CC(=	
)-N-				0)NC3=0)	
	acetyloluc			C31H51N	0)0)NC(=	
cpd u3aga	osamine	C04738	_2	3019P2	O(C)O(C)O(C)O(C)O(C)O(C)O(C)O(C)O(C)O(C)	Pubchem
opu_usugu	osamme	01750	<u>L</u>	501712		1 doenem
					CC(=0)0	
					$C^{1}C(C(OC))$	
					(C10)C0	
					(C10)C0)	
					O(-0)(0)	
	0DF-3-0-				$O(CC^2)$	
	(J-				$(C(C(\Omega)))$	
	radaaanayl				(C(C(O2)))	
					-0NC2-	
	J-D-			C201150N	-0)NC3-	
and u2haa	giucosaini	C06022	1	2018D2	O(O(O)N)	Dubaham
cpu_usnga	Ile	C00022	-1	3018F2	\mathbf{C}	Publieni
	Undecapre				CC(C(-0))	
	nyı-					
	aipnospho-				-0)NC(C)	
	IN-				CCC(C(-	
					-0)0)N)C(
	moyi-(IN-				=0)NC(C)	
	acetyigiuc				C(=0)NC(
	osamine)-				C)C(=0)0	
	L-alanyl-				$\mathcal{U}(=\mathcal{U}(\mathcal{U})$	
	D-				NC(=0)C(
	glutamyl-					
	meso-2,6-					
	diaminopi				C2C(C(C(
	meloyl-D-			00.0011.00	C(O2)CO)	
cpd_uaag	alanyl-D-			C95H152	O(O) O(O) NC(=	
mda	alanine	C05898	-4	N8O28P2	(U)C)CO)O	Pubchem

					P(=O)(O)	
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)OCC=C(
					C)CCC=C(
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	acetyl-3-				O2)N3C=	
	O-(1-				CC(=O)N	
	carboxyvin				C3=O)O)O	
	yl)-D-)CO)O)OC	
	glucosami			C20H26N	(=C)C(=O)	
cpd_uaccg	ne	C04631	-3	3O19P2	0	Pubchem
					CC(=O)N	
					C1C(C(C(
					OC1OP(=	
					O)(O)OP(
					=O)(O)OC	
					C2C(C(C(
	UDP-N-				O2)N3C=	
	acetyl-D-				CC(=O)N	
cpd uacga	glucosami			C17H25N	C3=O)O)O	
m	ne	C00043	-2	3O17P2)CO $)$ O $)$ O	Pubchem
	Undecapre				CC(C(=0))	
	nvl-				NC(CCC(
	diphospho-				=0)NC(C)	
	N-				CCC(C) =	
	acetylmura					
	movi_I _				=0)NC(C)	
	alanvl_D				C(=0)NC(
and warm	alutamy			C87H120	C(-0) = C(-0	
do	giulalityi-	C05807	А	N7022D2	C(-0)0	Dubaham
ua	meso-2,0-	C0309/	-4	IN/023P2	$\left \left(-0 \right) 0 \right)$	rubenem

	diaminopi				NC(=O)C(
	meloyl-D-				C)OC1C(C	
	alanyl-D-				(OC(C1O)	
	alanine				CO)OP(=	
					O)(O)OP(
					=O)(O)OC	
					C = C(C)CC	
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	UDP-N-				(O2)N3C=	
	acetylmura				CC(=O)N	
	moyl-L-			C23H33N	C3=O)O)O	
cpd_uama	alanine	C01212	-3	4O20P2)NC(=O)C	Pubchem
					CC(C(=O))	
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					=O)O)C(=	
					O)O)NC(=	
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					1C(C(OC(
					C(0)(0)	
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					0)000000	
					$C(C(\Omega))$	
					$N_{2}C = CC($	
	moul				-0NC2-	
and many	alamul D			CONTON	-0) $NC3=$	
cpa_uama	alanyi-D-	C00(02	4	C28H39N		D11
g	glutamate	C00692	-4	5023P2	(=U)C	Pubchem

	CC(C(=0))
	O(C(C(0)))
	O)CO)OP(
	=O)(O)OP
	(=O)(O)O
	CC2C(C(C
	(O2)N3C=
UDP-N-	CC(=O)N
acetylmura C20H28	N C3=O)OOO
cpd uamr mate C01050 -3 3019P2)NC(=O)C Pubchem
	CC1=C(C(
	=0)C(=C(
	$C_{1} = C_{1} = C_{1$
	CI=0,0C)
	OC)CC = C
	(C)CCC=C
Ubiquinon C49H740	O (C)CCC=C
cpd_ubq8 e-8 C17569 0 4	(C)C Pubchem
	CC1=C(C(
	=C(C(=C1))
	O)OC)OC)
	O)CC=C(
	$\dot{C}CCC=\dot{C}($
	C)CCC=C(
cpa_ubq8n Ubiquinoi-	$\int C C C = C C$
2 8 C00390 0 4	C)C Pubchem
	CC(=CCC
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cpd udcpd diphosphat C55H890	O (OP(=O))
p e C04574 -3 7P2	O)OP(=O) Pubchem

					(O)O)C)C)	
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1 1	nyı 	C00249	2	C33H89U	C(C)C(C)	D-1.1.
cpd_udcpp	pnospnate	C00348	-2	412	C	Pubchem
					CI=CN(C(
					=0)NCI=	
					0)020(0)	
					C(O2)COP	
					(=O)(O)O	
		~~~~		C9H11N2	P(=O)(O)	
cpd_udp	UDP	C00015	-3	012P2	0)0)0	Pubchem
					CI=CN(C(	
					=O)NCI=	
					O)C2C(C(	
					C(O2)COP	
					(=O)(O)O	
					P(=O)(O)	
					OC3C(C(C	
					(C(O3)CO	
	UDPgluco			C15H22N	)O)O)O)O)	
cpd_udpg	se	C00029	-2	2O17P2	0	Pubchem
					C1=CN(C(	
					=O)NC1=	
					O)C2C(C(	
					C(O2)COP	
					(=O)(O)O	
					P(=O)(O)	
					OC3C(C(C	
					(C(O3)CO	
cpd_udpga	UDPgalact			C15H22N	)0)0)0)0)	
1	ose	C00052	-2	2O17P2	0	Pubchem

					CC(C(=O))	
					NCICCCÍ	
					=0)NC(C)	
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					1C(C(OC(	
	UDP-N-				C10)C0)	
	acetylmura				OP(=O)(O	
	moyl-L-				)OP(=O)(	
	alanyl-D-				O)OCC2C	
	gamma-				(C(C(O2)))	
	glutamyl-				N3C=CC(	
	meso-2 6-				=0)NC3=	
	diaminoni			C35H51N	0)0)0)NC	
and uamd	malata	C20886	1	7026P2	(-0)C	Dubaham
cpu_uginu	metate	C20880	-4	702012	(-0)C	rubenem
					=O)NC(C	
					CCC(C(=	
					O)O)N)C(	
					=O)NC(C)	
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	UDP-N-				c) <del>)</del> <del>)</del> <del>)</del> <del>)</del> <del>)</del> <del>)</del> <del>)</del> <del>)</del>	
	acetylmura				(0C(C10))	
	movi-I -				CO)OP(=	
	alonyl D				O(O)OP(	
	alaliyi-D-				-0)(0)0F(	
	giutaniyi-				-0)(0)00	
	meso-2,6-				$C_2C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C(C$	
	diaminopi				$O_2$ )N3C=	
	meloyl-D-				CC(=O)N	
cpd_ugmd	alanyl-D-			C41H61N	C3=O)O)O	
a	alanine	C04882	-4	9O28P2	)NC(=O)C	Pubchem
					C1=CN(C(	
					=O)NC1=	
					O)C2C(C(	
					C(O2)COP	
				C9H11N2	(=0)(0)(0)	
end ump	UMP	C00105	_2	09P	(0)	Pubchem
-pa_ump	Uroporphy			C40H36N	C1C2=C(C)	1 ucenem
and unna?	rinogen III	C01051	0	4016	$\left  \begin{array}{c} -C(\mathbf{V}) \\ -C(\mathbf{V}) \\ \end{array} \right $	Dubaham
cpu_uppg3	mogen m	01031	-8	4010	(-U(NZ)U)	rubenem

					C3=C(C(=	
					C(N3)CC4	
					=C(C(=C(	
					N4)CC5=	
					C(C(=C1N))	
					5)CCC(=0	
					(0))))))))))))))))))))))))))))))))))))	
					)0)00(=0)	
					(0))))))))))))))))))))))))))))))))))))	
					(0)))))))))))(=	
					0)0)00(-	
					=0)0)000000000000000000000000000000000	
					=0)0)CC(	
					C(=0)0	
					C(-0)O	
				C4H4N2O	-0)NC1-	
and ura	Uracil	C00106	0	2	-0)	Pubchem
cpu_uia	Ulacii	00100	0	<i>Δ</i>	$C_{12} = C_{01}$	rubenem
					$C_{12} = C(N)$	
				C5U4N4O	NC(-0)NI	
and urata	umoto	C00266	0	C3H4N4O	$C_{2}=0$	Dubaham
cpu_urate	urate	00300	0	3	$C_2 = 0$	Fubchem
				CAUSNOO	-N1)C-C	
and man	Thereste	C00795	1	COHSN20	=NI)C=C	Durk als and
cpd_urcan	Urocanate	C00785	-1	2	C(=0)0	Pubchem
1 1 1	(S)-			CALLONO	C(C(=0))	
cpd_urdgly	Ureidoglyc	00000	0	C3H6N2O	)(NC(=0)	D 1 1
С	olate	C00603	0	4	N)O	Pubchem
1 1	Uranium		0	1100		<b>D</b> 1 1
cpd_urd10	dioxide	NA	0	002	O=[U]=O	Pubchem
		~~~~			C(=O)(N)	
cpd_urea	Urea	C00086	0	CH4N2O	N	Pubchem
					C1=CN(C(
					=O)NC1=	
					O)C2C(C(
			_	C9H12N2	C(O2)CO)	
cpd_uri	Uridine	C00299	0	06	0)0	Pubchem
					O=[U+2]=	
cpd_urnyl	Uranyl	NA	2	UO2	0	Pubchem
					C1=CN(C(
					=O)NC1=	
					O)C2C(C(
					C(O2)COP	
					(=O)(O)O	
					P(=O)(O)	
				C9H11N2	OP(=O)(O	
cpd_utp	UTP	C00075	-4	O15P3)O)O)O	Pubchem

				C5H11NO	CC(C)C(C	
cpd val-L	L-Valine	C00183	0	2	(=O)O)N	Pubchem
cpd_wo4	tungstate	C20679	-2	WO4	[O-][W](=O)(=O)[O-]	Pubchem
cpd_xan	Xanthine	C00385	0	C5H4N4O 2	C1=NC2= C(N1)C(= O)NC(=O) N2	Pubchem
cpd_xmp	Xanthosine 5'- phosphate	C00655	-2	C10H11N 4O9P	C1=NC2= C(N1C3C(C(C(O3)C OP(=O)([O-])[O-])O)O)NC(=O)NC2= O	Pubchem
cpd xtp	ХТР	C00700	-4	C10H11N 4O15P3	C1=NC2= C(N1C3C(C(C(O3)C OP(=O)(O)OP(=O)(O)OP(=O) (O)O)O(O) NC(=O)N C2=O	Pubchem
cpd_xtsn	Xanthosine	C01762	0	C10H12N 4O6	C1=NC2= C(N1C3C(C(C(O3)C O)O)O)NC (=O)NC2= O	Pubchem
cpd_xu5p- D	D- Xylulose 5- phosphate	C00231	-2	C5H9O8P	C(C(C(C(= O)CO)O)O)OP(=O)(O)O	Pubchem
cpd_trehal ose	Trehalose	C01083	0	C12H22O 11	C(C1C(C(C(C(01)O C2C(C(C(C(O2)CO) O)O)O)O) O)O)O	Pubchem
cpd_trehal ose6p	Trehalose 6- Phosphate	C00689	0	C12H23O 14P	C(C1C(C(C(C(O1)O C2C(C(C(C(O2)COP	Pubchem

					(=O)(O)O) O)O)O)O)	
					0)0)0	
					C(C1C(C(
					C(C(O1)O	
					C2(C(C(C(
					O2)CO)O)	
				C12H22O	O)CO)O)O	
cpd_sucr	Sucrose	C00089	0	11)O)O	Pubchem
cpd_sucr	Sucrose	C00089	0	11)0)0 C(C1C(C(Pubchem
cpd_sucr	Sucrose	C00089	0	11)0)0 C(C1C(C(C(C(01)0	Pubchem
cpd_sucr	Sucrose	C00089	0	11)0)0 C(C1C(C(C(C(01)0 C2(C(C(C(Pubchem
cpd_sucr	Sucrose	C00089	0	11)0)0 C(C1C(C(C(C(01)0 C2(C(C(C(02)C0P(=	Pubchem
cpd_sucr	Sucrose	C00089	0	11)O)O C(C1C(C(C(C(O1)O C2(C(C(C(O2)COP(= O)(O)O)O)	Pubchem
cpd_sucr	Sucrose 6-	C00089	0	11 C12H21O)0)0 C(C1C(C(C(C(01)0 C2(C(C(C(02)COP(= 0)(0)0)0) 0)C0)0)0	Pubchem

Data S1 Table D: Tables detailing the composition of each biomass component an	nd the
overall biomass reaction in the WP2 GEM.	

Biomass Objective Function Shewanella psychrophila WP2								
Requirements fo	r the production of	of 1g dry	-					
weight of Bioma	ss (gDW Cellular	·						
Biomass)								
Overall								
		Weight	Stoichiometry					
		Percentage (%	in Biomass					
		gDW)	Reaction	Data Source				
				Inferred from				
				other				
				Shewanella				
1 gDW DNA	cpd_dna_macro	5	0.05	models				
				Inferred from				
				other				
				Shewanella				
1 gDW RNA	cpd_rna_macro	9	0.09	models				
				Inferred from				
				other				
	cpd_protein_ma			Shewanella				
1 gDW Protein	cro	52.8	0.528	models				
				Inferred from				
				other				
	cpd_lipid_macr			Shewanella				
1 gDW Lipid	0	17.5	0.175	models				
				Inferred from				
				other				
1 gDW	cpd_peptidogly			Shewanella				
Peptidoglycan	can_macro	2.5	0.025	models				
				Inferred from				
				other				
1			0.004	Shewanella				
I gDW LPS	cpd_lps_macro	3.4	0.034	models				
				Interred from				
1 DW	1 1 1 1			other				
I gDW	cpd_carbohydra		0.077	Shewanella				
Carbonydrate	te_macro	1.1	0.077	models				
				Interred from				
	1 - 4			otner				
I gDW Irace	cpd_trace_macr	0.1	0.001	Snewanella				
Elements	0	2.1	0.021	models				

DNA

Requirements for the production of 1g dry weight of DNA (gDW DNA)

dNTP	Compositi on (p, mmol/mm ol)	cpd ID	MW (g/mol)	p*MW (g/mol)	(p/sum g/mmol)	Stoichiome try (mmol/gD W DNA)
				108.79672		
dATP	0.2215	cpd_datp	491.1816	44	0.454872	
				106.80027		
dTTP	0.2215	cpd_dttp	482.1683	85	0.454872	
				141.24990		
dGTP	0.2785	cpd dgtp	507.181	85	0.571927	
				130.10319		
dCTP	0.2785	cpd dctp	467.1569	67	0.571927	
			Molecular			
			weight of			
			DNA in S.			
			psyhcorphil	486.95010		
			a model:	8	2.053598	4.107196

RNA

Requirements for the production of 1g dry weight of RNA (gDW RNA)

DTP	Count in the genome cds	Mol Compositi on (p, mol/mol)	cpd ID	MW (g/mol)	p*MW (g/mol RNA)	Stoichiom etry (mmol/gD W RNA)
		0.2786591			141.33063	
ATP	1492316	714	cpd_atp	507.181	72	0.557645
		0.2667041			129.12246	
UTP	1428293	993	cpd_utp	484.1411	44	0.533721
		0.2396949			125.40368	
GTP	1283649	216	cpd_gtp	523.1804	5	0.479671
		0.2149417			103.85044	
CTP	1151087	078	cpd_ctp	483.1563	02	0.430135
				Molecular weight of		
				RNA in S.		
				psyhcorphil	499.70722	
				a model:	68	2.001172

Protein

Requirements for the production of 1g dry weight of Protein (gDW Protein)

			Count	Mol		P*MW	aa-	trna(a	Stoichi
			in	compo		(g/mol	trna	a)	ometry
Amino			genom	sition	MW	total	KEGG	KEGG	of aa
Acid	cpd	cpd	e	(P,	(g/mol)	aa)	ID	ID	(mmol/

				mol/m					gDW
				ol)					pro)
Alanin				0.0844	89.093	7.5205	cpd_al	cpd_trn	0.6554
e	ala	Α	144451	1242	2	7225	atrna	aala	75
Argini				0.0429	174.20	7.4770	cpd_ar	cpd_trn	0.3332
ne	arg	R	73450	2177	1	1447	gtrna	aarg	94
Aspar				0.0428	132.11	5.6593	cpd_as	cpd_trn	0.3326
agine	asn	N	73303	3586	79	8434	ntrna	aasn	27
Aspart		_		0.0567	133.10	7.5519	cpd_as	cpd_trn	0.4405
ate	asp	D	97093	3796	27	7534	ptrna	aasp	79
Cystei		G	1 = 1 = 2	0.0101	121.15	1.2356	cpd_cy	cpd_trn	0.0791
ne	cys	С	17453	9896	82	8757	strna	acys	96
Gluta		0	77000	0.0450	146.14	6.5834	cpd_gl	cpd_trn	0.3498
mine Claste	gin	Q	//088	4/69	45	259	ntrna	agin	02
Gluta	alu	Б	102710	0.0606	14/.12	8.91/5	cpa_gi	cpd_trn	0.4/06
Chusin	giu	L	103/19	0997	75 066	5 1940	utrna	agiu	40
Giyem	alv	C	110100	0.0090	/3.000	2706	cpd_gi	cpd_trn	0.3303
e Histidi	giy	U	110190	0.0215	155.15	3 3/12	cnd hi	agiy	0 1673
ne	his	н	36885	5438	155.15 46	6144	strna	ahis	73
Isoleuc	1115	11	50005	0.0654	131 17	8 5868	cnd ile	end trn	0 5083
ine	ile	т	112022	6197	29	3702	trna	aile	22
Leucin	ne	-	112022	0.1058	131.17	13,884	cpd le	cpd trn	0.8219
e	leu	L	181128	4525	29	0283	utrna	aleu	05
				0.0533	146.18	7.7974	cpd ly	cpd trn	0.4141
Lysine	lvs	K	91276	3869	76	5565	strna	alys	83
Methio	•			0.0262	149.21	3.9230	cpd m	cpd trn	0.2041
nine	met	Μ	44992	9185	13	4049	ettrna	amet	6
Phenyl									
alanin				0.0407	165.18	6.7234	cpd_ph	cpd_trn	0.3160
e	phe	F	69651	0175	91	8624	etrna	aphe	55
Prolin				0.0379	115.13	4.3656	cpd_pr	cpd_trn	0.2944
e	pro	Р	64889	19	05	3326	otrna	apro	47
				0.0730	105.09	7.6730	cpd_se	cpd_trn	0.5669
Serine	ser	S	124943	1258	26	8208	rtrna	aser	54
Threo		-		0.0546	119.11	6.5122	cpd_thr	cpd_trn	0.4245
nine	thr	Т	93554	6988	92	3264	trna	athr	2
Trypto		***	20(12	0.0120	204.22	2.4600	cpd_trp	cpd_trn	0.0935
pnan T '	trp	W	20613	4556	52	0682	trna	atrp	36
I yrosi	+****	V	57071	0.0308	181.18 0 <i>2</i>	5.5983	cpa_tyr	cpa_trn	0.2399
ne	tyr	1	328/4	9/83	83	3102 7 7015	una	alyr	20
Valine	vol	V	113671	0.0004	11/.14 62	1277	cpu_va	cpu_trn	0.3138
vanne	v ai	V	1130/1	250	U3 Molecul	12//	mna	aval	7 7651
					ar	120.70			52
					aı	0444			52

weight of
Protein
in S.
psyhcor
phila
model:

Lipids

Requirements for the production of 1g dry weight of Lipid (gDW Lipid)

	WP2T							
	10C							Stoichio
	(Wang,			Mol				metry
	2007)			composi				of aa
	%		Fatty	tion (P,			P*MW	(mmol/
Fatty	compos	Fatty	Acid	mol/mol	Formul	MW	(g/mol	gDW
acid	ition	Acid ID	ACP ID)	a	(g/mol)	total aa)	pro)
		cpd dod	cpd ddc		C12H24		11.8188	0.23905
12:00	5.9	ca	aACP	0.059	O2	200.32	8	4
iso-13 :		cpd_fa1	cpd_fa1		C13H25		15.5738	0.29577
0	7.3	3	3ACP	0.073	O2	213.34	2	8
		cpd_ttdc	cpd_my		C14H27		17.9614	0.32008
14:00	7.9	a	rsACP	0.079	O2	227.36	4	9
			cpd_fa1					
iso-13 :		cpd_fa1	30OH3		C13H25			0.07293
0 3- OH	1.8	30OH3	ACP	0.018	03	229.33	4.12794	2
iso-15 :			cpd_fa3		C15H30			
0	4	cpd_fa3	ACP	0.04	O2	242.4	9.696	0.16207
16 :		cpd_hdc	cpd_hde		C16H30		97.1846	1.54777
1ω7c	38.2	ea	ACP	0.382	O2	254.41	2	1
		cpd_hdc	cpd_pal		C16H32		32.5653	0.51457
16:00	12.7	a	mACP	0.127	O2	256.42	4	3
			cpd_fa1					
17:		cpd_fa1	71n8AC		C17H31			0.06482
108c	1.6	71n8	Р	0.016	O2	267.43	4.27888	8
			cpd_fa1					
18 :		cpd_fa1	81n7AC		C18H33			0.38086
1ω7t	9.4	81n7	Р	0.094	02	281.45	26.4563	5
	_	cpd_ocd	cpd_ocd		C18H35			0.08103
18:00	2	ca	ACP	0.02	02	283.47	5.6694	5
		cpd_epa		0.0-1	C20H30	202 i -	21.4739	0.28767
20 : 5ω3	7.1	apo	cpd_epa	0.071	02	302.45	5	5
			Molecula					
			r weight	0.0=0			246.806	• • • • • • •
			of Lipids	0.979			57	3.96667

in S. psyhcorp	
hila	
model:	

Cell Wall										
Requirements for the production of 1 gDW of peptidoglycan or 1 gDW of LPS										
		Molecular								
		Weight								
Metabolite	Metabolite ID	g/mol	mol/g	mmol/g						
Peptidoglycan	cpd_peptx	901.87	0.001108807256	1.108807256						
LPS	cpd_lps_Core[c	2849.04	0.000350995423	0.350995423						

Carbohydrates

Requirements for the production of 1 gDW of carbohydrate									
		Molecular							
		Weight							
Metabolite	Metabolite ID	g/mol	mol/g	mmol/g					
Glycogen 1									
gDW	[cpd_glycogen[c]]	666.58	0.001500195025	1.500195025					

Trace Elements

Requiremnets for the production of 1g dry weight of trace elements

1	-		0,00			
		iJO1366				
		Stoichiome				
		try	g/mol			
	Metabolite	(mmol/gD	Molecular	g/gDW of	g/g of	mmol/g of
Metabolite	ID	W of cell)	weight	cell	solute pool	Solutes
Biotin	cpd_btn[c]	2.00E-06	244.31	4.89E-07	2.63E-05	0.00
Succinyl-	cpd_succo					
CoA	a[c]	9.80E-05	867.61	8.50E-05	4.58E-03	0.01
				0.0001289		
CoA	cpd_coa[c]	0.000168	767.53	4504	6.95E-03	0.01
Acetyl-	cpd_accoa[0.0002258		
CoA	c]	0.000279	809.57	7003	1.22E-02	0.02
				0.0001751		
FAD+	cpd_fad[c]	0.000223	785.55	7765	9.44E-03	0.01
	cpd_nadh[
NADH	c]	4.50E-05	665.44	2.99E-05	1.61E-03	0.00
Undecapre						
nyl						
diphosphat	cpd_udcpd					
e	p[c]	5.50E-05	927.26	5.10E-05	2.75E-03	0.00

NADP+ c] 0.000112 745.42 8704 4.50E-03	0.01
Cobamide cpd coba 0.0003522	
coenzyme mcoa[c] 0.000223 1579.58 4634 1.90E-02	0.01
Menaquino cpd mqn7[0.0001447	
ne 7 c] 0.000223 649 27 7.80E-03	0.01
cpd sheme 0.0002044	
Siroheme [c] 0.000223 916.66 1518 1.10E-02	0.01
Thiamine	
diphosphat cpd thmpp 0.0000948	
e [c] 0.000223 425.31 4413 5.11E-03	0.01
Ubiquinol- cpd ubq8h 0.0001625	
8 2[c] 0.000223 729.12 9376 8.76E-03	0.01
S-	
Adenosyl-	
L- cpd amet[0.0000888	
methionine c] 0.000223 398.44 5212 4.79E-03	0.01
Chorismat cpd chor[c 0.0000504	
e] 0.000223 226.18 3814 2.72E-03	0.01
cpd phem 0.0001374	
Protoheme e[c] 0.000223 616.49 7727 7.41E-03	0.01
Pyridoxal	
5'phosphat cpd pydx5 0.0000551	
e p[c] 0.000223 247.14 1222 2.97E-03	0.01
cpd ribflv[0.0000839	
Riboflavin c] 0.000223 376.36 2828 4.52E-03	0.01
cpd nadph 0.0002497	
NADPH [c] 0.000335 745.42 157 1.35E-02	0.02
cpd amp[c 0.0003472	
AMP] 0.001 347.22 2 1.87E-02	0.05
0.0011873	
NAD cpd nad[c] 0.001787 664.43 3641 6.40E-02	0.10
UDP- cpd udpg	
Glucose c] 0.003 566.3 0.0016989 9.16E-02	0.16
Calcium 0.0001984	
2+ cpd ca2[c] 0.004952 40.08 7616 1.07E-02	0.27
0.0003567	
Iron 2+ cpd fe2[c] 0.006388 55.85 698 1.92E-02	0.34
Spermidin cpd spmd[0.0009795	
$\begin{bmatrix} 1 & 1 & -1 & 1 \\ 0.006744 & 145.25 & 66 & 5.28E-02 \end{bmatrix}$	0.36
Magnesiu cpd mg2[c 0.0002006	
$m 2^+$] 0.008253 24.31 3043 1.08E-02	0.45
Ammoniu 0.0002233	
m cpd nh4[c] 0.012379 18.04 1716 1.20E-02	0.67

	cpd_cobalt					
Cobalt 2+	2[c]	2.40E-05	58.93	1.41E-06	7.62E-05	0.00
				0.0000428		
Copper 2+	cpd_cu2[c]	0.000674	63.55	327	2.31E-03	0.04
Manganese	cpd_mn2[c			0.0000361		
2+]	0.000658	54.94	5052	1.95E-03	0.04
	cpd_mobd[
Molybdate	c]	7.00E-06	161.95	1.13E-06	6.11E-05	0.00
				0.0004046		
Sulfate	cpd_so4[c]	0.004126	98.08	7808	2.18E-02	0.22
				0.0001755		
Chlorine	cpd_cl[c]	0.004952	35.45	484	9.46E-03	0.27
	cpd_ptrc[c			0.0029327		
Putrescine]	0.03327	88.15	505	1.58E-01	1.79
5-						
Methyltetr						
ahydrofola	cpd_5mthf			0.0001024		
te	[c]	0.000223	459.45	5735	5.52E-03	0.01
				0.0072604		
Potassium	cpd_k[c]	0.18569	39.1	79	3.91E-01	10.00
		Molecular				
		weight of				
		Trace				
		Elements in				
		S.				
		psyhcorphil				
		a model:	1.86E-02	1.00E+00	14.95	

Reaction ID	Standard Gibbs Free Energy (kJ/mol)
2MAHMP	-32.3319
4HBTE	-20.3735
5DOAN	3.1817
5HPUDICDCs	-56.4442
A5PISO	-2.5059
AACPS10	39.8926
AACPS11	32.3752
AACPS12	24.8578
AACPS13	17.3404
AACPS14	-38.1024
AACPS15	-53.1317
AACPS16	55.2334
AACPS3	25.1638
AACPS4	-45.6153
AACPS5	-60.6501
AACPS6	32.6812
AACPS7	17.6464
AACPS8	10.1290
AACPS9	47.4101
AACPSFA130OH	206.5742
AACPSFA1718	-53.1325
AACPSFA1817	-60.6512
ABTA	8.0322
ACACCB	-27.0104
ACACCT	7.1852
ACACT10R	-27.0958
ACACt2	0.0000
ACALDi	-20.9198
ACBIPGT	1072.9123
ACCOAC	-600.8426
ACCOAL	5.7673
ACGAMK	-10.0797
ACGAt2	0.0000
ACGK	23.2061
ACGS	-22.6163

Data S1 Table E: Standard Gibbs Free Energy predictions for reactions in the WP2 GEM based on the Group Contribution method. Values are provided in kJ/mol.

ACHBS	-37.5569
ACKr	-14.1282
ACLS	-42.5482
ACMAT1	12.2573
ACNAMS	-65.3855
ACOAD10	42.5546
ACOAD8	42.5546
ACOAD9	51.7576
ACOATA	-4.0389
ACODA	-7.6529
ACONT	7.9076
ACOTA	-6.8947
ACS	-10.5274
ACt6	0.0000
ADA	-21.2807
ADCL	-89.9053
ADCOBAK	829.5900
ADCOBAS	-84.0023
ADCOBHEXS	-789.5845
ADCS	-16.6873
ADHMCYSSYN	35.4788
ADK1	-1.5889
ADK3	-1.6941
ADK4	0.6524
ADMDC	-386.9345
ADNCYC	-29.8265
ADNK1	-9.1420
ADNt2	0.0000
ADPRDP	-3.3598
ADPT	-16.3867
ADSK	-47.4721
ADSL1r	43.6293
ADSL2r	36.1607
ADSS	-28.2548
AEPPAT	-4.9380
AGDC	-3.6537
AGMAHYD	-51.3623
AGPEPHOS	-262.4762
AGPR	11.2357

AHAI	-11.9988
AHCYSNS	-16.6547
AICART	9.2504
AIRC2	-590.3691
AIRC3	31.1116
AKGD	-29.0756
ALAALA	-32.1185
ALAD_L	36.9584
ALAGLYX	-2.1955
ALAR	0.1480
ALATA_D2	5.8161
ALATA_L	0.4930
ALATA_L2	5.9641
ALA_Dt4	0.0000
ALAt4	0.0000
ALCD2x	22.5188
ALDD2x	-52.9600
ALLNRAC	0.0000
ALLTC	40.7525
ALLTN	-19.3822
AMAA	6.6165
AMALT1	21.8932
AMALT2	-49.2133
AMALT3	-4.0235
AMALT4	-23.2966
AMAOT	-0.6370
AMMQT7_2	-22.5975
AMPMS2	-174.5798
AMPTASECG	14.8248
AMPTASEPG	30.7607
ANPRT	-57.4517
ANS1	-106.5955
AOXS	13.5538
AP4AH	7.3520
AP5AH	-4481.7856
APRAUR	-17.4027
ARBABC	-28.4564
ARGDC	1.3864
ARGSL	10.2505

ARGSS	-0.7817
ARSRD2	-167.6156
ARSt1	0.0000
ASAD	4.8180
ASNN	-12.7136
ASNS1	-43.9536
ASP1DC	-17.0629
ASPCT	-21.5122
ASPK	18.4267
ASPO3	-137.0836
ASPO5	-21.1030
ASPO6	49.6899
ASPO8	47.0520
ASPO9	-15.0478
ASPTA1	2.9241
ASPTA4	-21.4896
ASPt2	0.0000
AST	-9.9090
ATPPRT	-94.9959
ATPS4r	28.4564
BETALDHx	-36.6929
BETALDHy	-35.4461
BPNT	-1.8987
BTS4	-213.7232
BUTSUCCCOA	-5.5095
BUT_T	0.0000
C120SN	-242.8593
C130ISN	-234.2998
C130OHISN	-11.7990
C140ISN	-312.3998
C140SN	-320.9593
C150ISN	-312.3998
C150SN	-390.4997
C151SN	-344.5762
C160ISN	-390.4997
C160SN	-399.0592
C161SN	-419.5231
C170ISN	-390.4997
C170SN	-468.5997

C171SN	-422.6762
C171n8SN	-422.6760
C180SN	-477.1592
C181SN	-497.6230
C181n7SN	-497.6229
C205SN	-132.5571
C50SN	66.3874
C60ISN	58.5640
C70ISN	51.0466
CAT	-469.5288
CBIAT	-564.2452
CBL1abc	-28.4564
CBLAT	-564.2452
CBPS	-612.6891
CDPG46D	-104.9434
CDPMEK	-8.9890
CHITINS	4.2064
CHOLDH1	12.8478
CHOLDH2	25.7139
CHOLDH3	26.9607
CHOLDH4	28.3864
CHOLDH5	-33.7134
CHOLt4	0.0000
CHORM	-44.6970
CHORS	-54.2881
CHRPL	-113.3597
CITT7	0.0000
CKDOAS	20.8014
CLAT	-17.4929
CO2t	0.0000
COBALTt3	0.0000
COBALTt5	0.0000
COBPS	-1074.7693
CONFALDD	-35.1930
CPPPGO	-370.9605
CRO4t6	0.0000
CS	-37.2457
CSND	-25.8642
CSNt2	0.0000

CTPS2	-17.1322
CU2t	-28.4564
CYCPOe	-404.7802
CYOO2	-170.0158
CYOR7	122.0250
CYSS	-56.3647
CYSTL	6.7668
CYTBD	-47.9908
CYTBO3_4	-47.9908
CYTD	-18.7127
CYTDH	3.0113
CYTDK1	-19.0820
CYTDK2	-19.1872
CYTDK3	-16.8407
CYTDt2	0.0000
CYTK1	3.4455
CYTK2	1.4770
CampHydrolyase	-12.7410
Clt	0.0000
Cut1	-28.4564
D-LACt2	0.0000
DADA	-17.7245
DADK	6.2712
DADNt2	0.0000
DAGK	-13.5785
DAHPS	-73.4702
DAPDC	-50.4450
DAPE	-0.6778
DASYN	-46.8030
DB4PS	-81.2807
DBTSr	-15.7897
DCYTD	-16.9033
DCYTt2	0.0000
DGALCT	0.0000
DGK1	0.7299
DHAD1	-42.9287
DHAD2	-42.9285
DHDPRy	-22.8764
DHDPS	-115.6186

DHFR	-25.3220
DHFS	-14.8557
DHNAOT7	-79.3129
DHNPA	-0.7509
DHORD2	-167.3374
DHORD4i	16.7982
DHORD8	-45.3016
DHORTS	-6.2540
DHPPDA2	26.2786
DHPRx	36.5043
DHPS3	-56.1496
DHPTPE	0.0000
DHQD1	-5.0321
DHQS	-124.8859
DIPEPabc10	-28.4564
DIPEPabc13	-28.4564
DKMPPD3	-66.2517
DMATT	-94.2693
DMOCT	-33.6612
DMPPS	-64.0817
DMQMT	-8.8454
DNMPPA	-18.7088
DNTPPA	-42.4220
DPCOAK	0.7018
DPR	-18.3304
DRBK	-16.8977
DRPA	21.6257
DTMPK	2.6577
DURIK1	-14.8571
DURIPP	14.1772
DURIt2	0.0000
DUTPDP	-59.1159
DXPRI	-15.8021
DXPS	-31.9101
E4PD	-38.9570
ECOAH2C	14.6247
ECOAH9	19.5288
EDA	16.9469
ENO	-3.9803

EPPP2	-24.7655
FAO4	-702.5430
FAO5	-837.9614
FAO6	-973.3797
FAO7	-1108.7980
FBA	23.1470
FBP	-12.2367
FCLT	3.0275
FDH10	-77.2869
FDH9	-15.1871
FE2abc	-28.4564
FE3abc	-28.4564
FGLU	-23.4058
FMNAT	796.4044
FMNRDDMBZ	-1824.7386
FMNRx	-17.0620
FORt	0.0000
FRD8	-68.1550
FRD9	-6.0552
FRTT	-91.9688
FTHFD	-23.0424
FTHFL	-5.4140
FUM	-3.3554
FUMACA	-51.9912
FUMt4_2	0.0000
G1PACT	-27.3289
G1PCT	-4.7267
G1PTMT	-1.3619
G1SATi	-9.3218
G35DP	-14.0308
G3PD2	28.4300
G3PD4	29.8556
G3PD8	-32.2442
G5SD	-13.6007
G6PDA	0.9313
G6PDHy	-4.1033
GAL1PURI	-7.4941
GALACN	7.2636
GALKr	-8.7593

GALU	-0.7036
GAPD	6.0739
GARFT	-8.2601
GBEZ	-26.5267
GCALDD	-70.7548
GF6PTA	-15.0310
GGLUGABDH	-36.6869
GGLUGABH	-10.6130
GGLUPTO	38.6237
GGLUPTS	-27.7762
GGTT	-91.9688
GHMT	-5.0624
GK1	-0.1999
GLCGSD	-1.9298
GLCP	63.3489
GLCS1	-76.1704
GLCt2	0.0000
GLGC	-12.4946
GLNS	-14.3568
GLU5K	30.0557
GLUCYSL	-38.2558
GLUDx	36.4654
GLUN	-14.0997
GLUPRT	-57.3985
GLUR	-1.0762
GLUSy	-51.8119
GLUt2	0.0000
GLUt4i	0.0000
GLYAT	29.0015
GLYBt4	0.0000
GLYCKb	-9.9458
GLYCL	17.0517
GLYCLTDXR	45.6904
GLYCLTt2r	0.0000
GLYCRt2	0.0000
GLYC_T	0.0000
GLYK	-20.2955
GLYOX	-25.4406
GLYt4	0.0000

GMHEPAT	-42.1009
GMHEPK	-11.8633
GMHEPPA	-10.1508
GMPS2	-69.9399
GP4GH	5.0237
GPDDA2	-38.3594
GPDDA4	-51.6379
GRTT	-91.9688
GSHPO	-452.3002
GSNK	-13.4399
GTHRD	13.1651
GTHRDH	8.8653
GTHRDabc	-28.4564
GTHS	-42.3471
GTPCI	-84.3269
GTPCII	-92.0689
GTPDPK	-32.3329
GUAD	23.7965
GUAPRT	-26.0846
HACD8	10.7512
HACOADr	-202.8887
HBZOPT	-91.2717
HCO3E	588.7135
HEMEOS	-81.2580
HEPTT	-91.9688
HEX1	-19.3379
HEXTT	-91.9688
HGT	0.0000
HIBHR	-22.4541
HISD1	4.3577
HISTD	-33.5316
HISTP	-14.8854
HIUH	-9.9416
HMBS	-139.9223
HMGDx	-3.7793
HMGL	-16.7829
HMGSs	-21.4948
HOMt2	0.0000
HOXPRx	33.1499

HPPDO1	-489.5702
НРРК	-14.8273
HPYRRx	-31.1897
HPYRRy	-32.4366
HSDy	22.6015
HSK	-11.4997
HSST	-20.4990
HSTPT	7.7854
HTHBPD	-149.8202
HXAD	-2.9286
HXPRT	-25.2301
ICDHxi	0.2701
ICDHy	1.5169
ICHORSi	0.9690
ICL	6.1298
IG3PS	-77.5508
IGPDH	-47.9232
IGPS	-55.0300
ILEDH2	24.4992
ILETA	-11.9662
ILEt4	0.0000
IMPC	3.2423
IMPD	10.5638
INDOLEt2	0.0000
INSK	-18.1939
IPDPS	-59.4799
IPMD	10.7808
IPPMIa	-19.5025
IPPMIb	11.0961
IPPS	-22.4440
IZPN	20.3024
KARA2i	-11.9989
KAS15	8.2185
KAS16	144.4009
KDOPP	-12.4409
KDOPS	-64.8318
Kt2i	0.0000
Kt3	0.0000
L-LACt2	0.0000

LDH Dir	-24 3489
LEUTA	-0.4372
LEUt4	0.0000
LGTHL	-24.3634
LLEUDr	36.0281
LPADSS	-2.2201
LYSt3	0.0000
MACPD	-18.5655
MALS	-29.2374
MALTt	0.0000
MAN1PT2	7.5288
MCCC	-604.6988
MCITD	-17.6248
MCITS	-42.9960
MCOATA	-1.8008
MDH	29.1413
MDRPD	-51.3109
ME2	9.0084
MEAMP1_GLU-ASP	1.5276
MEAMP1_GLY-ASP	5.1335
MEAMP1_GLY-GLU	-1.3250
MECDPDH	-1925.8360
MECDPS	1853.4811
MEPCT	-46.7152
MET-LABC	-28.4564
METAT	51.0181
METGL	188.0958
METS	-181.8689
MGCH	11.1261
MGt3	0.0000
MGt5	0.0000
MI1PP	-34.8893
MICITH	17.6236
MICITL	14.1583
MLACI	0.0000
MLTAM	-14.4523
MLTG1e	7.4409
MLTG2e	-36.5597
MLTG3e	34.5468

MLTG4e	-10.6430
MLTG5e	8.6301
MLTSp	-14.6665
MMSDHir	184.9999
MNabc	-28.4564
MOBDabc	-28.4564
MOHMT	0.5373
MTAN	-6.3914
MTHFC	-7.0021
MTHFD	9.8392
MTHFR2	-41.5579
MTHPTGHM	-201.8188
MTRI	-1.2217
MTRK	-11.3016
NADH12	-181.4631
NADH16	-59.4273
NADH4	2.6725
NADK	-8.9524
NADS1	48.3246
NAabcO	-28.4564
NAt3	0.0000
NAt3_2	0.0000
NAt9	0.0000
NDPK1	0.1052
NDPK2	-2.9123
NDPK3	10.2079
NDPK4	10.7254
NDPK5	0.9827
NDPK6	7.3017
NDPK7	9.7270
NDPK8	8.3746
NH4HNADOR	-465.9219
NH4HNADPOR	-469.6624
NH4t	0.0000
NIt3	0.0000
NMNAT	0.8877
NNAT	-42.3829
NNDMBRT	-41.3487
NNDPR	-13.0579

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NO3T7	0.0000
NODOx	-93.4530
NODOy	-94.6999
NPHS	-58.4858
NTD1	-13.5994
NTD10	0.2256
NTD11	-10.2625
NTD12	-27.6919
NTD2	-14.9848
NTD3_P	-17.2631
NTD4	-9.3745
NTD5_P	-10.1953
NTD6_P	-15.4962
NTD7	-19.3144
NTD8_P	-28.0640
NTD9	-15.0166
NTPP1	-45.8690
NTPP10	-48.3402
NTPP11	-48.3575
NTPP2	-44.0618
NTPP3	-55.3604
NTPP4	-57.8098
NTPP5	-58.8022
NTPP6	-42.5675
NTPP7	-57.5395
NTPP8	-45.4883
NTPP9	-31.0115
NTR4	-182.7447
NTR5	-120.6449
O2t	0.0000
OAADC	-21.3797
OBTFL	-13.2330
OCBT	-25.1184
OHPBAT	15.6051
OHPHM	-8.8293
OIVD1i	-31.2086
OIVD2	-25.5321
OIVD3	-25.5320
OMBZLM	3.1963

OMCDC	-10.7660
OMMBLHX	-213.6298
OMMBLHXAN	-41.0887
OMPDC	3.1964
OMPHHX	-213.6306
OMPHHXAN	-41.0894
OMP_AC	0.0000
OMP_ACGAM	0.0000
OMP_ADN	0.0000
OMP_ALA-D	0.0000
OMP_ALA-L	0.0000
OMP_ASP-L	0.0000
OMP_BGL	0.0000
OMP_CA2	0.0000
OMP_CBL1	0.0000
OMP_CHITOB	0.0000
OMP_CHOL	0.0000
OMP_CL	0.0000
OMP_CO2	0.0000
OMP_COBALT2	0.0000
OMP_CU2	0.0000
OMP_CYTD	0.0000
OMP_DAD-2	0.0000
OMP_DAMP	0.0000
OMP_DCMP	0.0000
OMP_DCYT	0.0000
OMP_DGMP	0.0000
OMP_DGSN	0.0000
OMP_DMS	0.0000
OMP_DMSO	0.0000
OMP_DODCA	0.0000
OMP_DTMP	0.0000
OMP_DURI	0.0000
OMP_FE2	0.0000
OMP_FOR	0.0000
OMP_FUM	0.0000
OMP_GAL	0.0000
OMP_GALTAN	0.0000
OMP_GLC-D	0.0000

OMP_GLU-L	0.0000
OMP_GLY	0.0000
OMP_GLY-ASP-L	0.0000
OMP_GLY-GLU-L	0.0000
OMP_GLYB	0.0000
OMP_GLYC	0.0000
OMP_GLYC-R	0.0000
OMP_GLYCLT	0.0000
OMP_GTHRD	0.0000
OMP_H2	0.0000
OMP_H2O2	0.0000
OMP_H2S	0.0000
OMP_HDCA	0.0000
OMP_ILE-L	0.0000
OMP_INDOLE	0.0000
OMP_INOSHP	0.0000
OMP_INOSPP1	0.0000
OMP_K	0.0000
OMP_LAC-D	0.0000
OMP_LAC-L	0.0000
OMP_LEU-L	0.0000
OMP_LYS-L	0.0000
OMP_MAL-L	0.0000
OMP_MALT	0.0000
OMP_MALTHP	0.0000
OMP_MALTTTR	0.0000
OMP_MET-L	0.0000
OMP_MG2	0.0000
OMP_MN2	0.0000
OMP_MOBD	0.0000
OMP_NH4	0.0000
OMP_NMN	0.0000
OMP_NO2	0.0000
OMP_NO3	0.0000
OMP_O2	0.0000
OMP_OCDCA	0.0000
OMP_PI	0.0000
OMP_PMCOA	0.0000
OMP_PPA	0.0000

OMD DDO I	0.000
OMP_PRO-L	0.0000
OMP_PIRC	0.0000
OMP_FIK	0.0000
OMP_SER-L	0.0000
OMP_SO3	0.0000
OMP_SUGG	0.0000
OMP_SUCC	0.0000
OMP_THR-L	0.0000
OMP_THYMD	0.0000
OMP_TMA	0.0000
OMP_TMAO	0.0000
OMP_TRP-L	0.0000
OMP_TSUL	0.0000
OMP_TTDCA	0.0000
OMP_TTTNT	0.0000
OMP_TYR-L	0.0000
OMP_URA	0.0000
OMP_UREA	0.0000
OMP_URI	0.0000
OMP_VAL-L	0.0000
OMP_XAN	0.0000
OMP_na1	0.0000
OPHBDC	-11.1587
OPHHX	-213.6356
OPHHXAN	-41.0945
ORNCD	-27.3416
ORPT	53.0230
OXGDC2	-26.5042
P5CD	-35.5741
P5CR	-50.2885
PANTS	-46.9966
PAP	-14.8779
PAPPT3	12.3438
PASYN_WP2	-4337.7399
PDH	-39.9381
PDX5PO	19.9222
PDX5PS	-245.3944
PERD	10.8037
PFL	-22.0785

PGAMT	-3.1968
PGCD	33.6222
PGDH	8.4651
PGDHY	-41.2653
PGI	2.5440
PGK	-18.9302
PGL	-22.8106
PGLYCP	-39.4018
PGM	5.3631
PGMT	-7.2012
PGPPH	-12.4368
PGSA	25.4994
PHE4MO	-442.9088
PHEAL	-3.2282
PHEMEabc	-28.4564
PHETA1	-0.4583
PHNabc	-28.4564
PIabc	-28.4564
PIt6	0.0000
PMANM	-5.7616
PMCOAt	0.0000
PMDPHT	-14.6176
PMPK	3.8755
PNTK	-17.3954
PPA	-12.7564
PPAtNa	0.0000
PPBNGS	-106.7508
PPC	-35.7028
PPCDC	-15.4095
РРСК	7.2463
PPM	-8.4638
PPM2	-3.7316
PPNCL	-56.7092
PPND	-81.8141
PPNDH	-88.7499
PPPGFUM	-137.4842
PPPGMEN	66.9810
PPPGNO3	-481.2531
PPPGO	-629.3985
PPS	1.7586
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PPTT	-91.9688
PRAGS	-34.8275
PRAIS	-42.6920
PRAIi	-5.3714
PRAMPC	24.2280
PRASCS	-43.6532
PRATPP	-44.1557
PRFGS	21.2756
PRKIN	-15.2390
PRMICIi	-5.3453
PRO1q	-132.4215
PROt4	0.0000
PRPPS	-6.3433
PSCVT	-36.1614
PSD	-17.6453
PSERT	-10.4317
PSP_L	-9.0827
PSSA	7.9993
PSUDS	-34.1782
PTAr	10.5445
PTPATi	-62.2738
PTRCabc	-28.4564
PULLNASE	32.7481
PUNP1	7.9407
PUNP2	14.7310
PUNP3	13.3408
PUNP4	20.9876
PUNP5	7.7323
PUNP6	10.9663
PUNP7	8.6224
PYAM5PO	36.3047
PYDXL5PSYN	-321.3548
РҮК	-28.6261
PYNP2	5.7115
PYRt2	0.0000
QULNS	-225.3764
RBFK	1340.6846
RBFSa	-135.0046

RBFSb	-30.0783
RBK	-27.0685
RBZP	-15.0572
RHCCE	-15.0514
RIBabc	-28.4564
RPE	-2.3946
RPI	0.8296
S7PI	9.0014
SADH	-82.8720
SADT2	13.0909
SDPDS	15.9013
SDPTA	-0.2408
SELNPS	796.6392
SERAT	-6.7919
SERD_D	-29.5449
SERD_L	-33.3421
SERGLYX	1.2458
SERt4	0.0000
SERt6	0.0000
SFGTH	-23.4579
SGDS	1.5712
SGSAD	-40.3701
SHCHCS2	-63.9442
SHCHD2	-11.7941
SHCHF	3.0258
SHK3D	-43.7709
SHKK	-2.9934
SHSL1	-65.4309
SLCYSS	-635.1769
SO4t2	0.0000
SOD	98.9507
SOTA	-5.5894
SPA	3.4413
SPMS	388.8698
SPRS	387.6919
SSALx	-41.7819
SUCBZL	-25.2725
SUCBZS	-54.9104
SUCCt4	0.0000

SUCCtex	0.0000
SUCD7	-115.9806
SUCOAS	-1.9778
SULR	654.5751
TAL	0.0878
TDP	-33.5401
TDP3AAAT	33.6580
TDPDRE	0.0000
TDPDRR	12.6029
TDPGDH	-80.1348
TDSK	868.9786
THD2	1.2469
THD5	-1.2469
THDPS	27.7727
THMDt2	0.0000
THMabc	-28.4564
THRA	3.4249
THRD	11.5065
THRD_L	-31.1538
THRHT	0.0000
THRLAD	1.0904
THRS	-21.0875
THRt3	0.0000
THRt4	0.0000
THZPSN	-238.8132
TKT1	-3.0475
TKT2	-9.2771
TMDK1	-18.2612
TMDPP	13.1461
TMDS	-54.1168
TMPKr	5.0836
TMPPP	-20.6844
TPI	6.6057
TRPOR	-414.2907
TRPS2	-54.5276
TRPS3	-27.3530
TRPt6	0.0000
TSULST	49.7466
TYRTA	-46.0259

TYRt6	0.0000
U23GAAT	-252.9035
UAAGDS	-38.5493
UAGAAT	-245.0629
UAGCVT	-44.0353
UAGDP	-31.1016
UAGPT3	-4.9579
UAMAGS	-34.9903
UAMAS	-35.0729
UAPGR	-53.0046
UDCPDP	-31.6685
UDCPDPS	-735.7502
UDPG4E	3.3284
UDPHEXURI	-6.7905
UGMDDS	-38.3237
UHGADA	-3.9573
UMPK	4.2442
UNK3	-156.3544
UPP3MT	161.8946
UPP3S	-242.5116
UPPDC1	-42.4884
UPPRT	-18.4871
UQOR	-181.4631
URAt6	0.0000
URCN	-5.8493
URDGLY	-31.8912
URHYDROX	-359.3361
URIDK2	7.6578
URIH	-4.1402
URIK1	-13.4717
URIK2	-13.5769
URIK3	-11.2304
URIt2	0.0000
USHD	-3.1930
UreaExp	0.0000
VALALAMOB	-5.5474
VALDHr	31.4110
VALTA	-5.0544
VALt4	0.0000

WO4abc	-28.4564
XAND	-50.2096
XANt	0.0000
ХРК	-58.5356
FFSD	-22.3563
FRUK	-17.7598
SUCP	0.9948
SUCRPTS	-54.7209
TRE6PP	-15.8962
TREH	-6.2194
TREHtex	-44.6792
OMP_SUCR	0.0000
OMP_CIT	0.0000
OMP_TREH	0.0000

Data S1 Table F: List of all reactions contained in the WP2 GEM that were excluded from the thermodynamic constraints.

TMAOR3e
DMSOR4e
DMSOR3e
2MAHMP
4HBASink
5DRIB_Sink
5HPUDICDCr
ACBIPGT
ACPS1
ACPSc
ADCOBAK
ALATRS
AMOB_Sink
ARGTRS
ASNTRS
ASPTRS
ATPM
Biomass_WP2
CBLAT
CPPPGOAN
CYSTRS
DNA_CUT
DNA_SYNTHESIS
EDTXS5
EDTXS6
FCLT
FMETTRS
FMNAT
FNOR
FRD10
FRD11
GLNTRS
GLUTRR
GLUTRS
GLYCLTDXR
GLYCOGEN_SYNTHESIS

GLYD
GLYTRS
Growth
H2Ot5
HCO3E
HISTRS
ILETRS
IPPMIa
KAS16
LEUTRS
LIPID_SYNTHESIS
LPS_SYNTHESIS
LPSSYN_core
LYSTRS
MECDPDH
MECDPS
METTRS
MLTS
MOAT3
NADH11
NADH13
NADH14
NMNP
NTD3
NTD5
NTD6
NTD8
OMP_H
OMP_H2O
PAPSR
PASYN_WP2
PEPTIDO_SYNTHESIS
PEPTIDOXe
PHETRS
PPTGSe
PRAMPC
PROT_SYNTHESIS
PROTRS
RBFK

RNA_SYNTHESIS		
RNDR1		
RNDR2		
RNDR3		
RNDR4		
RNTR1		
RNTR2		
RNTR3		
RNTR4		
SELNPS		
SERTRS		
SHCHF		
SPMS		
SULR		
TDSK		
THRTRS		
TRACE_ELEMENTS		
TRDR		
TRPTRS		
TYRTA		
TYRTRS		
UPP3MT		
VALTRS		

Data S1 Table G: Net number of protons and net charge transported from outside of the cell to inside of the cell for each transport reaction in the WP2 GEM.

Reaction ID	Net Charge Transported (out to in)	Net Protons Transporterd (out to in)
ACACt2	1	1
ACGALT2	1	1
ACGAt2	1	1
ACt6	1	1
ADNt2	1	1
AKGt6	1	1
ALA Dt4	1	0
ALAt4	1	0
ARBABC	0	0
ARGABC	0	0
ARGabc	0	0
ARSTATPASE	3	0
ARSt	1	1
ARSt1	-3	0
ASNt2	1	1
ASPt2	1	1
ASPt2_3	3	3
ATPS4r	3	3
BGLP	1	1
BGLP2	1	0
BUT_T	1	1
CAT4I	-1	1
CBL1abc	-3	0
CH4SXPORT	0	0
CHOLt4	2	0
CO2t	0	0
COBALTabc	2	0
COBALTt3	-1	1
COBALTt5	2	2
CRO4t6	-1	1
CSNt2	1	1
CU2t	2	0
CYOO2	-2	-2
CYOR7	-4	-4
CYSt2	1	1

CYTBD	-2	-2
CYTBO3_4	-4	-4
CYTDt2	1	1
Clt	-1	0
Cut1	-2	0
D-LACt2	1	1
DADNt2	1	1
DCYTt2	1	1
DGALCT	1	0
DGSNt2	1	1
DIPEPABC15	-2	0
DIPEPabc10	-1	
DIPEPabc13	-1	0
DODCAt2	0	1
DURIt2	1	1
ETOHT1	0	0
FE2abc	2	0
FE3abc	3	0
FORt	0	0
FRMDT	0	0
FUMT2_2	2	2
FUMt4	3	3
FUMt4_2	1	0
G3PGABC	0	0
GLCPTS	0	0
GLCt2	1	1
GLNT2	1	1
GLUt2	1	1
GLUt4i	1	0
GLYBt4	1	0
GLYCLTt2r	1	1
GLYCRt2	1	1
GLYC_T	0	0
GLYt4	1	0
GSNT	0	0
GTHRDabc	0	0
GUAT	0	0
H2Ot5	0	0
HDCAT2	0	-1

HGT	2	0
HIST2R	1	1
HOMt2	1	1
HYXNT	0	0
ILEt4	1	0
INDOLEt2	1	1
INST2	1	1
Kt2i	2	1
Kt3	0	1
L-LACt2	1	1
LEU_ABC	0	0
LEUt4	1	0
LYSt3	1	1
MALT2_2	2	2
MALTt	1	1
MALt2_3	3	3
MET-LABC	0	0
MGt3	-1	1
MGt5	2	0
MNabc	2	2
MOBDabc	0	0
NADH11	-4	-4
NADH13	-4	-4
NADH16	-4	-4
NAabcO	-1	0
NAt3	0	1
NAt3_2	1	2
NAt9	-1	0
NH4t	0	0
NIt3	-1	1
NMNP	0	0
NO3T7	0	0
NOT2	1	1
O2t	0	0
OCDCAT2	0	1
PHEMEabc	0	0
PHET2R	1	1
PHNabc	0	0
PIabc	0	0

PIt6	1	1
PMCOAt	0	0
PPAT2	1	1
PPAtNa	1	0
PRO_LABC	0	0
PROt4	1	0
PTRCORNT7	0	0
PTRCT2	1	1
PTRCabc	0	0
PYRt2	1	1
SABC	0	0
SERt4	1	0
SERt6	1	1
SO4T4	1	0
SO4t2	1	1
SUCCT2_2	2	2
SUCCt2_3	3	3
SUCCt4	1	0
SUCCtex	1	1
SUCFUMtdc	0	0
SUCRPTS	0	0
SULabc	0	0
THD2	2	2
THMDt2	1	1
THMabc	1	0
THRHT	1	1
THRt3	1	1
THRt4	1	0
THYMT6	1	1
TRPt6	1	1
TSULABC	-1	0
TTDCAT2	0	1
TYRt6	1	1
UQOR	-2	0
URAt6	1	1
URIt2	1	1
UreaExp	0	0
VALt4	1	1
WO4abc	0	0

XANt	0	0

Data S1 Table H: Non-default concentration bounds used in the WP2 TMFA simulations. Concentrations are based on the LMO-812 media composition for all compounds except cpd_cbasp and cpd_dhor-S which were modified based on previous literature (Materials and Methods).

	Lower Concentration	Upper Concentration
Metabolite ID	Bound (M)	Bound (M)
cpd_cbasp[c]	1.00E-06	5.00E-02
cpd_dhor-S[c]	1.00E-06	5.00E-02
cpd_4abz[e]	5.46E-08	5.46E-06
cpd_4abz[p]	5.46E-08	5.46E-06
cpd_4abz[c]	5.46E-08	5.46E-06
cpd_btn[e]	2.43E-08	2.43E-06
cpd_btn[p]	2.43E-08	2.43E-06
cpd_btn[c]	2.43E-08	2.43E-06
cpd_ca2[e]	1.00E-05	1.55E-01
cpd_ca2[p]	1.00E-05	1.55E-01
cpd_ca2[c]	1.00E-05	1.55E-01
cpd_cl[e]	1.00E-05	2.82E+00
cpd_cl[p]	1.00E-05	2.82E+00
cpd_cl[c]	1.00E-05	2.82E+00
cpd_cobalt2[e]	2.46E-07	2.46E-05
cpd_cobalt2[p]	2.46E-07	2.46E-05
cpd_cobalt2[c]	2.46E-07	2.46E-05
cpd_cu2[e]	1.34E-08	1.34E-06
cpd_cu2[p]	1.34E-08	1.34E-06
cpd_cu2[c]	1.34E-08	1.34E-06
cpd_adcoba[e]	6.75E-07	6.75E-05
cpd_adcoba[p]	6.75E-07	6.75E-05
cpd_adcoba[c]	6.75E-07	6.75E-05
cpd_fe2[e]	1.00E-05	3.18E-04
cpd_fe2[p]	1.00E-05	3.18E-04
cpd_fe2[c]	1.00E-05	3.18E-04
cpd_k[e]	1.00E-05	5.07E-02
cpd_k[p]	1.00E-05	5.07E-02
cpd_k[c]	1.00E-05	5.07E-02
cpd_mobd[e]	7.38E-08	7.38E-06
cpd_mobd[p]	7.38E-08	7.38E-06
cpd_mobd[c]	7.38E-08	7.38E-06
cpd_na1[e]	1.00E-05	2.79E+00

cpd_na1[p]	1.00E-05	2.79E+00
cpd_na1[c]	1.00E-05	2.79E+00
cpd_nh4[e]	1.00E-05	1.60E-02
cpd_nh4[p]	1.00E-05	1.60E-02
cpd_nh4[c]	1.00E-05	1.60E-02
cpd_ni2[e]	3.10E-08	3.10E-06
cpd_ni2[p]	3.10E-08	3.10E-06
cpd_ni2[c]	3.10E-08	3.10E-06
cpd_nac[e]	1.23E-07	1.23E-05
cpd_nac[p]	1.23E-07	1.23E-05
cpd_nac[c]	1.23E-07	1.23E-05
cpd_pnto-R[e]	1.19E-07	1.19E-05
cpd_pnto-R[p]	1.19E-07	1.19E-05
cpd_pnto-R[c]	1.19E-07	1.19E-05
cpd_pi[e]	1.00E-05	1.36E-02
cpd_pi[p]	1.00E-05	1.36E-02
cpd_pi[c]	1.00E-05	1.36E-02
cpd_so4[e]	1.00E-05	5.66E-01
cpd_so4[p]	1.00E-05	5.66E-01
cpd_so4[c]	1.00E-05	5.66E-01
cpd_thm[e]	3.36E-07	3.36E-05
cpd_thm[p]	3.36E-07	3.36E-05
cpd_thm[c]	3.36E-07	3.36E-05
cpd_acgam[e]	1.00E-05	5.00E-03
cpd_acgam[p]	1.00E-05	5.00E-03
cpd_acgam[c]	1.00E-05	5.00E-03
		0.00032952 (4C),
		0.00025746 (15C),
cpd_o2[e]	1.00E-05	0.00023388 (20C)
		0.00032952 (4C),
		0.00025746 (15C),
cpd_o2[p]	1.00E-05	0.00023388 (20C)
		0.00032952 (4C),
		0.00025746 (15C),
cpd_o2[c]	1.00E-05	0.00023388 (20C)

Data S1 Table I: Exchange Constraints used for the temperature-dependent model simulations based on the LMO-812 media.

Compound ID	Compound Name	Lower Limit	Upper Limit
cpd_na1[e]	Sodium	-1000	1000
cpd_pro-L[e]	L-Proline	0	1000
cpd_h2o2[e]	Hydrogen peroxide	0	1000
cpd_damp[e]	dAMP	0	1000
cpd_dcmp[e]	dCMP	0	1000
cpd_dgmp[e]	dGMP	0	1000
cpd_dtmp[e]	dTMP	0	1000
cpd_met-L[e]	L-Methionine	0	1000
cpd_adn[e]	Adenosine	0	1000
cpd_dad-2[e]	Deoxyadenosine	0	1000
cpd_dgsn[e]	Deoxyguanosine	0	1000
cpd_glyc-R[e]	(R)-Glycerate	0	1000
cpd_indole[e]	Indole	0	1000
cpd_ura[e]	Uracil	0	1000
cpd_CrOH3[e]	Cr(OH)3	0	1000
cpd_ac[e]	Acetate	0	1000
	N-Acetyl-D-		
cpd_acgam[e]	glucosamine	-5	1000
cpd_ala-D[e]	D-Alanine	0	1000
cpd_ala-L[e]	L-Alanine	0	1000
cpd_asp-L[e]	L-Aspartate	0	1000
cpd_bgl[e]	cellobiose	0	1000
cpd_ca2[e]	Calcium	-1000	1000
cpd_cl[e]	Chloride	-1000	1000
cpd_co2[e]	CO2	0	1000
cpd_cobalt3[e]	Co3+	0	1000
cpd_cobalt2[e]	Co2+	-1000	1000
cpd_cro4[e]	chromate	0	1000
cpd_cu2[e]	Cu2+	-1000	1000
cpd_cytd[e]	Cytidine	0	1000
cpd_dcyt[e]	Deoxycytidine	0	1000
cpd_dms[e]	Dimethyl sulfide	0	1000
cpd_dmso[e]	Dimethyl sulfoxide	0	1000
cpd_dna[e]	Dimethyl sulfoxide	0	1000
	Dodecanoic acid		
cpd_dodcan[e]	(neutral)	0	1000

cpd_duri[e]	Deoxyuridine	0	1000
cpd_fe2[e]	Fe2+	-1000	1000
cpd_fe3[e]	Fe3+	0	1000
cpd_for[e]	Formate	0	1000
cpd_fum[e]	Fumarate	0	1000
cpd_galactan[e]	Galactan	0	1000
cpd_gal[e]	D-Galactose	0	1000
cpd_glc-D[e]	D-Glucose	0	1000
cpd_glu-L[e]	L-Glutamate	0	1000
cpd_gly[e]	glycyl-L-glutamic acid	0	1000
cpd_gly-asp-L[e]	glycyl-L-aspartic acid	0	1000
cpd_gly-glu-L[e]	glycyl-L-glutamic acid	0	1000
cpd_glyc[e]	(R)-Glycerate	0	1000
cpd_glyclt[e]	Glycolate	0	1000
cpd_h[e]	H+	-1000	1000
cpd_h2o[e]	H2O	-1000	1000
cpd_h2s[e]	Hydrogen sulfide	0	1000
cpd_hdcan[e]	hexadecanoate (n- C16:0) (neutral)	0	1000
cpd_ile-L[e]	L-Isoleucine	0	1000
cpd k[e]	K+	-1000	1000
cpd lac-D[e]	D-Lactate	0	1000
cpd_lac-L[e]	L-Lactate	0	1000
cpd_lami[e]	laminarin	0	1000
cpd_leu-L[e]	L-Leucine	0	1000
cpd_mal-L[e]	L-Malate	0	1000
cpd_panose[e]	Panose	0	1000
cpd_malt[e]	Maltose	0	1000
cpd_malthp[e]	Maltoheptaose	0	1000
cpd_malthx[e]	Maltohexaose	0	1000
cpd_maltpt[e]	Maltopentaose	0	1000
cpd_malttr[e]	Maltotriose	0	1000
cpd_maltttr[e]	Maltotetraose	0	1000
cpd_mg2[e]	Mg	-1000	1000
cpd_mn2[e]	Mn2+	-1000	1000
	Manganese(IV)		
cpd_mn4o[e]	oxide	0	1000

cpd_nh4[e]	Ammonium	-5.6	1000
cpd_no2[e]	Nitrite	0	1000
cpd_no3[e]	Nitrate	0	1000
cpd o2[e]	Oxygen	-0.32952261 (4C), - 0.25745959 (15C), - 0.23387845 (20C)	1000
	octadecanoate (n-		
cpd_ocdcan[e]	C18:0) neutral	0	1000
cpd_pi[e]	Phosphate	-0.7	1000
cpd_pmcoa[e]	Pimeloyl-CoA	-1000	1000
cpd_ptrc[e]	Putrescine	0	1000
cpd_pyr[e]	Pyruvate	0	1000
cpd_ser-L[e]	L-Serine	0	1000
cpd_so3[e]	Sulfite	0	1000
cpd_so4[e]	Sulfate	-9.8	1000
cpd_succ[e]	Succinate	0	1000
cpd_thr-L[e]	L-Threonine	0	1000
cpd_tma[e]	Trimethylamine	0	1000
cpd_tmao[e]	Trimethylamine N- oxide	0	1000
cpd_tsul[e]	Thiosulfate	0	1000
	tetradecanoate		1000
cpd_ttdcan[e]	(C14:0) (neutral)	0	1000
cpd_tttnt[e]	tetrathionate	0	1000
cpd_tyr-L[e]	L-Tyrosine	0	1000
cpd_urdio[e]	Uranium dioxide	0	1000
cpd_uri[e]	Uridine	0	1000
cpd_urnyl[e]	Uranyl	0	1000
cpd_val-L[e]	L-Valine	0	1000
cpd_thymd[e]	Thymidine	0	1000
cpd_mobd[e]	Molybdate	-1000	1000
cpd_cbl1[e]	Cob(I)alamin	-1000	1000
cpd_ppa[e]	Propionate	0	1000
cpd_urea[e]	Urea	0	1000
cpd_chitin[e]	Methanethiol	0	1000
cpd_lys-L[e]	L-Lysine	0	1000
cpd_trp-L[e]	L-Tryptophan	0	1000
cpd_xan[e]	Xanthine	0	1000
cpd_etoh[e]	Ethanol	0	1000
cpd_akg[e]	2-Oxoglutarate	0	1000

cpd_gln-L[e]	L-Glutamine	0	1000
cpd_asn-L[e]	L-Asparagine	0	1000
cpd_ins[e]	Inosine	0	1000
cpd_thym[e]	Thymine	0	1000
cpd_hxan[e]	Hypoxanthine	0	1000

Appendix IV Data S2 for Manuscript II

Natah	Lower	Upper	Dones	Lower	Upper	Danas	Lower	Upper	Deves
olite ID	Bound 4	Bound 4	Kange 4	Bound 15	Bouna 15	Kange 15	Bound 20	Bound 20	Range 20
Biomas	- 1.00E-	-	0.0199	1.00E-	15	0.0199	1.00E-	20	0.0199
s[c]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0002		0.0197	0.0001		0.0198	0.0001		0.0198
cpd_10	087677		912322	859027		140972	768629		231370
fthf[c]	907	0.02	1	951	0.02	1	373	0.02	6
cpd_12									
dag3p[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_12	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dgr[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_13	1.00E-	0.02	0.0199	1.00E-	3.98E-	2.98E-	1.00E-	8.43E-	7.43E-
	05	0.02	9	05	05	0.0100	1.005	05	05
cpa_1p	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
and 22	05	0.02	9	05	0.02	9	05	0.02	9
dbdp[c	1 00F-		0 0100	1 00F-		0 0100	1 00F-		0 01 99
	1.00L-	0.02	0.0199 q	1.000	0.02	0.0199 Q	1.00L-	0.02	0.0199 Q
cpd 23	03	0.02			0.02		03	0.02	
dhmb[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_23									
dhmp[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0006		0.0193	0.0003		0.0196	0.0002		0.0197
cpd_25	532782		467217	588680		411319	774170		225829
aics[c]	848	0.02	2	821	0.02	2	274	0.02	7
cpd_25	0.0028			0.0023		0.0176	0.0009		0.0190
dhpp[c	719315	0.00	0.0171	309650	0.00	690349	127681	0.00	872318
]	99	0.02	280684	44	0.02	6	899	0.02	1
cpa_26	1 005		0.0100	1 005		0.0100	1 005		0.0100
uap-	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
cnd 26	05	0.02	9	05	0.02	9	05	0.02	9
dan-	1 00F-		0 0199	1 00F-		0 0199	1 00F-		0 0199
M[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd 2a	1.00E-	2.02	0.0199	1.00E-	2.02	0.0199	1.00E-		0.0199
hbut[c]	05	0.02	9	05	0.02	9	05	0.02	9

Data S2 Table A Metabolite concentration ranges from TMFA simulations.

cpd_2a									
hhmd[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2a									
hhmp[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2a	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
obut[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pr5p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
da7p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dg6p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2d									
mmq7[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0041	0.0041						
cpd_2d	1.00E-	297679	197679	1.00E-		0.0199	1.00E-		0.0199
r1p[c]	05	46	46	05	0.02	9	05	0.02	9
			0.0199						
cpd_2d	1.35E-		865343	1.00E-		0.0199	1.00E-		0.0199
r5p[c]	05	0.02	1	05	0.02	9	05	0.02	9
cpd_2h									
3opp[c	1.00E-		0.0199						
]	05	0.02	9	NA	NA	NA	NA	NA	NA
cpd_2i	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ppm[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2k	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mb[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2									
maaco	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2									
mahm	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2									
mb2co	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_2 mbcoa[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2 mcacn[c]	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
	1.005	0.02	9	1.005	0.02	9	1.005	0.02	9
cpa_2	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199
mcit[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_2 me4p[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd 2									
mecdp[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cl	05	0.02	9	05	0.02	9	05	0.02	9
cpd 2									
mp2co	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd 2o	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
but[c]	05	0.02	9	05	0.02	9	05	0.02	9
cnd_{20}	1 00F-		0 0199	1 00F-		0 0199	1 00F-		0 0199
hph[c]	05	0.02	9	05	0.02	9	05	0.02	9
			0 0199	0.0002		0 0197			0 0199
cpd 20	2.01F-		799486	576389		423610	9.24F-		076347
mbzl[c]	05	0.02	5	267	0.02	7	05	0.02	1
cnd 20		0.02		207	0.02	-	00	0.02	
mhmhl	1 00F-		0 0199	1 00F-		0 0199	1 00F-		0 0199
	1.002	0.02	0.0133 Q	1.002	0.02	9	1.002	0.02	0.0133 Q
cnd 20	05	0.02		00	0.02	0.0007	05	0.02	0.0021
mmbl[c	1 00F-	743925	643925	1 00F-	762802	662802	1 00F-	653155	553155
1	05	59	59	05	094	094	05	04	04
rnd 20	1 00F-		0 0199	1 00F-		0.0199	1 00F-	• •	0 0199
mph[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd 20	1.00F-	0.01	0.0199	1.00F-	0.01	0.0199	1.00F-		0.0199
ph[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd 2p									
4c2me[1 00F-		0 0199	1 00F-		0 0199	1 00F-		0 0199
cl	05	0.02	9	05	0.02	9	05	0.02	9
<u></u>		0.02		00	0.0003	0 0003	00	0.0006	0,0006
cpd 2n	1.00F-		0.0199	1.00F-	569053	469053	1.00F-	824595	724595
a[c]	05	0.02	9.0155 Q	05	504	504	05	055	055
cpd 2n	1.00F-	3.02	0.0199	1.00F-		0.0199	1,00F-		0.0199
glyc[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_2s	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hchc[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_34	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hpp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3c	0.0002		0.0197			0.0199			0.0199
2hmp[c	156185		843814	8.10E-		190076	5.32E-		468256
]	343	0.02	7	05	0.02	2	05	0.02	6
cpd_3c									
3hmp[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3c		0.0009	0.0009		0.0024	0.0024		0.0037	0.0037
4mop[c	1.00E-	275640	175640	1.00E-	693682	593682	1.00E-	612125	512125
]	05	455	455	05	4	4	05	12	12
cpd_3d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hq[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hsk[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3h									
mbcoa[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3h	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3h									
tdACP[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3i	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
g3p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3									
mb2co							1.00E-		0.0199
a[c]	NA	NA	NA	NA	NA	NA	05	0.02	9
cpd_3									
mgcoa[1.00E-		0.0199						
c]	05	0.02	9	NA	NA	NA	NA	NA	NA
cpd_3	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mob[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mop[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3o	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
phb[c]	05	0.02	9	05	0.02	9	05	0.02	9
					0.0033	0.0032		0.0061	0.0060
cpd_3p	1.00E-		0.0199	9.38E-	475710	537766	9.03E-	612960	710152
g[c]	05	0.02	9	05	49	85	05	04	48

cpd_3p	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_3p	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
sme[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_4a	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
but[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_4a	5.46E-	5.46E-	5.41E-	5.46E-	5.46E-	5.41E-	5.46E-	5.46E-	5.41E-
bz[c]	08	06	06	08	06	06	08	06	06
cpd_4a	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dcho[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_4a									
mpm[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_4c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
2me[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_4f									
umaca	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_4h	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ba[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd 4h	1.00E-		0.0199				1.00E-		0.0199
.' -, ,									
bcoa[c]	05	0.02	9	NA	NA	NA	05	0.02	9
bcoa[c] cpd_4h	05 1.00E-	0.02	9 0.0199	NA 1.00E-	NA	NA 0.0199	05 1.00E-	0.02	9 0.0199
bcoa[c] cpd_4h bz[c]	05 1.00E- 05	0.02	9 0.0199 9	NA 1.00E- 05	NA 0.02	NA 0.0199 9	05 1.00E- 05	0.02	9 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz	05 1.00E- 05 1.00E-	0.02	9 0.0199 9 0.0199	NA 1.00E- 05 1.00E-	NA 0.02	NA 0.0199 9 0.0199	05 1.00E- 05 1.00E-	0.02	9 0.0199 9 0.0199
bcoa[c] cpd_4h bz[c] cpd_4iz p[c]	05 1.00E- 05 1.00E- 05	0.02 0.02 0.02	9 0.0199 9 0.0199 9	NA 1.00E- 05 1.00E- 05	NA 0.02 0.02	NA 0.0199 9 0.0199 9	05 1.00E- 05 1.00E- 05	0.02 0.02 0.02	9 0.0199 9 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac	05 1.00E- 05 1.00E- 05	0.02	9 0.0199 9 0.0199 9	NA 1.00E- 05 1.00E- 05	NA 0.02 0.02	NA 0.0199 9 0.0199 9	05 1.00E- 05 1.00E- 05	0.02 0.02 0.02	9 0.0199 9 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac	05 1.00E- 05 1.00E- 05	0.02	9 0.0199 9 0.0199 9 0.0199	NA 1.00E- 05 1.00E- 05	NA 0.02 0.02	NA 0.0199 9 0.0199 9	05 1.00E- 05 1.00E- 05	0.02 0.02 0.02	9 0.0199 9 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c]	05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 0.02	9 0.0199 9 0.0199 9 0.0199 9	NA 1.00E- 05 1.00E- 05 NA	NA 0.02 0.02 NA	NA 0.0199 9 0.0199 9 NA	05 1.00E- 05 1.00E- 05 NA	0.02 0.02 0.02 NA	9 0.0199 9 0.0199 9 NA
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mon[c]	05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 0.02	9 0.0199 9 0.0199 9 0.0199 9 0.0199	NA 1.00E- 05 1.00E- 05 NA 1.00E- 05	NA 0.02 0.02 NA	NA 0.0199 9 0.0199 9 NA 0.0199	05 1.00E- 05 1.00E- 05 NA 1.00E- 05	0.02 0.02 0.02 NA	9 0.0199 9 0.0199 9 NA 0.0199
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mop[c] cpd_4	05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 0.02 0.02	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9	NA 1.00E- 05 1.00E- 05 NA 1.00E- 05	NA 0.02 0.02 NA 0.02	NA 0.0199 9 0.0199 9 NA 0.0199 9	05 1.00E- 05 NA 1.00E- 05	0.02 0.02 0.02 NA 0.02	9 0.0199 9 0.0199 9 NA 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mop[c] cpd_4 mop[c] cpd_4 mop[c]	05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E-	0.02 0.02 0.02 0.02 0.02	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9	NA 1.00E- 05 1.00E- 05 NA 1.00E- 05	NA 0.02 0.02 NA 0.02	NA 0.0199 9 0.0199 9 NA 0.0199 9	05 1.00E- 05 1.00E- 05 NA 1.00E- 05	0.02 0.02 0.02 NA 0.02	9 0.0199 9 0.0199 9 NA 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mop[c] cpd_4 mop[c] cpd_4 mpetz[c]	05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 0.02 0.02	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9	NA 1.00E- 05 NA 1.00E- 05 1.00E- 05	NA 0.02 0.02 NA 0.02	NA 0.0199 9 0.0199 9 NA 0.0199 9 0.0199	05 1.00E- 05 NA 1.00E- 05 1.00E- 05	0.02 0.02 0.02 NA 0.02	9 0.0199 9 0.0199 9 NA 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mop[c] cpd_4 mpetz[c]	05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 0.02 0.02 0.02 0.0134	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9 0.0134	NA 1.00E- 05 1.00E- 05 1.00E- 05	NA 0.02 0.02 NA 0.02 0.02 0.0104	NA 0.0199 9 0.0199 9 NA 0.0199 9 0.0199 9	05 1.00E- 05 NA 1.00E- 05 1.00E- 05	0.02 0.02 0.02 NA 0.02 0.02	9 0.0199 9 0.0199 9 NA 0.0199 9 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mop[c] cpd_4 mop[c] cpd_4 mpetz[c] cpd_4	05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 0.02 0.02 0.0134 661897	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9 0.0134 561897	NA 1.00E- 05 NA 1.00E- 05 1.00E- 05 1.00E-	NA 0.02 0.02 NA 0.02 0.0104 675067	NA 0.0199 9 0.0199 9 NA 0.0199 9 0.0104 575067	05 1.00E- 05 NA 1.00E- 05 1.00E- 05	0.02 0.02 0.02 NA 0.02	9 0.0199 9 0.0199 9 NA 0.0199 9 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mop[c] cpd_4 mpetz[c] cpd_4 mpetz[c]	05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 0.02 0.02 0.02 0.0134 661897 4	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9 0.0134 561897 4	NA 1.00E- 05 NA 1.00E- 05 1.00E- 05 1.00E- 05	NA 0.02 0.02 NA 0.02 0.02 0.0104 675067 5	NA 0.0199 9 0.0199 9 NA 0.0199 9 0.0104 575067 5	05 1.00E- 05 NA 1.00E- 05 1.00E- 05	0.02 0.02 NA 0.02 0.02 0.02	9 0.0199 9 0.0199 9 NA 0.0199 9 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mop[c] cpd_4 mpetz[c] cpd_4 mpetz[c]	05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 0.0002	0.02 0.02 0.02 0.02 0.02 0.0134 661897 4	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9 0.0134 561897 4 0.0197	NA 1.00E- 05 NA 1.00E- 05 1.00E- 05 1.00E- 05	NA 0.02 0.02 NA 0.02 0.0104 675067 5	NA 0.0199 9 0.0199 9 NA 0.0199 9 0.0104 575067 5	05 1.00E- 05 NA 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 NA 0.02 0.02 0.02	9 0.0199 9 0.0199 9 NA 0.0199 9 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mop[c] cpd_4 mpetz[c] cpd_4 mpetz[c] cpd_4p asp[c]	05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 0.0002 177701	0.02 0.02 0.02 0.02 0.02 0.0134 661897 4	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9 0.0134 561897 4 0.0197 822298	NA 1.00E- 05 NA 1.00E- 05 1.00E- 05 1.00E- 05 1.00E-	NA 0.02 0.02 NA 0.02 0.0104 675067 5	NA 0.0199 9 0.0199 9 NA 0.0199 9 0.0104 575067 5	05 1.00E- 05 NA 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 NA 0.02 0.02 0.02	9 0.0199 9 0.0199 9 NA 0.0199 9 0.0199 9 0.0199
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mop[c] cpd_4 mpetz[c] cpd_4 mpetz[c] cpd_4p asp[c]	05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 0.0002 177701 476	0.02 0.02 0.02 0.02 0.02 0.0134 661897 4 0.02	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9 0.0134 561897 4 0.0197 822298 5	NA 1.00E- 05 NA 1.00E- 05 1.00E- 05 1.00E- 05	NA 0.02 0.02 NA 0.02 0.0104 675067 5 0.02	NA 0.0199 9 0.0199 9 NA 0.0199 9 0.0104 575067 5 0.0199 9	05 1.00E- 05 NA 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 NA 0.02 0.02 0.02	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9 0.0199 9
bcoa[c] cpd_4h bz[c] cpd_4iz p[c] cpd_4 mlacac [c] cpd_4 mop[c] cpd_4 mpetz[c] cpd_4 mpetz[c] cpd_4p asp[c] cpd_4p asp[c]	05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 0.0002 177701 476 1.00E-	0.02 0.02 0.02 0.02 0.02 0.0134 661897 4 0.02	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9 0.0134 561897 4 0.0197 822298 5 0.0199	NA 1.00E- 05 NA 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	NA 0.02 0.02 NA 0.02 0.0104 675067 5 0.02	NA 0.0199 9 0.0199 9 NA 0.0199 9 0.0104 575067 5 0.0199 9 0.0199	05 1.00E- 05 NA 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 NA 0.02 0.02 0.02	9 0.0199 9 0.0199 9 0.0199 9 0.0199 9 0.0199 9 0.0199

cpd_4p	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pcys[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_4r	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
5au[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_56									
78thh[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_5a	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
izc[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_5a	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
op[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_5a	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
prbu[c]	05	0.02	9	05	0.02	9	05	0.02	9
								0.0002	0.0002
cpd_5a	1.00E-	6.96E-	5.96E-	1.00E-	8.58E-	7.58E-	1.00E-	191136	091136
pru[c]	05	05	05	05	05	05	05	832	832
cpd_5c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
aiz[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_5d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
rib[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_5h	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
iu[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_5									
mdr1p[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_5									
mdru1	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_5	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mta[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_5	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mthf[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_5									
mthglu	1.00E-		0.0199						
[c]	05	0.02	9	NA	NA	NA	NA	NA	NA
cpd_5	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mtr[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_6p	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
gc[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_6p	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
gl[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_78	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dhp[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_7c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ltrp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_8a	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
onn[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_aa	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
coa[c]	05	0.02	9	05	0.02	9	05	0.02	9
			0.0199						
cpd_ac	1.00E-		899999	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0199	0.0199		0.0199	0.0199		0.0199	0.0199
cpd_ac	1.00E-	999739	899739	1.00E-	999916	899916	1.00E-	999917	899917
[e]	05	6	6	05	5	5	05	9	9
		0.0199	0.0199						
cpd_ac	1.00E-	999826	899826	1.00E-		0.0199	1.00E-		0.0199
[p]	05	4	4	05	0.02	9	05	0.02	9
cpd_ac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ac[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ACP[c]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0001		0.0198						
cpd_ac	131090		868909	1.00E-		0.0199	1.00E-		0.0199
ald[c]	407	0.02	6	05	0.02	9	05	0.02	9
cpd_ac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
coa[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0016	0.0016		0.0014	0.0014		0.0029	0.0029
cpd_ac	1.00E-	923110	823110	1.00E-	238524	138524	1.00E-	321641	221641
g5p[c]	05	22	22	05	77	77	05	13	13
cpd_ac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
g5sa[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ac	1.00E-		0.0049	1.00E-		0.0049	1.00E-		0.0049
gam[c]	05	0.005	9	05	0.005	9	05	0.005	9
			0.0049			0.0049			0.0049
cpd_ac	1.00E-		899999	1.00E-		899999	1.00E-		899999
gam[e]	05	0.005	96	05	0.005	96	05	0.005	96
		0.0049	0.0049		0.0049	0.0049		0.0049	0.0049
cpd_ac	1.00E-	999978	899978	1.00E-	999979	899979	1.00E-	999979	899979
gam[p]	05	3	3	05	13	13	05	49	49
cpd_ac									
gam1p[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ac									
gam6p[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9

	0.0001		0.0198	0.0001		0.0198			0.0199
cpd_ac	181815		818184	404639		595360	6.82E-		317909
glu[c]	857	0.02	1	899	0.02	1	05	0.02	9
cpd ac									
mam[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ac									
mama[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ac									
mana[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
nam[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
orn[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd AC	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
P[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ser[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tACP[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ad	6.75E-	6.75E-	6.68E-						
coba[c]	07	05	05	NA	NA	NA	NA	NA	NA
cpd ad									
cobap[1.00E-		0.0199						
c]	05	0.02	9	NA	NA	NA	NA	NA	NA
cpd ad	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
e[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ad									
gcoba[1.00E-		0.0199						
c]	05	0.02	9	NA	NA	NA	NA	NA	NA
		0.0004	0.0004		0.0007	0.0007		0.0009	0.0009
cpd ad	1.00E-	115728	015728	1.00E-	408054	308054	1.00E-	536688	436688
n[c]	05	908	908	05	122	122	05	061	061
cpd ad	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ad	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n[p]	05	0.02	9	05	0.02	9	05	0.02	9

		0.0006	0.0006		0.0009	0.0009		0.0011	0.0011
cpd_ad	1.00E-	909099	809099	1.75E-	787102	612530	1.00E-	366959	266959
p[c]	05	549	549	05	14	102	05	91	91
cpd_ad	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pglc[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ad									
phep-	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
DD[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ag	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
m[c]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0004		0.0195	0.0002		0.0197	0.0002		0.0197
cpd_ah	859406		140593	699764		300235	097164		902835
cys[c]	547	0.02	5	293	0.02	7	117	0.02	9
cpd_ah	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dt[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0003	0.0002		0.0005	0.0005		0.0007	0.0007
cpd_aic	1.00E-	061482	961482	1.00E-	573078	473078	1.00E-	209362	109362
ar[c]	05	445	445	05	522	522	05	81	81
cpd_air	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0021	0.0020						
cpd_ak	1.00E-	038649	938649	1.00E-		0.0199	1.00E-		0.0199
g[c]	05	9	9	05	0.02	9	05	0.02	9
cpd_ak	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
g[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_al	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a-B[c]	05	0.02	9	05	0.02	9	05	0.02	9
					0.0188	0.0187		0.0188	0.0188
cpd_al	1.00E-	0.0187	0.0187	1.00E-	017309	917309	1.00E-	215543	115543
a-D[c]	05	556825	456825	05	1	1	05	1	1
								0.0199	0.0199
cpd_al	1.00E-		0.0199	1.00E-		0.0199	1.00E-	999917	899917
a-D[e]	05	0.02	9	05	0.02	9	05	9	9
cpd_al	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a-D[p]	05	0.02	9	05	0.02	9	05	0.02	9
			0.0199			0.0199			0.0199
cpd_al	1.07E-		893365	1.06E-		893626	1.06E-		893738
a-L[c]	05	0.02	7	05	0.02	9	05	0.02	9
cpd_al	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_al	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a-L[p]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_al	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
aala[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_al	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ac-S[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_al									
atrna[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_all	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tn-R[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_all	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tn-S[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_all	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tt[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0009	0.0009						
cpd_a	1.00E-	701326	601326	1.00E-	3.98E-	2.98E-	1.00E-	8.43E-	7.43E-
met[c]	05	528	528	05	05	05	05	05	05
cpd_a									
metam	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_a	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mob[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_a	1.00E-	1.20E-	1.98E-	1.00E-	2.47E-	1.47E-	1.00E-	3.37E-	2.37E-
mp[c]	05	05	06	05	05	05	05	05	05
cpd_an	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
th[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ap									
oACP[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ap	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
s[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ar	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a5p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ar							1.00E-		0.0199
ab-L[c]	NA	NA	NA	NA	NA	NA	05	0.02	9
cpd_ar							1.00E-		0.0199
ab-L[p]	NA	NA	NA	NA	NA	NA	05	0.02	9
cpd_ar	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
g-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ar	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
gsuc[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ar									
gtrna[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_as	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_as	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_as									
ntrna[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
			0.0199			0.0199			
cpd_as	1.49E-		851479	1.91E-		808932	1.00E-		0.0199
p-L[c]	05	0.02	9	05	0.02	5	05	0.02	9
cpd_as	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_as	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_as	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
psa[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_as									
ptrna[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0040		0.0159	0.0100		0.0099	0.0068		0.0131
cnd at	076823		023176	270946		729053	898792		101207
cpu_at	070823		925170	270540		123033	050752		101207
p[c]	56	0.02	⁹²³¹⁷⁰	1	0.02	92	35	0.02	7
p[c] cpd_be	56 1.00E-	0.02	4 0.0199	1	0.02	92	35	0.02	7
p[c] cpd_be tald[c]	56 1.00E- 05	0.02	4 0.0199 9	1 NA	0.02 NA	92 NA	35 NA	0.02 NA	7 NA
p[c] cpd_be tald[c] cpd_bg	56 1.00E- 05 1.00E-	0.02	4 0.0199 9 0.0199	1 NA 1.00E-	0.02 NA	92 92 NA 0.0199	35 NA 1.00E-	0.02 NA	NA 0.0199
p[c] cpd_be tald[c] cpd_bg l[e]	56 1.00E- 05 1.00E- 05	0.02 0.02 0.02	4 0.0199 9 0.0199 9	1 NA 1.00E- 05	0.02 NA 0.02	92 92 NA 0.0199 9	35 NA 1.00E- 05	0.02 NA 0.02	NA 0.0199 9
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt	56 1.00E- 05 1.00E- 05 1.00E-	0.02 0.02 0.02	4 0.0199 9 0.0199 9 0.0199	1 NA 1.00E- 05 1.00E-	0.02 NA 0.02	92 92 NA 0.0199 9 0.0199	35 NA 1.00E- 05 1.00E-	0.02 NA 0.02	NA 0.0199 9 0.0199
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c]	56 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 0.02	4 0.0199 9 0.0199 9 0.0199 9	1 NA 1.00E- 05 1.00E- 05	0.02 NA 0.02 0.02	92 92 NA 0.0199 9 0.0199 9	35 NA 1.00E- 05 1.00E- 05	0.02 NA 0.02 0.02	NA 0.0199 9 0.0199 9
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt	56 1.00E- 05 1.00E- 05 1.00E- 05 2.43E-	0.02 0.02 0.02 0.02 2.43E-	4 0.0199 9 0.0199 9 0.0199 9 2.41E-	1 NA 1.00E- 05 1.00E- 05 2.43E-	0.02 NA 0.02 0.02 2.43E-	92 92 NA 0.0199 9 0.0199 9 2.41E-	35 NA 1.00E- 05 1.00E- 05 2.43E-	0.02 NA 0.02 0.02 2.43E-	NA 0.0199 9 0.0199 9 2.41E-
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c]	56 1.00E- 05 1.00E- 05 1.00E- 05 2.43E- 08	0.02 0.02 0.02 0.02 2.43E- 06	4 0.0199 9 0.0199 9 0.0199 9 2.41E- 06	1 NA 1.00E- 05 1.00E- 05 2.43E- 08	0.02 NA 0.02 0.02 2.43E- 06	92 NA 0.0199 9 0.0199 9 2.41E- 06	35 NA 1.00E- 05 1.00E- 05 2.43E- 08	0.02 NA 0.02 0.02 2.43E- 06	NA 0.0199 9 0.0199 9 2.41E- 06
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bu	56 1.00E- 05 1.00E- 05 1.00E- 05 2.43E- 08 1.00E-	0.02 0.02 0.02 0.02 2.43E- 06	0.0199 9 0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199	1 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E-	0.02 NA 0.02 0.02 2.43E- 06	92 NA 0.0199 9 0.0199 9 2.41E- 06 0.0199	35 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E-	0.02 NA 0.02 0.02 2.43E- 06	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bu t[c]	56 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05	0.02 0.02 0.02 2.43E- 06 0.02	4 0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199 9	1 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05	0.02 NA 0.02 0.02 2.43E- 06 0.02	92 NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9	35 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05	0.02 NA 0.02 0.02 2.43E- 06 0.02	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bu t[c] cpd_ca	56 1.00E- 05 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E-	0.02 0.02 0.02 2.43E- 06 0.02 0.1547	0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547	1 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E-	0.02 NA 0.02 0.02 2.43E- 06 0.02 0.1547	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547	35 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E-	0.02 NA 0.02 0.02 2.43E- 06 0.02 0.1547	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bu t[c] cpd_ca 2[c]	56 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05	0.02 0.02 0.02 2.43E- 06 0.02 0.1547 52988	4 0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988	1 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988	35 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bu t[c] cpd_ca 2[c] cpd_ca	56 1.00E- 05 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 2.43E- 06 0.02 0.1547 52988 0.1547	0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547	1 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05 1.00E-	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547	35 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05 1.00E-	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bt t[c] cpd_ca 2[c] cpd_ca 2[e]	56 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988	4 0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988	1 NA 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988	35 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bu t[c] cpd_ca 2[c] cpd_ca 2[e] cpd_ca	56 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988 0.1547	0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547	1,005-10 1,00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988 0.1547	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547	35 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988 0.1547	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bt t[c] cpd_ca 2[c] cpd_ca 2[e] cpd_ca 2[p]	56 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988 0.1547 529208	4 0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429208	1 NA 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 529234	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429234	35 NA 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 529245	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bu t[c] cpd_ca 2[c] cpd_ca 2[e] cpd_ca 2[p] cpd_ca	56 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988 0.1547 529208	0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429208 0.0199	1 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988 0.1547 529234	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429234 0.0199	35 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988 0.1547 529245	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429245 0.0199
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bt t[c] cpd_ca 2[c] cpd_ca 2[e] cpd_ca 2[p] cpd_ca mp[c]	56 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988 0.1547 529208	4 0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429208 0.0199 9	1 NA 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 529234 0.1547	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429234 0.0199 9	35 NA 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 529285 0.1547 529245	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429245 0.0199 9
p[c] cpd_be tald[c] cpd_bg l[e] cpd_bt coa[c] cpd_bt n[c] cpd_bu t[c] cpd_ca 2[c] cpd_ca 2[e] cpd_ca 2[p] cpd_ca 2[p] cpd_ca mp[c] cpd_ca	56 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 0.02 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988 0.1547 529208	0.0199 9 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429208 0.1547 9 0.0199 9 0.0199	1,005-10 1,00E- 05 1,00E- 05 2,43E- 08 1,00E- 05 1,00E- 05 1,00E- 05 1,00E- 05 1,00E- 05 1,00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 529234 0.1547	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429234 0.1547 9 0.0199 9 0.0199	35 NA 1.00E- 05 1.00E- 05 2.43E- 08 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05 1.00E- 05	0.02 NA 0.02 2.43E- 06 0.02 0.1547 52988 0.1547 52988 0.1547 529245	NA 0.0199 9 0.0199 9 2.41E- 06 0.0199 9 0.1547 42988 0.1547 42988 0.1547 429245 0.0199 9 0.0199

rate_m acro[c]									
			0.0499			0.0499			0.0499
cpd_cb	1.51E-		849106	1.36E-		863957	1.30E-		869881
asp[c]	05	0.05	3	05	0.05	1	05	0.05	3
cpd_cb	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
l1[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cb	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
l1[e]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0199	0.0199		0.0199	0.0199		0.0199	0.0199
cpd_cb	1.00E-	999913	899913	1.00E-	999916	899916	1.00E-	999917	899917
l1[p]	05	2	2	05	5	5	05	9	9
cpd_cb	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cd	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cd									
p4d6dg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0003		0.0196	0.0002		0.0197	0.0001		0.0198
cpd_cd	197212		802787	095618		904381	747724		252275
pdag[c]	782	0.02	2	253	0.02	7	501	0.02	5
cpd_cd	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pg[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ch	1.00E-		0.0199				1.00E-		0.0199
4s[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_ch	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
itin[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ch	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
itob[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ch	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
itob[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ch	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ol[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ch	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ol[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ch	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ol[p]	05	0.02	9	05	0.02	9	05	0.02	9
			0.0199			0.0199			
cpd_ch	1.52E-		847725	1.50E-		850150	1.49E-		0.0199
or[c]	05	0.02	9	05	0.02	8	05	0.02	851181
cpd_ci	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
nnm[c]	05	0.02	9	05	0.02	9	05	0.02	9

	0.0003		0.0196	0.0002		0.0197	0.0002		0.0197
cpd_cit	092576		907423	712864		287135	564362		435637
[c]	375	0.02	6	511	0.02	5	34	0.02	7
cpd_cit	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cit	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cit	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ck	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
do[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ck									
do8n[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cl[1.00E-	0.7797	0.7797	1.00E-	0.8255	0.8255	1.00E-	0.8459	0.8459
c]	05	78977	68977	05	972559	872559	05	146659	046659
cpd_cl[3.62E-	2.8244	2.8243	3.42E-	2.8244	2.8244	3.34E-	2.8244	2.8244
e]	05	35219	98998	05	35219	01008	05	35219	0183
cpd_cl[3.62E-	2.8244	2.8243	3.42E-	2.8244	2.8243	3.34E-	2.8244	2.8244
p]	05	33993	97772	05	3404	99829	05	3406	00671
		0.0006	0.0006		0.0009	0.0009		0.0011	0.0011
cpd_c	1.00E-	255448	155448	1.00E-	543722	443722	1.00E-	443451	343451
mp[c]	05	532	532	05	944	944	05	18	18
			0.0199			0.0199			
cpd_co	1.00E-		899999	1.00E-	0.00	899999	1.00E-		0.0199
2[c]	05	0.02	9	05	0.02	9	05	0.02	9
	4 005	0.0199	0.0199	4 005	0.0400	0.0400	4 005		0.0400
cpa_co	1.00E-	999826	899826	1.00E-	0.0199	0.0199	1.00E-	0.02	0.0199
zlej	05	4	4	05	999833	899833	05	0.02	9
	1 005	0.0199	0.0199	1 005	0.0199	0.0199	1 005		0.0100
2[p]	1.00E-	999913	299912	1.00E-	999910	2333T0	1.00E-	0.02	0.0199
2[b]	05	∠ 0.0002	2 0.0002	05	0,0002	0,0002	05	0.02	9
and co	1 005	0.0002	0.0002	1 005	0.0003	0.0003	1 005	0.0004	0.0004
	1.002-	552554 76E	252554	1.002-	095259	052259	1.00E-	014	405065
a[c]	05	705	705	05	630	630	05	914	914
hal+2[c	2 165	2 165	2 125	2 165	2 165	2 125	2 165	2 165	2 125
	2.40L-	2.401-	2.43L-	2.40L-	2.40L-	2.43L-	2.40L-	2.40L-	2.43L-
	07	05	05	07	05	05	07	05	05
halt2[e	2 /6F-	2 /6F-	2 12F-	2 /6F-	2 /6F-	2 12F-	2 /6F-	2 16F-	2 /I3E-
]	07	05	05	2. <u></u> 40€ 07	05	05	2.40L	05	25C 05

cpd_co									
balt2[p	2.46E-	2.46E-	2.43E-	2.46E-	2.46E-	2.43E-	2.46E-	2.46E-	2.43E-
]	07	05	05	07	05	05	07	05	05
cpd_co									
balt3[e	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_co									
bamco	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_co	1.00E-		0.0199				1.00E-		0.0199
nfald[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_cp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ppg3[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
o4[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_Cr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
OH3[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd cs	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd cs	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
. <u> </u>	05	0.02	9	05	0.02	9	05	0.02	9
cpd ct	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd cu	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
2[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd cu	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
2[e]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0199	0.0199		0.0199	0.0199		0.0199	0.0199
cpd_cu	1.00E-	999913	899913	1.00E-	999916	899916	1.00E-	999917	899917
2[p]	05	2	2	05	5	5	05	9	9
cpd_cy	1.00E-		0.0199				1.00E-		0.0199
an[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_cy	1.00E-		0.0199				1.00E-		0.0199
s-gly[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_cy	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
s-gly[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cy	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
s-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cy	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
sth-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cy									
strna[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9

cpd cy	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
td[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd cy	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
td[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_cy	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
td[p]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0200	0.0199						
cpd_da	1.00E-	000000	900000	1.00E-		0.0199	1.00E-		0.0199
d-2[c]	05	1	1	05	0.02	9	05	0.02	9
cpd_da	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
d-2[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_da	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
d-2[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_da	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
d-5[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_da	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_da	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_da	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_da	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_da	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
nn[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_da	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_db	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
4p[c]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0166		0.0033	0.0081			0.0059		0.0140
cpd_dc	983753		016246	054519		0.0118	413374		586625
amp[c]	3	0.02	68	03	0.02	945481	83	0.02	2
cpd_dc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tp[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_dc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yt[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yt[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yt[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dd									
caACP[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
sn[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
sn[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
sn[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ap[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
bpt[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
f[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dh									
mptp[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
na[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
npt[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0033	0.0033		0.0036	0.0036		0.0038	0.0038
cpd_dh	1.00E-	135914	125914	1.00E-	753119	743119	1.00E-	426454	416454
or-S[c]	06	53	53	06	95	95	06	59	59
cpd_dh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pmp[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_dh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pt[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ptd[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_di	1.00E-		0.0199				1.00E-		0.0199
mp[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_di	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dit	1.00E-		0.0199				1.00E-		0.0199
p[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_dk	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mpp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mlz[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mpp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ms[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ms[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mso[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_d	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mso[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dn									
a_macr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
o[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dn	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[e]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0040		0.0159	0.0050		0.0149	0.0023		0.0176
cpd_dn	076823		923176	271313		728686	735217		264782
ad[c]	56	0.02	4	15	0.02	9	94	0.02	1
cpd_do	1.00E-		0.0199				1.00E-		0.0199
dca[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_do	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dcan[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_do	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dcan[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
coa[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dri	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
b[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
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bt[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt									
dp3adg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
alp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt									
dp3ddg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
alp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt									
dp6dm	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt									
dpddg[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt									
dpddm	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt									
dpglc[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_dt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_du	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_du	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_du	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ri[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_du	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ri[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_du	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ri[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_du	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tp[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_dx	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yl5p[c]	05	0.02	9	05	0.02	9	05	0.02	9
				0.0001		0.0198			0.0199
cpd_e4	1.00E-		0.0199	037733		962266	4.60E-		540167
p[c]	05	0.02	9	517	0.02	5	05	0.02	5
cpd_ei	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
g3p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ep	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_et	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ha[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_et	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
oh[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_et	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
oh[e]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0005		0.0194	0.0004		0.0195	0.0004		0.0195
cpd_f6	178151		821848	453863		546136	174609		825390
p[c]	736	0.02	3	487	0.02	5	489	0.02	5
cpd_fa	1.00E-		0.0199				1.00E-		0.0199
1[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_fa	1.00E-		0.0199				1.00E-		0.0199
11[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_fa									
11ACP[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_fa	1.00E-		0.0199				1.00E-		0.0199
13[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_fa									
130OH	1.00E-		0.0199				1.00E-		0.0199
3[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_fa									
130OH									
3ACP[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_fa									
13ACP[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_fa									
14ACP[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_fa									
171n8[1.00E-		0.0199				1.00E-		0.0199
c]	05	0.02	9	NA	NA	NA	05	0.02	9

cpd_fa 171n8 ACP[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_fa 181n7[c]	1.00E- 05	0.02	0.0199 9	NA	NA	NA	1.00E- 05	0.02	0.0199 9
cpd_fa 181n7 ACP[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_fa 1ACP[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_fa 3[c]	1.00E- 05	0.02	0.0199 9	NA	NA	NA	1.00E- 05	0.02	0.0199 9
cpd_fa 3ACP[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_fa 6[c]	1.00E- 05	0.02	0.0199 9	NA	NA	NA	1.00E- 05	0.02	0.0199 9
cpd_fa 6ACP[c 1	1.00E- 05	0.02	0.0199	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199
cpd_fa 7ACP[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_fa 8ACP[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_fa d[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_fa dh2[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_fal d[c]	1.00E- 05	0.02	0.0199 9	NA	NA	NA	1.00E- 05	0.02	0.0199 9
cpd_fd p[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_fd xo- 4:2[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_fd xr- 4:2[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9

cpd_fe	1.00E-	0.0003	0.0003	1.00E-	0.0003	0.0003	1.00E-	0.0003	0.0003
2[c]	05	17736	07736	05	17736	07736	05	17736	07736
			0.0003			0.0003			0.0003
cpd_fe	1.00E-	0.0003	077359	1.00E-	0.0003	077359	1.00E-	0.0003	077359
2[e]	05	17736	957	05	17736	958	05	17736	959
		0.0003	0.0003		0.0003	0.0003		0.0003	0.0003
cpd_fe	1.00E-	177358	077358	1.00E-	177358	077358	1.00E-	177358	077358
2[p]	05	621	621	05	674	674	05	696	696
cpd_fe	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
3[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_fg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
am[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_fgl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ut-S[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_fic	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ytcc[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_fm									
ettrna[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_fm	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tm	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
nRD[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_to	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cytcc[c]	05	0.02	9	05	0.02	9	05	0.02	9
	4 005		0.0400	4 005		0.0199	4 005		0.0199
	1.00E-	0.02	0.0199	1.00E-	0.02	899999	1.00E-	0.02	899999
r[c]	05	0.02	9	05	0.02	9	05	0.02	9
and fo	1 005		0.0100	1 005	0.0100	0.0100	1 005	0.0199	0.0199
cpu_io	1.00E-	0.02	0.0199	1.00E-	0.0199	0.0199	1.00E-	999835	0226669
I[e]	05	0.02	9	05	0.0100	0 0 1 0 0	05	9	9
and fo	1 00E		0 0100	1 00E	0.0199	0.0199 800016	1 00E	0.0199	0.0199
r[n]	1.001-	0.02	0.0199	1.00L-	555510	555510	1.00L-	0	0
cpd fo	1 00F-	0.02	0 0100	1 00F-	J	0 0100	1 00F-		0 0100
rglu[c]	1.000	0.02	0.0155 Q	1.000	0.02	0.0155 Q	1.000	0.02	0.0155 Q
cnd fn	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199
ram[c]	1.000	0.02	9.0199 9	1.000	0.02	9	1.000	0.02	0.0155 Q
ranijej	05	0.02	0.0110	05	0.02	0 0199	05	0.02	0 0199
cnd fn	4 81F-	0 0110	072037	1 91F-		808850	1 29F-		871374
rica[c]	4.01C	552575	7	1.510	0.02	4	1.29C 05	0.02	6,13,4 6
cnd fr	1 00F-	552575	, 0,0199	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199
	05	0.02	9	05	0.02	9	05	0.02	9
In I n I		3.52			3.52			0.02	

cpd_frl1.00E- (0)0.0199NANANA1.00E- (0)1.00E- (0)0.01990.0190.01990.01990.01990.01990.01990.01990.01990.01990.01990.01990.01990.01990.01990.01990.019 <t< th=""><th>0.0199 9 0.0199 9 2.37E- 05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9</th></t<>	0.0199 9 0.0199 9 2.37E- 05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
t[c]0.050.029NANANA0.050.02cpd_fr1.00E-0.01991.00E-0.01991.00E-0.01991.00E-u[c]0.050.0290.050.0290.050.02cpd_fr1.00E-1.20E-1.98E-1.00E-2.47E-1.47E-1.00E-3.37E-m[c]0.050.050.060.050.050.050.050.050.02cpd_fu1.00E-1.20E-1.98E-1.00E-2.47E-1.47E-1.00E-3.37E-m[c]0.050.050.050.050.050.050.050.050.02cpd_fu1.00E-1.00E-0.01991.00E-0.0290.050.020.02m[p]0.050.0290.50.0290.50.020.020.0190.019m[p]0.050.0290.50.0290.50.020.020.0190.019cpd_g11.00E-7871876871871.00E-90557805571.00E-0.0190.0190.019cpd_g31.00E-525624256227131372868732170.020.020.020.02cpd_g31.00E-52562426282713130.01990.0190.020.020.020.020.020.020.020.020.020.020.020.020.020.020.020.02 </td <td>9 0.0199 9 2.37E- 05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9</td>	9 0.0199 9 2.37E- 05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
cpd_fr1.00e- 000.01991.00e- 000.01991.00e- 0000.01991.00e- 000md[c]050.029050.029050.0290.02cpd_fr1.00e- 0050.029050.029050.0290.02cpd_fu1.00e- 0050.0506050505050.020.02cpd_fu1.00e- 0050.029050.029050.020.02cpd_fu1.00e- 0050.029050.029050.020.02cpd_fu1.00e- 0050.029050.029050.020.02cpd_fu1.00e- 0050.029050.029050.020.02cpd_fu1.00e- 0050.029050.029050.020.02cpd_g11.00e- 1.00e-7871876871871.00e- 00590557805571.00e- 005421355cpd_g31.00e- 1.00e-5256284256282713137286867321772868673217cpd_g31.00e- 00.01991.00e-1.00e- 00.01990.0190.0190.019cpd_g31.00e- 00.01991.00e-0.01990.0010.0190.0190.019cpd_g31.00e- 00.01990.01990.01990.0190.0190.019<	0.0199 9 0.0199 9 2.37E- 05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
md[c]0.050.0290.050.0290.0199cpd_fr1.00E-0.01991.00E-0.01991.00E-0.01991.00E-0.01990.01090.01990.01010.01010.01010.01010.011010.011010.011010.0111<	9 0.0199 9 2.37E- 05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
cpd_fr1.00E- 00.01991.00E- 00.01991.00E- 00.021.00E- 00.02u[c]050.029050.029050.02cpd_fu1.00E- 050.05060505050505cpd_fu1.00E- 050.029050.029050.02m[e]050.029050.029050.02cpd_fu1.00E- 100E0.01991.00E- 0.020.01991.00E-0.01990.0199m[p]050.029050.029050.02cpd_fu1.00E- 100E0.00080.00090.0090.0010.001cpd_g11.00E- 100E7871876871871.00E- 100E9005578005571.00E- 100E421355p[c]05937937059469460561cpd_g31.00E- 525628425622713137286867352177p[c]050.029050.0290.020.02cpd_g31.00E- 50.020.01991.00E- 50.020.0290.020.02cpd_g31.00E- 50.020.01970.00191.00E- 50.020.020.01970.001cpd_g31.00E- 50.020.01970.0020.01970.0210.020.020.02cpd_g31.00E- 50.020.0290	0.0199 9 2.37E- 05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
u[c]0050.029050.029050.02cpd_fu1.00E-1.20E-1.98E-1.00E-2.47E-1.47E-1.00E-3.37E-m[c]05050605050505050505cpd_fu1.00E-0.01991.00E-0.01990.0191.00E-0.029050.02cpd_fu1.00E-0.0191.00E-0.01991.00E-0.029050.02cpd_fu1.00E-0.0029050.0290.0191.00E-0.02cpd_fu1.00E-0.0029050.0290.0290.02cpd_g11.00E-0.00290.0090.0091.00E-0.0140.023cpd_g31.00E-7871876871871.00E-900557805571.00E-421355p[c]059379370594694605611p[c]051.011.01E-0.01490.00231.01E-0.02p[c]051.011.01E-0.0191.00E-0.0190.020.02p[c]050.029050.0290.020.02p[c]050.0290.0191.00E-0.0190.0010.019p[c]050.0290.0190.0290.020.020.02p[c]050.029 <td< td=""><td>9 2.37E- 05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9</td></td<>	9 2.37E- 05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
cpd_fu1.00e- 1.00e-1.20e- 1.98e-1.00e- 0.0192.47e- 0.051.47e- 0.051.00e- 0.053.37e- 0.5m[c]050.0000.01991.00e- 0.0190.01991.00e- 0.020.01991.00e- 0.02m[e]050.029050.029050.02cpd_fu1.00e- 0.050.01991.00e- 0.0190.01991.00e- 0.020.02m[p]050.029050.0290.01990.021cpd_f11.00e- 0.0550.0290.01991.00e- 0.0210.01900.0010cpd_g11.00e- 0.0559379370594694605611cpd_g31.00e- 1.05593793705946946052612cpd_g31.00e- 1.0550.0191.00e- 1.0520.0219005578005771.00e- 1.00E-60.02cpd_g31.00e- 1.0550.0190.01931.00e- 1.020.0191.00e- 1.020.0191.00e- 1.02cpd_g31.00e- 1.0020.0191.00E- 1.0020.0191.00E- 1.00E0.0191.00E- 1.00E0.0191.00E- 1.00Ep[c]0.0020.0191.00E- 0.0190.0191.00E- 0.0190.0191.00E- 0.0190.0190.0190.019p[c]0.0020.0190.0191.00E- 0.0190.0190.0190.0190.019	2.37E- 05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
m[c]050506050505cpd_fu1.00E-0.0191.00E-0.0191.00E-m[e]050.029050.0290.02cpd_fu1.00E-0.0191.00E-0.0191.00E-0.02m[p]050.029050.0290.02m[p]050.0290.0191.00E-0.010cpd_g11.00E-7871876871871.00E-90057800571.00E-cpd_g31.00E-7871876871871.00E-90057800571.00E-421355p[c]05937937059469460561cpd_g31.00E-5256284256827131372868673521772866p[c]051.0141.150.02990.02cpd_g31.00E-0.01991.00E-1.00E-0.0191.00E-p[c]050.029050.0290.02cpd_g31.00E-0.01991.00E-1.00E-0.0191.00E-p[c]050.029050.0290.02cpd_g41.00E-0.01971.00E-0.0191.00E-p[c]050.0291.00E-0.0191.00E-p[c]050.0291.00E-0.0191.00E-p[c]980.0290.0190.0191.00E- <td>05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9</td>	05 0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
cpd_fu1.00E-0.01991.00E-0.01991.00E-m[e]050.029050.029050.02cpd_fu1.00E-0.0191.00E-0.01991.00E-0.01991.00E-m[p]050.029050.029050.02cpd_g11.00E-7871876871871.00E-9005578005571.00E-421355p[c]059379370594694605661cpd_g31.00E-5256284256282713137286867352177p[c]050.029050.02990.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.0190.02p[c]050.029050.029900.02cpd_g31.00E-0.0191.00E-0.01991.00E-0.0190.020.02p[c]050.029050.029050.02900.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.0190.0200.02p[c]050.029050.029050.02900.02cpd_g31.00E-0.01991.00E-0.01990.00E0.0190.0200.02p[c]050.029050.029050.02	0.0199 9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
m[e]050.029050.029050.02cpd_fu1.00E-0.01991.00E-0.01991.00E-0.01991.00E-m[p]050.029050.029050.02cpd_g11.00E-7871876871871.00E-9005578005571.00E-421355p[c]059379370594694605661cpd_g31.00E-5256284256282713137286867352177p[c]0511150.02990.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.0290.02pe[c]050.029050.029050.0290.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.0290.020.02pg[c]050.029050.029050.0290.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.0190.0010.02pg[c]050.029050.029050.0290.00.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.0191.00E-0.0190.0190.0190.019cpd_g41.00E-0.01991.00E-0.01991.00E-0.0190.0190.0290.02 </td <td>9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9</td>	9 0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
cpd_fu1.00E-0.01991.00E-0.01991.00E-0.01991.00E-m[p]050.029050.0290.00.02cpd_g11.00E-7871876871871.00E-9005578005571.00E-421355p[c]0.05937937059469460.061cpd_g31.00E-5256284256282713137286867352177p[c]0.051.00E-5256284256282713137286867352177p[c]0.050.0290.01991.00E-9.01991.00E-9.01991.00E-p[c]0.050.0290.050.0290.01991.00E-p[c]0.050.0290.050.0290.01991.00E-p[c]0.050.0290.050.0290.020.02pg[c]0.050.0290.050.0290.020.02pg[c]0.0020.0290.01991.00E-0.01991.00E-pg[c]0.00020.01970.00290.01970.0011.00E-pg[c]0.00020.01970.00290.01970.00290.0197pg[c]0.00020.01970.00290.01970.0020.01970.002p[c]9980.027239591.02E-0.01991.00E-0.01990.0197 <td>0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9</td>	0.0199 9 0.0010 321355 61 0.0176 264782 1 0.0199 9
m[p]050.029050.029050.02cpd_g11.00E-7871876871871.00E-9005578005571.00E-421355p[c]05937937059469460561cpd_g31.00E-5256284256282713137286867352177p[c]0511150.029940.022cpd_g31.00E-5256284256282713137286867352177p[c]0511150.02990.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.02pe[c]050.029050.0290.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.02pe[c]050.029050.0290.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.02pe[c]050.029050.0290.02cpd_g62760400.01970200889799119191360.02p[c]9980.027239591720.0281220.02cpd_g81.00E-0.01991.00E-0.01991.00E-0.0191.00E-[c]050.029050.0290.0290.02cpd_g81.00E-0.01991.00E-0.0199	9 0.0010 321355 61 0.0176 264782 1 0.0199 9
cpd_g10.00080.00090.00090.0010cpd_g11.00E-7871876871871.00E-9005578005571.00E-421355p[c]0.05937937059469460.02361cpd_g31.00E-5256284256282713137286867352177p[c]0.051.00E-5256284256282713130.01991.00E-940.023cpd_g31.00E-5256284256282713130.01991.00E-940.02cpd_g31.00E-0.0191.00E-0.01991.00E-940.02cpd_g31.00E-0.0191.00E-0.0191.00E-0.0190.019pg[c]0.50.0290.50.0290.50.02cpd_g31.00E-0.0191.00E-0.0191.00E-0.0190.019pg[c]0.50.0290.50.0290.50.02cpd_g31.00E-0.0191.00E-0.0191.00E-0.0190.019pg[c]0.50.0290.50.0290.50.02pg[c]0.50.0290.50.0290.50.02pg[c]0.50.0290.50.0290.50.02pg[c]0.50.0290.50.0290.50.02p[c]9980.02723591.720	0.0010 321355 61 0.0176 264782 1 0.0199 9
cpd_g11.00E-7871876871871.00E-9005578005571.00E-421355p[c]05937937059469460561cpd_g31.00E-525628425628271313728686735217p[c]0511150.029940.02cpd_g31.00E-5256284256282713137286867352177p[c]0511150.029940.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01991.00E-pe[c]050.029050.029050.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01990.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.02pe[c]050.029050.029050.02pg[c]050.029050.029050.02pg[c]050.029050.0290.0190.019p[c]9980.027239591720.0281220.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.0190.02[c]050.029050.029050.02p[c]050.029050.0290.0190.019[321355 61 0.0176 264782 1 0.0199 9
p[c]05937937059469460561cpd_g31.00E-5256284256282713130.01490.0023p[c]0511150.029940.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01991.00E-pe[c]050.029050.029050.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01990.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01990.029050.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01991.00E-0.01990.020.02cpd_g31.00E-0.01970200889799119191360.020.020.020.020.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-0.01990.020.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990.020.020.020.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990.020.020.020.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990.020.020.020.020.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990.02 <td< td=""><td>61 0.0176 264782 1 0.0199 9</td></td<>	61 0.0176 264782 1 0.0199 9
cpd_g30.01480.01480.00500.01490.0023cpd_g31.00E-525628425628271313728686735217p[c]0511150.029940.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01991.00E-pe[c]050.029050.029050.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01990.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.02pg[c]050.029050.029050.02pg[c]050.029050.029050.02p[c]9980.027239591720.0281220.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.020.020.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.020.020.02[c]050.029050.029050.020.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990.02[c]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990.02[c]050.029050.029050.02 </td <td>0.0176 264782 1 0.0199 9</td>	0.0176 264782 1 0.0199 9
cpd_g31.00E-525628425628271313728686735217p[c]051150.029940.02cpd_g31.00E-0.01991.00E-0.01991.00E-pe[c]050.029050.02905cpd_g31.00E-0.01991.00E-0.01991.00E-pg[c]050.029050.02905pg[c]050.029050.02905pg[c]050.029050.02905cpd_g62760400.0197020088979911919136p[c]9980.027239591720.028122cpd_ga1.00E-0.01991.00E-0.01991.00E-l[c]050.029050.02905l[e]050.029050.0290.02l[e]050.029050.0290.02l[e]050.029050.029050.02l[p[c]050.029050.029050.02l[p[c]050.029050.029050.02l[p[c]050.029050.029050.02l[p[c]050.029050.029050.02l[p[c]05	264782 1 0.0199 9
p[c]0511150.029940.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01991.00E-pe[c]050.029050.029050.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01991.00E-pg[c]050.029050.029050.02pg[c]050.029050.029050.02cpd_g62760400.0197020088979911919136919136p[c]9980.027239591720.0281220.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-l[c]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-l[e]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990.02l[p[c]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990.0199l[p[c]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990	0.0199 9
cpd_g31.00E-0.01991.00E-0.01991.00E-pe[c]050.029050.02905cpd_g31.00E-0.01991.00E-0.01991.00E-pg[c]050.029050.02905opd_g62760400.0197020088979911919136p[c]9980.027239591720.028122cpd_ga1.00E-0.01991.00E-0.01991.00E-[c]050.029050.02905cpd_ga1.00E-0.01991.00E-0.01991.00E-[c]050.029050.02905cpd_ga1.00E-0.01991.00E-0.01991.00E-[e]050.029050.02905cpd_ga1.00E-0.01991.00E-0.01991.00E-[lpc]050.029050.02905cpd_ga1.00E-0.01991.00E-0.01991.00E-[lpc]050.029050.02905cpd_ga1.00E-0.01991.00E-0.01991.00E-[lpc]050.029050.029050.029050.029050.02	0.0199 9
pe[c]050.029050.029050.02cpd_g31.00E-0.01991.00E-0.01991.00E-0.01991.00E-pg[c]050.029050.029050.02cpd_g62760400.01970200889799119191360.02p[c]9980.027239591720.0281220.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-l[c]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-l[e]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-l[e]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990.02lp[c]050.029050.029050.02	9
cpd_g31.00E-0.01991.00E-0.01991.00E-pg[c]050.029050.029050.00020.00020.00020.01970.0001cpd_g62760400.0197020088979911919136p[c]9980.027239591720.028122cpd_ga1.00E-0.01991.00E-0.01991.00E-[c]050.029050.02905cpd_ga1.00E-0.01991.00E-0.01991.00E-[e]050.029050.02905cpd_ga1.00E-0.01991.00E-0.01991.00E-[le]050.029050.02905lp[c]050.029050.02905lp[c]050.029050.02905	
pg[c]050.029050.029050.020.00020.00020.00020.01970.00010.01970.0001cpd_g62760400.0197020088979911919136p[c]9980.027239591720.0281220.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-l[c]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-l[e]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01990.02lp[c]050.029050.029050.02	0.0199
0.00020.00020.00020.01970.0001cpd_g62760400.0197020088979911919136p[c]9980.027239591720.0281220.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-l[c]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-l[e]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-lp[c]050.029050.0290.01991.00E-	9
cpd_g62760400.0197020088979911919136p[c]9980.027239591720.0281220.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-l[c]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-l[e]050.029050.029050.02cpd_ga1.00E-0.01991.00E-0.01991.00E-0.01991.00E-lp[c]050.029050.029050.02	0.0198
p[c] 998 0.02 723959 172 0.02 8 122 0.02 cpd_ga 1.00E- 0.0199 1.00E- 0.0199 1.00E- l[c] 05 0.02 9 05 0.02 9 05 0.02 cpd_ga 1.00E- 0.0199 1.00E- 0.0199 1.00E- 0.0199 1.00E- l[e] 05 0.02 9 05 0.02 9 05 0.02 cpd_ga 1.00E- 0.0199 1.00E- 0.0199 1.00E- 0.02 0.02 0.02 0.02 cpd_ga 1.00E- 0.0199 1.00E- 0.0199 1.00E- 0.02 <	080863
cpd_ga1.00E-0.01991.00E-0.01991.00E-I[c]050.029050.02905cpd_ga1.00E-0.01991.00E-0.01991.00E-I[e]050.029050.02905cpd_ga1.00E-0.01991.00E-0.01991.00E-l[e]050.029050.02905cpd_ga1.00E-0.01991.00E-0.01991.00E-l[p[c]050.029050.02905	9
I[c] 05 0.02 9 05 0.02 1p[c]050.029050.029050.029050.02	0.0199
cpd_ga 1.00E- 0.0199 1.00E- 0.0199 1.00E- l[e] 05 0.02 9 05 0.02 9 05 0.02 cpd_ga 1.00E- 0.0199 1.00E- 0.0199 1.00E- 0.0199 0.02 l[p[c] 05 0.02 9 05 0.02 9 05 0.02	9
I[e] 05 0.02 9 05 0.02 9 05 0.02 cpd_ga 1.00E- 0.0199 1.00E- 0.0199 1.00E- 0.0199 1.00E- l1p[c] 05 0.02 9 05 0.02 9 05 0.02	0.0199
cpd_ga 1.002- 0.0199 1.002- 0.0199 1.002- l1p[c] 05 0.02 9 05 0.02 9 05	9
	0.0199
and an	9
Lactor 1 00E 0 0100 1 00E 0 0100 1 00E	0 0100
$\begin{bmatrix} 1.001^{-1} \\ 0.0139 \\ 1.001^{-1} \\ 0.001^$	0.0199
	0.0053
cnd ga 1 00F- 950862 850862 1 00F- 667495 567495 1 00F- 879861	779861
m1n[c] 05 07 07 05 33 33 05 13	
	13
cpd ga 4.00F- 599606 3.80F- 620259 3.71F-	13
m6p[c] 05 0.02 5 05 0.02 1 05 0.02	13 0.0199 628803
cpd ga 1.00E- 0.0199 1.00E- 0.0199 1.00F-	13 0.0199 628803 8
r[c] 05 0.02 9 05 0.02 9 05 0.02	13 0.0199 628803 8 0.0199

cpd_gc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ald[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gd	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gd	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pdp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gd									
pmann	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gd	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ptp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gg									
luaba[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gg									
luabt[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gg	4 0 0 5			4 9 9 5			4 9 9 5		
	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199
C]	05	0.02	9	05	0.02	9	05	0.02	9
cpa_gic	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
	1.005	0.02	9	1.005	0.02	9	1.005	0.02	9
cpa_gic	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
-D[e]	1.005	0.02	9	1.005	0.02	9		0.02	9
Cpu_gic	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
cod al	1.005	0.02	0 0100	1.005	0.02	0 0100	1.005	0.02	0 0100
cpu_gi n-l[c]	1.001-	0.02	0.0199 Q	1.00L-	0.02	0.0199 Q	1.00L-	0.02	0.0199
cnd gl	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199	1 00F-	0.02	0 0100
cpu_gi n_l [ɕ]	1.000	0.02	0.0155 Q	1.000	0.02	0.0155 Q	1.000	0.02	0.0155 Q
cnd gl	00	0.02		05	0.02		00	0.02	
ntrna[c	1 00F-		0 0199	1 00F-		0 0199	1 00F-		0 0199
1	1.002	0.02	9	1.002	0.02	9	1.002	0.02	9
cpd gl		0.02		00	0.02			0.02	
u-asp-	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
L[C]	05	0.02	9	05	0.02	9	05	0.02	9
L - J		0.0125	0.0125		0.0127	0.0127		0.0128	0.0128
cpd gl	1.00E-	371220	271220	1.00E-	626506	526506	1.00E-	608106	508106
u-D[c]	05	6	6	05	7	7	05	6	6

			0.0199			0.0199			0.0199
cpd_gl	9.51E-		049368	1.57E-		843292	1.56E-		844488
u-L[c]	05	0.02	7	05	0.02	8	05	0.02	8
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
u-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
u-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
u1sa[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
u5p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
u5sa[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ucys[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd gl									
utrna[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
1	05	0.02	9	05	0.02	9	05	0.02	9
- cpd gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
x[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd gl									
y-asp-	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd gl									
y-asp-	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl									
y-asp-	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl									
y-glu-	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl									
y-glu-	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl									
y-glu-	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
L[p]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0001		0.0198						
cpd_gl	131090		868909	1.00E-		0.0199	1.00E-		0.0199
y[c]	407	0.02	6	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
y[e]	05	0.02	9	05	0.02	9	05	0.02	9

cpd gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
y[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yb[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yb[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yb[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yc-R[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yc-R[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl							1.00E-		0.0199
yc-R[p]	NA	NA	NA	NA	NA	NA	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yc[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yc[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yc[p]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0003		0.0196	0.0002		0.0197	0.0001		0.0198
cpd_gl	197212		802787	095618		904381	747724		252275
yc3p[c]	782	0.02	2	253	0.02	7	501	0.02	5
cpd_gl	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199
ycit[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gl	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
ycitlej	1.005	0.02	9	1.005	0.02	9	05	0.02	9
cpa_gi	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
ycit[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpu_gi	1 005		0.0100	1 005		0.0100	1 005		0.0100
fcl	1.002-	0.02	0.0199	1.002-	0.02	0.0199	1.002-	0.02	0.0199
cod al	05	0.02	9	05	0.02	9	05	0.02	9
vtrna[c	1 00F-		0 0100	1 00F-		0 0100	1 00F-		0 0100
junale	1.001-	0.02	0.0199 Q	1.00L-	0.02	0.0199	1.000	0.02	0.0199 Q
ι cnd σ	05	0.02	J	05	0.02		05	0.02	J
mh17h	1 00F-		0 0199	1 00F-		0 0199	1 00F-		0 0199
	05	0.02	9	05	0.02	9	05	0.02	9
cod a		0.02			0.02			0.02	
mh1plc	1.00F-		0.0199	1.00F-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_g		0.0004	0.0003		0.0004	0.0004		0.0004	0.0004
mh7p[c	1.00E-	023114	923114	1.00E-	670079	570079	1.00E-	979145	879145
]	05	491	491	05	777	777	05	976	976
cpd_g	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gs	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hox[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hrd[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hrd[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hrd[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_gu	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_h2	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_h2	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199	1.00E-		0.0199
[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_h2	4 005		0.0400	4 005		0.0400	4 005		0.0400
mb4p[c	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
and h2	1 005	0.0001	0.0001	1 005		0.0100	1 005		0.0100
	1.00E-	109414	127	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
02[c]	1 005	127	0.0100	1 005	0.02	9	1 005	0.02	9
02[0]	1.002-	0.02	0.0199	1.002-	0.02	0.0199	1.00E-	0.02	0.0199
$\frac{02[e]}{cnd}$	1 00F-	0.02	0 0100	1 00F-	0.02	0 0100	1 00F-	0.02	0 0100
02[n]	1.001-	0.02	0.0199 Q	1.00L-	0.02	0.0199 Q	1.00L-	0.02	0.0199 Q
$\frac{02[p]}{cnd}$	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199	1 00F-	0.02	0 0100
s[c]	1.000	0.02	0.0155 9	1.000	0.02	0.0155 9	1.000	0.02	0.0155 Q
cnd h2	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199
s[e]	1.002	0.02	9	1.002	0.02	9	1.000	0.02	9
cpd h2	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199
s[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd hc	1.00F-	0.02	0.0199	1.00F-	0.02	0.0199	1.00F-	0.02	0.0199
o3[c]	05	0.02	9	05	0.02	9	05	0.02	9

		0.0004	0.0004		0.0007	0.0007		0.0009	0.0009
cpd_hc	1.00E-	115728	015728	1.00E-	408054	308054	1.00E-	536688	436688
ys-L[c]	05	908	908	05	122	122	05	061	061
cpd_hd	1.00E-		0.0199				1.00E-		0.0199
ca[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_hd	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
can[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hd	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
can[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hd	1.00E-		0.0199				1.00E-		0.0199
cea[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_hd									
eACP[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_he	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
meO[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_he	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pdp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_he	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
xdp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hg	1.00E-		0.0199						
entis[c]	05	0.02	9	NA	NA	NA	NA	NA	NA
cpd_hi	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
bcoa[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hi	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
s-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hi	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
sp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hi	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
std[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hi									
strna[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_h	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mbil[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_h									
mgcoa[1.00E-		0.0199						
c]	05	0.02	9	NA	NA	NA	NA	NA	NA
cpd_h									
mglut-	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
S[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ho	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
m-L[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_hp									
dACP[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hp	1.00E-		0.0199				1.00E-		0.0199
dca[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_hp	1.00E-		0.0199				1.00E-		0.0199
de[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_hp									
deACP[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
yr[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hx	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
an[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_hx	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
an[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ias	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ib	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
coa[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0131	0.0131		0.0133	0.0133		0.0134	0.0134
cpd_ic	1.00E-	342082	242082	1.00E-	467513	367513	1.00E-	391422	291422
hor[c]	05	6	6	05	4	4	05	7	7
		0.0006	0.0006		0.0007	0.0007		0.0007	0.0007
cpd_ici	1.00E-	467099	367099	1.00E-	372281	272281	1.00E-	799209	699209
t[c]	05	782	782	05	188	188	05	841	841
cpd_id	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ile	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ile	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ile	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ile	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
trna[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_im	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
acp[c]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0001		0.0198			0.0199			0.0199
cpd_im	962395		037604	7.40E-		260214	4.86E-		513553
p[c]	871	0.02	1	05	0.02	2	05	0.02	7
cpd_in	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dole[c]	05	0.02	9	05	0.02	9	05	0.02	9

								0.0199	0.0199
cpd_in	1.00E-		0.0199	1.00E-		0.0199	1.00E-	999917	899917
dole[e]	05	0.02	9	05	0.02	9	05	9	9
cpd_in	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dole[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_in	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
oshp[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_in									
oshp[p	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_in									
ospp1[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_in									
ospp1[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_in	1.00E-	0.00	0.0199	1.00E-		0.0199	1.00E-		0.0199
OST[C]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_in	1.00E-	0.00	0.0199	1.00E-		0.0199	1.00E-		0.0199
s[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_in	1.00E-	0.00	0.0199	1.00E-		0.0199	1.00E-		0.0199
s[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ip	1.00E-	0.02	0.0199	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199
ap[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpa_itp	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
	1.005	0.02	9	1.005	0.02	9	1.005	0.02	9
	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
	1.005		9	1.005	0.02	9	1.005	0.02	9
сра_к[1.00E-	0.0500	0.0500	1.00E-	0.0500	0.0506 71275	1.00E-	0.0500	0.0500
cj opd k[1.005	01275	0.0506	1 005	01275	0.0506	1 005	01275	0.0506
cpu_k[o]	1.00E-	0.0500 91275	71275	1.00E-	0.0500 91275	71275	1.00E-	0.0500 91275	0.0500
ej	05	0.0506	0.0506	05	0.0506	0.0506	05	0.0506	0.0506
and k[1 00F-	0.0500 812530	712520	1 00F-	Q1252Q	712538	1 00F-	8125 <i>1</i> 2	712542
cpu_k[n]	1.000	1	1 12550	1.000	512555	5	1.000	1	1 12342
cnd kd	1 00F-	-	0 0199	1 00F-		0 0199	1 00F-		0 0199
	1.000	0.02	9	1.000	0.02	9	1.000	0.02	9.0155
cpd kd	00	0.02			0.02			0.02	
o8nlina	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd kd									
iailn8o	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
d4[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_kd									
o8nlipi	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
d4L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_kd	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
o8p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd lac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-D[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-D[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-D[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_la	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mi[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_le	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
u-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_le	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
u-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_le	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
u-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_le									
utrna[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lgt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-S[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lip									
id_mac	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ro[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lip	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
idA[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lip									
idAds[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lip	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
idX[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lp									
s_Core[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_lp									
s_macr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
o[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lys	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lys	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lys	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_lys	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
trna[c]	05	0.02	9	05	0.02	9	05	0.02	9
					0.0001				0.0199
cpd_m	1.00E-	5.14E-	4.14E-	1.00E-	001125	9.01E-	3.96E-		603847
al-L[c]	05	05	05	05	738	05	05	0.02	8
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
al-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
al-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m									
alACP[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m									
alcoalc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
J	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-	0.02	0.0199	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199
alt[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpa_m	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
ait[e]	1 005	0.02	9		0.02	9	1.005	0.02	9
cpa_m	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
ait[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpu_m	1 005		0.0100	1 005		0.0100	1 005		0.0100
annp[c	1.001-	0.02	0.0199	1.00L-	0.02	0.0199	1.001-	0.02	0.0199
rnd m	05	0.02	5	05	0.02	5	05	0.02	5
althn[e	1 00F-		0 0199	1 00F-		0 0199	1 00F-		0 0199
1	1.001	0.02	9	1.002	0.02	9	1.002	0.02	9
rnd m	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199
althx[c]	05	0.02	9	0.5	0.02	9	05	0.02	9
cpd m									
althx[e	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
altpt[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
altpt[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
alttr[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
alttr[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
altttr[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m									
altttr[e	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
an1p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-		0.0199				1.00E-		0.0199
an6p[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_m									
ercppy	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r[c]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0002		0.0197	0.0050		0.0149	0.0023		0.01/6
cpa_m	061573	0.02	938426	2/1313	0.00	/28686	/3521/	0.02	264782
et-L[C]	/39	0.02	3	1.005	0.02	9	94	0.02	1
cpa_m	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
et-L[e]	1.005	0.02	9	1.005	0.02	9	1.005	0.02	9
cpu_m	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
et-r[b]	05	0.02	9	05	0.02	9	05	0.02	9
and m	1 005	0.0009 E00021	0.0009	1 005	750210	0.0010	1 005	202101	0.0011
cpu_m	1.002-	868	400021	1.002-	736510	5/	1.002-	506191	208191
cnd m	05	000	000	05	54	54	05	,	/
ettrnal	1 00F-		0 0199	1 00F-		0 0199	1 00F-		0 0199
cl	1.001	0.02	9	1.001	0.02	9	1.001	0.02	9
c]	00	0.0015	0.0015	03	0.0017	0.0016	03	0.0017	0.0017
cpd m	1.00E-	244394	144394	1.00E-	088486	988486	1.00E-	939908	839908
g2[c]	05	56	56	05	64	64	05	54	54
0 1 1	0.0001		0.0198	0.0001		0.0198	0.0001		0.0198
cpd m	311957		688042	170378		829621	114832		885167
	646	0.02	4	654	0.02	3	885	0.02	1
	0.0001	0.0199	0.0198	0.0001	0.0199	0.0198	0.0001	0.0199	0.0198
cpd_m	311957	999913	687956	170378	999916	829538	114832	999917	885085
g2[p]	076	2	1	166	5	4	428	9	5
cpd_mi	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
1p-D[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_mi	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cit[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ml	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
thf[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd m									
malsa[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mql7[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m									
mqn7[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n2[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n2[e]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0199	0.0199		0.0199	0.0199		0.0199	0.0199
cpd_m	1.00E-	999913	899913	1.00E-	999916	899916	1.00E-	999917	899917
n2[p]	05	2	2	05	5	5	05	9	9
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n4o[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	7.38E-	7.38E-	7.31E-	7.38E-	7.38E-	7.31E-	7.38E-	7.38E-	7.31E-
obd[c]	08	06	06	08	06	06	08	06	06
cpd_m	7.38E-	7.38E-	7.31E-	7.38E-	7.38E-	7.31E-	7.38E-	7.38E-	7.31E-
obd[e]	08	06	06	08	06	06	08	06	06
cpd_m	7.38E-	7.38E-	7.31E-	7.38E-	7.38E-	7.31E-	7.38E-	7.38E-	7.31E-
obd[p]	08	06	06	08	06	06	08	06	06
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ql7[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
qn7[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_m									
yrsACP	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_na	1.00E-	2.7857	2.7857	1.00E-	2.7857	2.7857	1.00E-	2.7857	2.7857
1[c]	05	91739	81739	05	91739	81739	05	91739	81739
cpd_na	1.00E-	2.7857	2.7857	1.00E-	2.7857	2.7857	1.00E-	2.7857	2.7857
1[e]	05	91739	81739	05	91739	81739	05	91739	81739
cpd_na	1.00E-	2.7857	2.7857	1.00E-	2.7857	2.7857	1.00E-	2.7857	2.7857
1[p]	05	91739	81739	05	91739	81739	05	91739	81739
					0.0001			0.0001	0.0001
cpd_na	1.00E-	4.99E-	3.99E-	2.79E-	111257	8.32E-	1.86E-	567561	381529
d[c]	05	05	05	05	514	05	05	763	663

		0.0009	0.0009						
cpd_na	1.00E-	183995	083995	1.00E-	3.98E-	2.98E-	1.00E-	8.43E-	7.43E-
dh[c]	05	246	246	05	05	05	05	05	05
cpd_na	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_na	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dph[c]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0032		0.0127	0.0040		0.0119	0.0018		0.0140
cpd_nh	027529	0.0159	803150	174490	0.0159	656189	968080	0.0159	862599
4[c]	81	83068	2	83	83068	2	11	83068	9
		0.0159	0.0159		0.0159	0.0159		0.0159	0.0159
cpd_nh	1.00E-	830541	730541	1.00E-	830546	730546	1.00E-	830548	730548
4[e]	05	3	3	05	6	6	05	9	9
		0.0159	0.0159		0.0159	0.0159		0.0159	0.0159
cpd_nh	1.00E-	830610	730610	1.00E-	830613	730613	1.00E-	830614	730614
4[p]	05	7	6	05	3	3	05	4	4
cpd_ni	3.10E-	3.10E-	3.07E-	3.10E-	3.10E-	3.07E-	3.10E-	3.10E-	3.07E-
2[c]	08	06	06	08	06	06	08	06	06
cpd_ni	3.10E-	3.10E-	3.07E-	3.10E-	3.10E-	3.07E-	3.10E-	3.10E-	3.07E-
2[p]	08	06	06	08	06	06	08	06	06
cpd_ni	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
crnt[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_n	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mn[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_n	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mn[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_no	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_no	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
2[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_no	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
2[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_no	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
2[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_no	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
3[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_no	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
3[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_no	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
3[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_o2	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
-[c]	05	0.02	9	05	0.02	9	05	0.02	9

		0.0003	0.0003		0.0002	0.0002		0.0002	0.0002
cpd_o2	2.84E-	295197	010984	1.00E-	574597	474597	1.00E-	338798	238798
[c]	05	14	876	05	851	851	05	081	081
			0.0003			0.0002			0.0002
cpd_o2	2.84E-	0.0003	010987	1.00E-	0.0002	474599	1.00E-	0.0002	238799
[e]	05	2952	49	05	5746	917	05	3388	918
		0.0003	0.0003		0.0002	0.0002		0.0002	0.0002
cpd_o2	2.84E-	295198	010986	1.00E-	574598	474598	1.00E-	338799	238798
[p]	05	57	183	05	925	884	05	04	999
cpd_oa	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_oc									
dACP[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_oc	1.00E-		0.0199				1.00E-		0.0199
dca[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_oc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dcan[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_oc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dcan[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_oc	1.00E-		0.0199				1.00E-		0.0199
dcea[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_oc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
tdp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_oc									
teACP[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_oh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cu[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0009	0.0009						
cpd_oh	1.00E-	183995	083995	1.00E-		0.0199	1.00E-		0.0199
pb[c]	05	247	247	05	0.02	9	05	0.02	9
cpd_or	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_or	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ot[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_or	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ot5p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pa									
ImACP[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pa	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n4p[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_pa	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
nose[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pa	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
nt-R[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pa	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pa	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ps[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pd	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ACP[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pd	1.00E-		0.0199				1.00E-		0.0199
e[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_pd									
eACP[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0017		0.0182						
cpd_pd	250091		749908	1.00E-		0.0199	1.00E-		0.0199
x5p[c]	69	0.02	3	05	0.02	9	05	0.02	9
cpd_pe	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pe	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ndp[c]	05	0.02	9	05	0.02	9	05	0.02	9
					0.0018	0.0018		0.0034	0.0034
cpd_pe	1.00E-		0.0199	1.00E-	796339	696339	1.00E-	937409	837409
p[c]	05	0.02	9	05	97	97	05	41	41
cpd_pe									
ptido[p	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pe									
ptidogl									
ycan_									
macro[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pe	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ptx[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pg	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ly[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0006	0.0006		0.0009	0.0009		0.0011	0.0011
cpd_pg	1.00E-	255448	155448	1.00E-	543722	443722	1.00E-	443451	343451
lyp[c]	05	532	532	05	944	944	05	18	18
cpd_ph	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
e-L[c]	05	0.02	9	05	0.02	9	05	0.02	9

1		1						1	1
cpd_ph	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
eme[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ph	1.00E-		0.0199	1.00E-		0.0199			
eme[p]	05	0.02	9	05	0.02	9	NA	NA	NA
cpd_ph									
etrna[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ph	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
om[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ph	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pyr[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0021	0.0020						
cpd_ph	1.00E-	038649	938649	1.00E-		0.0199	1.00E-		0.0199
thr[c]	05	89	89	05	0.02	9	05	0.02	9
		0.0009	0.0009	0.0005	0.0022	0.0016	0.0003	0.0032	0.0028
cpd_pi[1.00E-	701326	601326	677779	588545	910766	854689	480757	626068
c]	05	528	528	281	74	45	284	45	17
						0.0135			0.0135
cpd_pi[1.00E-	0.0135	0.0135	5.68E-	0.0135	079642	3.85E-	0.0135	261948
e]	05	64741	54741	05	64741	9	05	64741	4
		0.0135	0.0135		0.0135	0.0135		0.0135	0.0135
cpd_pi[1.00E-	647351	547351	5.68E-	647353	079586	3.85E-	647354	261892
p]	05	1	1	05	4	5	05	3	9
cpd_p		0.0199	0.0199					0.0199	0.0199
mcoa[c	1.00E-	999826	899826	1.00E-	0.0199	0.0199	1.00E-	999835	899835
]	05	4	4	05	999833	899833	05	9	9
cpd_p			0.0199			0.0199			0.0199
mcoa[e	1.00E-		899999	1.00E-		899999	1.00E-		899999
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_p		0.0199	0.0199		0.0199	0.0199		0.0199	0.0199
mcoa[p	1.00E-	999913	899913	1.00E-	999916	899916	1.00E-	999917	899917
]	05	2	2	05	5	5	05	9	9
cpd_pn	1.19E-	1.19E-	1.17E-	1.19E-	1.19E-	1.17E-	1.19E-	1.19E-	1.17E-
to-R[c]	07	05	05	07	05	05	07	05	05
cpd_pp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
bng[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd pp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
coa[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hn[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pp	1.00E-	4.99E-	3.99E-	1.00E-	1.99E-	9.95E-	1.00E-	2.90E-	1.90E-
i[c]	05	05	05	05	05	06	05	05	05
cpd_pp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p9[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pg9[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
am[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
an[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr									
bamp[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
batp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
fp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_prl	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr	1.00E-		0.0199				1.00E-		0.0199
o-gly[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_pr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
o-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
o-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
o-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr									
otein_									
macro	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
C]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr				4 9 9 5			4 9 9 7		
otrnalc	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199
J	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pr	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199
pp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ps	1.00E-		0.0199	1.00E-		0.0199	1.00E-	0.00	0.0199
[C]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_ps	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
d5p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ps	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
er-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pt	1.00E-		0.0199				1.00E-		0.0199
dca[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_pt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
rc[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
rc[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_pt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
rc[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_py									
am5p[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0001	0.0001						
cpd_py	1.00E-	159414	059414	1.00E-		0.0199	1.00E-		0.0199
dx5p[c]	05	127	127	05	0.02	9	05	0.02	9
cpd_py	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_py	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_py	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199	1.00E-	0.00	0.0199
r[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpa_qu	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
IN[C]	05	0.02	9	05	0.02	9	05	0.02	9
and rit	1.005	0.0005	0.0004	1 005	0.0005	0.0005	1.005	0.0006	0.0006
cpu_ri	1.00E-	000101	980181	1.00E-	844849	744849	1.00E-	207858	10/858
p[c]	0.0002	000	0.0106	0.0002	994	994	0.0002	740	740
and rE	0.0003		0.0190	0.0003		0.0190	0.0003		0.0190
cpu_rs	50007	0.02	005152	421015	0.02	576164	70	0.02	770277
cnd rh	1 00F-	0.02	4 0 0100	1 00F-	0.02	0 0100	1 00F-	0.02	0 0100
15bp[c]	1.000	0.02	0.0155 Q	1.000	0.02	0.0199 Q	1.000	0.02	0.0195 Q
cnd rh	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199
cvs[c]	1.002	0.02	9	1.002	0.02	9	1.002	0.02	9
cnd rib	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199	1 00F-	0.02	0 0199
-d[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd rih							1.00E-		0.0199
-d[e]	NA	NA	NA	NA	NA	NA	05	0.02	9
cpd rib	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
flv[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_rn									
a_macr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
o[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0139	0.0139		0.0141	0.0141		0.0142	0.0142
cpd_ru	1.00E-	531201	431201	1.00E-	462151	362151	1.00E-	300138	200138
5p-D[c]	05	8	8	05	2	2	05	5	5
	0.0004		0.0195	0.0004		0.0195	0.0004		0.0195
cpd_s7	971272		028727	282582		717417	016753		983246
p[c]	889	0.02	1	087	0.02	9	093	0.02	9
cpd_sb	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
zcoa[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_sel	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_sel	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
np[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_se	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_se	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_se	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_se	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
rtrna[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_sh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cl[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_sh	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
eme[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_sk	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
m[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_sk	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
m5p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_sl2	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
6da[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0002	0.0002		0.0003	0.0003		0.0004	0.0004
cpd_sl2	1.00E-	332534	232534	1.00E-	695239	595239	1.00E-	503085	403085
a6o[c]	05	765	765	05	856	856	05	914	914
cpd_slc	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ys[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_so	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
3[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_so	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
3[e]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_so	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
3[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_so	1.00E-	0.5662	0.5662	1.00E-	0.5662	0.5662	1.00E-	0.5662	0.5662
4[c]	05	37304	27304	05	37304	27304	05	37304	27304
cpd_so	1.00E-	0.5662	0.5662	1.00E-	0.5662	0.5662	1.00E-	0.5662	0.5662
4[e]	05	37304	27304	05	37304	27304	05	37304	27304
cpd_so	1.00E-	0.5662	0.5662	1.00E-	0.5662	0.5662	1.00E-	0.5662	0.5662
4[p]	05	370583	270583	05	370677	270677	05	370717	270717
cpd_sp	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
md[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_sp							1.00E-		0.0199
rm[c]	NA	NA	NA	NA	NA	NA	05	0.02	9
cpd_sr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ch[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ss									
altpp[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c6p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
carg[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cbz[c]	05	0.02	9	05	0.02	9	05	0.02	9
						0.0199			0.0199
cpd_su	1.00E-		0.0199	4.67E-		532595	2.91E-		709130
cc[c]	05	0.02	9	05	0.02	2	05	0.02	3
								0.0199	0.0199
cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-	999917	899917
cc[e]	05	0.02	9	05	0.02	9	05	9	9
cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cc[b]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0008		0.0191	0.0005		0.0194	0.0004		0.0195
cpd_su	574363		425636	412368		587631	441398		558601
ccoa[c]	093	0.02	9	555	0.02	4	716	0.02	3
cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cglu[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cgsa[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_su									
chms[c	1.00E-	_	0.0199	1.00E-	-	0.0199	1.00E-	_	0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
corn[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cr[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cr[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_su	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
csal[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tc	1.00E-		0.0199				1.00E-		0.0199
ynt[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
bpt[c]	05	0.02	9	05	0.02	9	05	0.02	9
	0.0008		0.0191	0.0005		0.0194	0.0004		0.0195
cpd_th	574363		425636	412368		587631	441398		558601
dp[c]	093	0.02	9	555	0.02	4	716	0.02	3
		0.0023	0.0022		0.0122	0.0122			
cpd_th	1.00E-	006036	906036	1.00E-	719098	619098	1.00E-		0.0199
f[c]	05	54	54	05	4	4	05	0.02	9
cpd_th	1.00E-		0.0199						
glu[c]	05	0.02	9	NA	NA	NA	NA	NA	NA
cpd_th									
mmp[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mpp[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0017	0.0017						
cpd_th	1.00E-	682052	582052	1.00E-		0.0199	1.00E-		0.0199
r-L[c]	05	54	54	05	0.02	9	05	0.02	9
cpd_th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r-LA[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
rtrna[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ym[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ym[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ymd[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ymd[e]	05	0.02	9	05	0.02	9	05	0.02	9

cpd th	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ymd[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_t	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ma[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_t	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ma[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_t	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mao[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_t	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mao[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tr									
ace_m	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
acro[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dox[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
drd[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tr									
ehalos	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
e[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tr	1.005		0.0100	1 005		0.0100	1 005		0.0100
enaios	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199	1.00E-	0.02	0.0199
e[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpu_ti ebalos	1 00F-		0 0100	1 00F-		0 0100	1 00F-		0 0100
enaios e6n[c]	1.000	0.02	0.01 <i>99</i>	1.001-	0.02	0.0199 Q	1.000	0.02	0.0199 Q
cod tr	05	0.02	5	05	0.02	5	05	0.02	J
naala[c	1 00F-		0 0199	1 00F-		0 0199	1 00F-		0 0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd tr		0.01			0.01			0.01	-
naarg[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
1	05	0.02	9	05	0.02	9	05	0.02	9
cpd tr									
naasn[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tr									
naasp[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tr									
nacys[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_tr nagln[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr naglu[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr nagly[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr nahis[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr naile[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr naleu[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr nalys[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr namet[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr naphe[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr napro[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr naser[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr nathr[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr natrp[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9
cpd_tr natyr[c]	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9	1.00E- 05	0.02	0.0199 9

cpd_tr									
naval[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
								0.0199	0.0199
cpd_tr	1.00E-		0.0199	1.00E-		0.0199	1.00E-	999917	899917
p-L[e]	05	0.02	9	05	0.02	9	05	9	9
cpd_tr	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tr									
ptrna[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ts	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ul[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ts	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ul[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ts	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ul[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dcan[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_tt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dcan[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ttt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
nt[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ttt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
nt[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ty	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
								0.0199	0.0199
cpd_ty	1.00E-		0.0199	1.00E-		0.0199	1.00E-	999917	899917
r-L[e]	05	0.02	9	05	0.02	9	05	9	9
cpd_ty	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
r-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ty	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
rtrna[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_u2	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
3ga[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_u3	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
aga[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_u3	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
hga[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_ua									
agmda[1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ua	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ccg[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ua									
cgam[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ua									
gmda[c	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ua	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ma[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ua	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mag[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ua	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mr[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ub	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
q8[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ub	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
	05	0.02	9	05	0.02	9	05	0.02	9
cpd ud	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cpdp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd ud	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
cpp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ud	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
			0.0199			0.0199			
cpd_ud	4.24E-		576066	4.01E-		598809	3.92E-		0.0199
pg[c]	05	0.02	6	05	0.02	3	05	0.02	608204
		0.0047	0.0047		0.0049	0.0049		0.0051	0.0050
cpd_ud	1.00E-	177223	077223	1.00E-	851609	751609	1.00E-	046974	946974
pgal[c]	05	21	21	05	81	81	05	57	57
cpd_ug	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
md[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ug	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mda[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_u	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
mp[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_up	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
pg3[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ur	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_ur	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ur	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
a[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ur	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ate[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ur	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
can[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ur									
dglyc[c	1.00E-		0.0199						
]	05	0.02	9	NA	NA	NA	NA	NA	NA
cpd_ur	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
dio[e]	05	0.02	9	05	0.02	9	05	0.02	9
			0.0199			0.0199			0.0199
cpd_ur	1.00E-		899999	1.00E-		899999	1.00E-		899999
ea[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0199	0.0199					0.0199	0.0199
cpd_ur	1.00E-	999826	899826	1.00E-	0.0199	0.0199	1.00E-	999835	899835
ea[e]	05	4	4	05	999833	899833	05	9	9
		0.0199	0.0199		0.0199	0.0199		0.0199	0.0199
cpd_ur	1.00E-	999913	899913	1.00E-	999916	899916	1.00E-	999917	899917
ea[p]	05	2	2	05	5	5	05	9	9
cpd_uri	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_uri	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_uri	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ur	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
nyl[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_ut	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
p[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_va	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
I-L[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_va	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
l-L[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_va	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
l-L[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_va	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
ltrna[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_w	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
o4[c]	05	0.02	9	05	0.02	9	05	0.02	9

cpd_w	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
o4[p]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_xa	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n[c]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_xa	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n[e]	05	0.02	9	05	0.02	9	05	0.02	9
cpd_xa	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
n[p]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0010	0.0010		0.0027	0.0026		0.0041	0.0041
cpd_x	1.00E-	191623	091623	1.00E-	034852	934852	1.00E-	114504	014504
mp[c]	05	56	56	05	66	66	05	91	91
cpd_xt	1.00E-		0.0199				1.00E-		0.0199
p[c]	05	0.02	9	NA	NA	NA	05	0.02	9
cpd_xt	1.00E-		0.0199	1.00E-		0.0199	1.00E-		0.0199
sn[c]	05	0.02	9	05	0.02	9	05	0.02	9
		0.0036	0.0036		0.0045	0.0045		0.0046	0.0046
cpd_xu	1.00E-	207330	107330	1.00E-	309870	209870	1.00E-	471986	371986
5p-D[c]	05	68	68	05	46	46	05	5	5

Reacti	Lower Bound	Upper Bound	Rango	Lower Bound	Upper Bound	Rango	Lower Bound	Upper Bound	Range
on ID	4	4	4	15	15	15	20	20	20
2MAH	-	-	-						
MP	NA	NA	NA	NA	NA	NA	NA	NA	NA
4HBASi									
nk	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-					-	-	
	64.418	22.130	42.287				66.961	20.628	46.332
4HBTE	5	6	9	NA	NA	NA	3	7	6
	-			-			-		
	40.863	-1.00E-	40.863	42.611	-1.00E-	42.611	43.406	-1.00E-	43.406
5DOAN	33653	06	33553	4697	06	4687	07569	06	07469
5DRIB_									
Sink	NA	NA	NA	NA	NA	NA	NA	NA	NA
5HPUD		N1 A					N1 A		
ICDCr	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-	E2 E4E						
	100.48	47.943	32.343	ΝΑ	ΝΑ	ΝΑ	ΝΑ	ΝΑ	ΝΑ
ICDCS	9257	74791	46900	INA	INA	INA	INA	INA	INA
	- 19 191		19 191	19 886		19 886	20 202		20 202
ASPISO	4	0	4	15.000	0	15.000	20.202	0	20.202
			•				-		
AACPS	12.652	43.596	56.249				15.686	43.969	59.655
10	84383	93911	78294	NA	NA	NA	31977	36233	6821
	-						-		
AACPS	20.170	36.079	56.249				23.203	36.451	59.655
11	25009	53285	78294	NA	NA	NA	72603	95607	6821
	-						-		
AACPS	27.687	28.562	56.249				30.721	28.934	59.655
12	65635	12659	78294	NA	NA	NA	13229	54981	6821
	-						-		
AACPS	35.205	21.044	56.249				38.238	21.417	59.655
13	06261	72033	78294	NA	NA	NA	53855	14355	6821
	-	-					-	-	
AACPS	90.647	34.398	56.249				93.681	34.025	59.655
14	93863	15569	78294	NA	NA	NA	41457	73246	6821
	-	-	FC 343				-	-	
AACPS	105.67	49.427	56.249				108./1	49.054	59.655
12	/1/05	38/59	78294	NA	INA	INA	06465	96437	68211

Data S2 Table B Reaction Gibbs Free Energy Ranges from TMFA simulations.

							-		
AACPS	2.6879	58.937	56.249				0.3455	59.310	59.655
16	52891	73583	78294	NA	NA	NA	230499	15906	6821
	_						_		
ΔΔCPS	27 381	28 868	56 249				30 415	29 240	59 655
2	67215	1100	79204	ΝΑ	ΝΑ	ΝΑ	1/200	52/02	6921
3	07215	1108	70294	INA	INA	INA	14009	5540Z	0021
	-	-					-	-	
AACPS	98.160	41.911	56.249				101.19	41.538	59.655
4	8145	03156	78294	NA	NA	NA	42904	60833	6821
	-	-					-	-	
AACPS	113.19	56.945	56.249				116.22	56.573	59.655
5	5627	84408	78294	NA	NA	NA	9103	42085	68211
	-						-		
AACPS	19.864	36.385	56.249				22.897	36.757	59.655
6	26589	51705	78294	NA	NA	NA	74183	94028	6821
		0						0.010	
	2/ 200	21 250	56 2/0				27 022	21 722	50 655
AACF3	07041	21.330	70204				57.952	12776	29.000
/	07841	70454	78294	NA	NA	INA	55455	12776	0821
	-						-		
AACPS	42.416	13.833	56.249				45.449	14.205	59.655
8	48467	29828	78294	NA	NA	NA	96061	7215	6821
	-						-		
AACPS	5.1354	51.114	56.249				8.1689	51.486	59.655
9	37573	34537	78294	NA	NA	NA	13513	76859	6821
AACPS									
FA130	154.02	210.27	56.249				150.99	210.65	59.655
OH	87383	85213	78294	NA	NA	NA	52624	09445	68211
		00210	70231				52021	-	00211
	105 67	10 120	56 240				100 71		
	105.07	49.420	70204				100.71	49.055	CO211
FA1/18	80387	2558	78294	NA	NA	NA	15147	83258	68211
	-	-					-	-	
AACPS	113.19	56.946	56.249				116.23	56.574	59.655
FA1817	67377	95474	78294	NA	NA	NA	02136	53152	6821
	-			-			-		
	4.2936	43.062	47.356	13.356	44.452	57.809	14.926	45.084	60.011
ABTA	37385	55138	18876	3189	89452	21342	93368	86867	80235
	_			_			_		
ACACC	51,783		59,803	45.348		54,758	46.841	10.042	56.883
B	<u>בבר כס</u> כ	8.0199	22.203	6	9,4102	8	3	20.0.12	5
		0.0100	2	0	5.7102	0		2	5
	- 27 0 / F	12 215	70.060	20.225	24 725	62 071	20 067	26 401	66 260
	27.845	42.215	/0.060	29.235	34./35	22540	29.80/	30.401	100.209
1	0954	55634	651/4	44154	89364	33518	41569	/82/4	19843

	-			-			-		
ACACT	51.868	7.9345	59.803	45.433	9.3248	54.758	46.926	9.9568	56.883
10R	59757	47476	14504	94789	90615	8385	62445	6477	48922
	-			-			-		
	13.850	24.246	38.097	14.263	22.412	36.675	14.450	24.154	38.605
ACALDi	96249	85889	82138	30693	35735	66429	73623	92457	6608
ACBIPG									
т	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
ACCOA	653.38	580.54	72.847	641.15	576.87	64.277	642.56	575.20	67.351
С	80696	06005	46909	33464	56429	70358	13294	97538	57562
	-			-			-		
ACGA	41.915	-1.00E-	41.915	41.844	-1.00E-	41.844	43.753	-1.00E-	43.753
MK	56521	06	56421	25091	06	24991	46183	06	46083
	-			-			-		
ACGAt	19.626	-1.00E-	19.626	20.405	-1.00E-	20.405	20.759	-1.00E-	20.759
2	66603	06	66503	64257	06	64157	72282	06	72182
	-			-			-		
	11.824	-1.00E-	11.824	11.879	-1.00E-	11.879	13.846	-1.00E-	13.846
ACGK	24835	06	24735	72326	06	72226	56564	06	56464
	-	-		-	-		-	-	
	51.955	12.048	39.906	52.706	5.3543	47.352	54.989	3.8616	51.127
ACGS	67528	87005	80523	32176	17363	0044	15122	40799	51042
	-	-		-	-		-	-	
	72.587	2.5266	70.060	73.977	1.1362	72.841	74.609	0.5042	74.105
ACHBS	25492	02184	65274	59806	59044	33902	57422	848902	28933
	-			-			-		
	25.532		25.532	25.395		25.395	26.224		26.224
ACKr	4	0	4	9	0	9	2	0	2
	-	-		-	-		-	-	
	77.578	7.5178	70.060	78.968	6.1274	72.841	79.600	5.4955	74.105
ACLS	48499	32244	65274	82812	89105	33902	80428	14951	28933
	-			-			-		
ACMAT	49.302	32.619	81.921	51.746	30.492	82.238	52.856	33.719	86.576
1	82406	01665	84072	12881	58054	70935	72387	36275	08662
	-	-		-	-		-	-	
ACNA	100.41	37.328	63.087	83.155	34.189	48.965	84.089	32.763	51.326
MS	58672	31131	55592	57086	835	73586	57319	25485	31833
ACOAD	21.335	66.781	45.446				17.320	59.567	42.247
10	2	3	1	18.575	58.304	39.729	4	9	5
ACOAD							17.320	59.567	42.247
8	NA	NA	NA	NA	NA	NA	35	93237	58237

ACOAD	30.538	75.984	45.446				26.523		42.247
9	2	3	1	27.778	67.507	39.729	4	68.771	6
	-			-			-		
ACOAT	39.069	20.733	59.803	40.459	14.299	54.758	41.091		56.883
А	2	9	1	5	3	8	5	15.792	5
	_			_			_		
	51.697	-1.00E-	51.697	53.446	-1.00E-	53.446	54.240	-1.00E-	54.240
ACODA	86893	06	86793	00561	06	00461	6116	06	6106
				_			_		
				10.302		10.302	10.618		10.618
ACONT	-9.6076	0	9.6076	7	0	7	7	0	7
		28.135	28.135		29.525	29.525		30.157	30.157
АСОТА	0	6	6	0	9	9	0	9	9
ACPS1	NA	NA	NA	NA	NA	NA	NA	NA	NA
	ΝΛ	ΝΛ	ΝΛ	ΝΛ	ΝΛ		ΝΛ	ΝΛ	ΝΛ
ACFJU			INA					INA	
	52 915	6 8 2 2 0	15 002	26.006	7 7012	20 201	28 261	6 4506	21 21/
100	22/012	64605	43.992	07/0	10202	29.204	6615	20202	07217
ACS	55465	17 515	27024	0749	42505	10 505	0013	20.662	20 662
A C+C		17.515	17.515		19.595	19.595		20.003	20.003
ACI6	0	Z	2	0	/	/	0	3	3
	-	-	20 705	-	-	20.020	-	42.025	24 622
	43.082	13.296	29.785	41.616	12.979	28.636	44.469	12.835	31.633
ADA	49921	83876	66046	/0135	96257	/38/8	86163	92793	9337
	-	-	45 6 40	-	-		-	-	40.070
	145.95	100.31	45.643	148.18	100.72	47.455	149.19	100.91	48.279
ADCL	6/335	27801	95344	13966	58484	54821	2607	36067	00037
ADCOB									
AK	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
	46.528	-1.00E-	46.528	52.031	-1.00E-	52.031	52.663	-1.00E-	52.663
ADCS	31671	06	31571	74103	06	74003	71518	06	71418
	-			-			-		
ADHM	8.5662	-1.00E-	8.5662	10.314	-1.00E-	10.314	11.108	-1.00E-	11.108
CYSSYN	05888	06	04888	33906	06	33806	94505	06	94405
	-			-					
	19.519		19.519	17.129		17.129			
ADK1	8	0	8	5	0	5	-20.351	0	20.351
	-			-					
	19.519	25.373	44.892	17.129	26.415	43.545		26.889	47.240
ADK3	8	1	9	5	8	3	-20.351	8	8
	-			-			-		
	17.278	27.719	44.998	16.223	28.762	44.985	18.109	29.236	
ADK4	6	6	2	1	3	4	7	3	47.346

	-	-		-	-		-	-	
ADMD	424.00	378.43	45.572	417.82	378.09		420.19	377.94	42.247
С	64	4	4	56	66	39.729	08	33	5
	-	-		-	-		-	-	
ADNCY	73.871	52.652	21.219	75.619	55.755	19.864	76.414	55.290	21.123
С	52105	06548	45557	65423	15105	50318	26022	46903	79119
	-	-		_	-		-	-	
	35.223	14.837	20.386	33.135	13.920	19.214	35.816	12.613	23.202
ADNK1	40813	26695	14118	57425	80991	76434	78209	896	88609
	-			-			-		
	22.821	8.5662	31.387	23.726	10.101	33.828	24.138	11.647	35.786
ADNt2	17884	03888	38273	94459	51943	46402	6563	7548	4111
	-	-		-	-		-	-	
	51.417	12.682	38.734	52.807	13.650	39.156	53.439	12.309	41.129
ADPT	0126	39334	61926	35574	57404	7817	32989	97012	35977
	_	_		_	_		-	_	
	82.502	36.067	46.434	82.557	36.204	46.353	84.524	35.376	49.148
ADSK	44394	93363	51031	91885	43819	48066	76123	14319	61804
ADSL1r	-0.4158	0	0.4158	-2.1639	0	2.1639	-2.9585	0	2.9585
ADSI 2r	-7 8843	0	7 8843	-9 6324	0	9 6324	-10 427	0	10 427
TIDGEZI	-	0	7.0045	-	0	5.0524	-	0	10.427
	63 595	-1 00F-	63 595	52 413	-1 00F-	52 413	54 300	-1 00F-	54 300
	68227	1.001	68127	92075	1.001	91975	5226	1.001	5216
11000		00	00127	-	00	51575	5220	00	5210
	44 501	-1 00F-	44 501	46 250	-1 00F-	46 250	47 044	-1 00F-	47 044
AGDC	94915	1.001	94815	08533	1.001	08433	69132	1.001	69032
NODE			54015	-		00433	-		05052
ΔGMΔ	95 407	42 861	52 545	97 155	42 524	54 631	97 950	42 371	55 578
HYD	28602	79696	48906	4192	41543	00376	02519	06019	965
	20002	67 104	62 653	7172	/1 729	10 585	02313	12 553	12 553
AGPR	4 4515	+100.00 و	02.055 4	1 1443	91.723 9	-0.505 6	0	42.555 3	42.555
				1.1-1-5					5
	17 029	-1 00F-	17 029	37 53/	-1 00F-	37 53/	38 989	-1 00F-	38 989
ΔΗΔΙ	09992	1.001	09892	50923	1.001	50823	9068	1.001	9058
			05052			50025	-		5050
ΔΗΟΥς	60 699	17 103	13 596	62 117	15 712	16 735	63 242	15 080	18 161
	71182	17956	53226	02.447 8/15	83642	00857	15098	86227	58872
145	, 1102	1,220	55220	U+J	03042	00057	-3030	00227	50072
	12 521		12 521	- 17 0/0		17 0/0	- 19 020		19 020
AICART	12.551	0	۵.21	17.040 2	0	17.040 2	15.009 A	0	15.005 A
	9	0	9	2	0	2	4	0	+
	6/2 01	570.06	77 017	-	566 10	64 277	632 00	561 72	67 251
	16001	71212	12.041	030.07	200.40 21727	70250	79602	504.75	57567
AINUZ	40004	1212	40909	30//3	21/3/	10558	10002	02040	57502
	13.596	48.626	35.030	12.901	49.321	36.420	12.585	49.637	37.052
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AIRC3	4	8	4	3	9	6	3	9	6
	-			-			-		
	34.848	12.666	47.514	43.252	4.8840	48.136	44.822	6.4640	51.286
AKGD	26271	19995	46266	14516	83984	22914	76194	19369	78131
	-	_		-			-		
ALAAL	84.367	11.816	72.551	72.133		63.981	73.541		67.055
А	9	5	4	2	-8.1515	7	2	-6.4856	6
ALAD_	6.2076	48.259	42.051	3.0691	42.650	39.580	1.6425	43.742	42.099
L	24801	41945	79465	48485	13357	98509	68342	12943	56109
				-			-		
ALAGL				38.616		38.616	39.248		39.248
YX	-31.636	0	31.636	2	0	2	2	0	2
	-			-			-		
	17.367		17.367	18.062		18.062	18.378		18.378
ALAR	1	0	1	3	0	3	3	0	3
	-			-			-		
ALATA	17.197	40.846	58.044	30.456	42.236	72.693	31.088	42.868	73.957
_D2	87684	41017	28701	56644	75331	31974	54059	72746	26805
	-			-			-		
ALATA	11.832		43.961	20.895	36.765	57.661	22.466	37.397	59.863
_L	8	32.129	8	5	7	2	1	7	8
	-			-			-		
ALATA	17.197	37.600	54.797	30.456	42.236	72.693	31.088	42.868	73.957
_L2	87784	11214	98998	56743	75231	31974	54159	72646	26805
ALATRS	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
ALA_Dt	28.127	-1.00E-	28.127	23.726	-1.00E-	23.726	50.379	20.515	70.894
4	19299	06	19199	94359	06	94259	49806	244	74206
	-			-			-		
	27.979	35.030	63.009	23.578	36.420	59.999	50.231	20.663	70.894
ALAt4	17171	32637	49808	92231	66951	59182	47678	26627	74306
		46.745	39.856		38.268			39.532	42.247
ALCD2x	6.8892	5	3	-1.4608	2	39.729	-2.7155	1	6
	-	-		-	-				
ALDD2	74.179	34.323	39.856	76.670	37.210	39.460			
х	43208	14651	28557	76265	60965	153	NA	NA	NA
	-			-			-		
ALLNR	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
AC	2	2	4	3	3	6	3	3	6
		49.252	52.545						
ALLTC	-3.2926	9	5	NA	NA	NA	NA	NA	NA

	-			-			-		
	36.897		35.030	37.592		36.420	37.908		37.052
ALLTN	3	-1.867	3	5	-1.1718	7	5	-0.8559	6
	-			-			-		
	37.280	15.116	52.397	39.028	15.454	54.482	39.823	15.607	55.430
AMAA	47944	99034	46978	61262	37187	98449	21861	72711	94572
	-			-			-		
AMALT	13.137	56.923	70.060	14.527	58.313	72.841	15.159	58.945	74.105
1	13199	52275	65474	47513	86589	34102	44928	84005	28933
	-	-		-	-		-	-	
AMALT	84.243	14.183	70.060	85.634	12.792	72.841	86.265	12.160	74.105
2	66906	01432	65474	0122	67118	34102	98636	69703	28933
	-			-			-		
AMALT	39.053	31.006	70.060	40.444	32.397	72.841	41.076	33.029	74.105
3	85832	79642	65474	20146	13956	34102	17561	11372	28933
	-			-			-		
AMALT	58.326	11.733	70.060	59.717	13.124	72.841	60.349	13.756	74.105
4	93936	71538	65474	2825	05852	34102	25665	03268	28933
	-			-			-		
AMAO	28.694		28.694	22.155		22.155	24.358		24.358
Т	3	0	3	7	0	7	3	0	3
	-			-			-		
AMMQ	41.705	-1.00E-	41.705	36.220	-1.00E-	36.220	38.901	-1.00E-	38.901
T7_2	78185	06	78085	18602	06	18502	39387	06	39287
AMOB									
_Sink	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-	~~ ~~~	-	-		-	-	
AMPM	248.85	168.38	80.476	253.72	177.57	76.149	255.93	176.63	79.300
52	89507	25104	44033	50509	5378	67288	69164	66934	22304
	-	~~~~					-		
AMPTA	23.630	23.325	46.955				31.762	22.04.6	55.578
SECG	4	3	/	NA	NA	NA	9	23.816	9
AMPIA	7 60 45	39.261	46.955				45 007	39.751	55.578
SEPG	-7.6945	2	/	NA	NA	NA	-15.827	9	9
	-	-	56 9 49	-	-		-	-	50 470
ANDDT	92.482	36.232	56.249	93.872	37.587	56.285	94.504	36.327	58.176
ANPRI	03845	25551	78294	38159	2079	1/369	35574	91989	43585
	-	-	04 447	-	-	00 450	-	-	00 740
4.116.1	162.96	81.548	81.417	169.52	81.070	88.452	1/0.63	80.916	89./16
ANS1	63216	81394	50767	2/0/5	297	41054	33006	941/6	35885
	-		40.000	-			-		
	48.006	_	48.006	50.449	_	50.449	51.560	_	51.560
AOXS	4	0	4	7	0	7	3	0	3

	-			-			-		
APRAU	39.390	-1.00E-	39.390	29.877	-1.00E-	29.877	33.391	-1.00E-	33.391
R	05795	06	05695	80661	06	80561	75847	06	75747
							-		
ARBAB							79.710		48.825
С	NA	NA	NA	NA	NA	NA	3	-30.885	3
	_			_			_		
	42.658	-1.00E-	42.658	44.406	-1.00E-	44.406	45.201	-1.00E-	45.201
ARGDC	64024	06	63924	77342	06	77242	38141	06	38041
	_			_			_		
	33 794		33 794	35 542		35 542	36 337		36 337
ARGSI	55.754	0	55.754	55.542	0	55.542	20.337	0	50.557
ANGSE	5	0	5	0	0	0	2	0	Z
	- 	1 005	E2 227	EE /12	2 2 2 2 2 0	E2 070	56 260	0 1 1 6 2	EE 01/
ADCSS	33.327	-1.002-	22.527	74054	2.5525	00176	70177	160107	20105
ARGSS	22565	00	22405	74054	10//2	82170	/01//	109197	30403
ARGIR									
5	NA	NA	NA	NA	NA	NA	NA	NA	NA
		65.466	65.466		40.091	40.091			
ASAD	0	6	6	0	6	6	0	40.915	40.915
	-	-					-	-	
	42.552	4.7297	37.823				41.656	4.2688	37.388
ASNN	86739	35479	13191	NA	NA	NA	88717	24657	06252
	-	-		-	-		-	-	
	117.83	50.175	67.664	125.09	54.877	70.213	126.51	53.153	73.364
ASNS1	96286	47165	15699	11861	25023	93591	77663	28021	48607
ASNTR									
S	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
ASP1D	61.107	9.4738	51.634	62.855	9.7761	53.079	63.650	8.0716	55.578
С	86476	63049	00171	99794	78175	81976	60593	38932	967
	_			_			_		
	55.594	-1.00E-	55.594	47.518	-1.00E-	47.518	49.022	-1.00E-	49.022
ASPCT	52319	06	52219	42489	06	42389	13162	06	13062
	_			_					
	16.603		16.603	16.659		16.659			
ASPK	7	0	7	2	0	2	-18.626	0	18.626
	-	-	,	-	-	<u> </u>		-	_3.320
	165 68	102.96	62 722	157 71	102 21	55 199	159 39	100.03	59 262
	87270	47922	94566	40712	<u>102.21</u> <u>11158</u>	9255	22221	09876	32/170
731 03	51515	77 723	54500	-0713	-1-1-0	5255	55524	0,070	54473
	20 022	12 01	52 040	- רסד דב	12 766	51 540	20 005	15 040	55 025
	33.033	12.012	75706	057502	13./00	2015	33.303	10.949 60506	05150
ASPUS	32003	00042	75700	03/39	44091	5045	44052	00200	02128

	24.120	63.886	39.765	23.697	84.559	60.862	23.480	86.742	63.262
ASPO6	94053	59779	65726	33573	42278	08706	43609	58094	14485
	12.021	81.170	69.149	10.631	81.921	71.290	9.9993	84.104	74.105
ASPO8	67906	84646	1674	33592	49294	15702	61763	65109	28933
	-			-			-		
	50.078	19.071	69.149	51.468	19.821	71.290	52.100	22.004	74.105
ASPO9	12517	04223	1674	46831	68871	15702	44246	84687	28933
ASPTA		37.042	37.042		37.793	37.793		39.976	39.976
1	0	9	9	0	5	5	0	7	7
	-			-			-		
ASPTA	33.815	13.540	47.356	42.878	14.931	57.809	44.448		60.011
4	5	7	2	2	1	3	8	15.563	8
ASPTRS	NA								
	-			-			-		
	21.909	17.515	39.424	22.175	19.595	41.771	24.138	20.663	44.801
ASPt2	6915	16269	85418	76059	65182	41241	6563	26827	92457
	-	_		-	_		_	_	
	44.939	2.6513	42.287	46.329	1.2610	45.068	46.961	0.6290	46.332
AST	34752	66163	98136	69066	23024	66764	66481	488694	61594
ATPM	NA								
	-	-		-	-		-	-	
ATPPR	130.02	91.291	38.734	131.41	93.341	38.074	132.04	92.398	39.650
Т	62654	64615	61926	66085	77011	83844	85827	46918	11352
	36.281	72.501		33.732	60.776	27.044	32.574	62.399	29.825
ATPS4r	4	4	36.22	8	9	1	4	9	5
	-	-		-	-		-	-	
	45.943	17.470	28.472	38.014	14.332	23.682	39.585	12.905	26.679
BPNT	71061	72872	98189	81004	25241	55763	42481	67226	75255
	-	-		-	-		-	-	
	282.03	190.96	91.069	277.09	190.06	87.037	280.03	189.65	90.379
BTS4	41	46	5	91	14	7	06	08	8
	-			-			-		
BUTSU	40.539	19.263	59.803	38.235	21.348	59.584	39.959	22.296	62.256
CCCOA	8	3	1	7	9	6	7	8	5
Biomas									
s_WP2	NA								
	-	-		-	-		-	-	
C120S	572.46	278.89	293.57	517.49	270.19	247.30	532.38	266.24	266.14
Ν	87948	55539	32409	62345	5705	05295	47584	12263	35321
	-	-		-	-		-	-	
C130IS	468.58	264.83	203.74	433.84	259.96	173.87	443.37	257.75	185.62
Ν	09223	34189	75034	20049	72179	4787	82789	53083	29705

	-	-		-	-		-	-	
C130O	231.97	32.901	199.07	204.01	30.140	173.87	212.41	26.789	185.62
HISN	495	21926	37307	57807	99368	4787	26442	67366	29705
	-	-		-	-		-	-	
C140IS	618.93	358.94	259.98	572.38	352.69	219.69	584.99	349.84	235.14
N	61751	96131	65621	58948	30689	28259	55977	91852	64125
	_	_		_	_		_		
C140S	719 83	373 01	346 82	656 04	362 92	293 11	674 00	358 33	315 66
N	47365	17481	29885	01244	15561	85683	20772	51032	69741
	47303	17401	25005		15501	05005	20772	51052	05741
C150IS	619 02	258 01	250.08	572 20	252 60	210 60	58/ 00	210 81	225 1/
	61751	06121	65621	572.30	20600	219.09	564.33	01050	6/175
	01/51	90131	05021	30940	50089	20259	55977	91052	04125
C1 F.O.C	-	452.00	216 22	-	-		-	-	204.00
C1505	/69.29	453.06	316.22	/10.92	445.41	265.51	/26.61	441.94	284.66
N	1428	58072	56207	97847	892	08647	29166	30621	98545
				-	-		-	-	
C151S				718.12	425.00	293.11	735.74	420.07	315.66
N	NA	NA	NA	48452	6277	85683	19956	50215	69741
	-	-		-	-		-	-	
C160IS	769.29	453.06	316.22	710.92	445.41	265.51	726.61	441.94	284.66
Ν	1428	58072	56207	97847	892	08647	29166	30621	98545
	-	-		-	-		-	-	
C160S	867.20	467.12	400.07	794.58	455.64	338.93	815.61	450.42	365.19
N	06783	79423	2736	40142	74071	66071	93961	898	0416
	-	-		-	-		-	-	
C161S	870.14	492.84	377.30	807.72	482.58	325.13	827.61	477.92	349.69
N	9404	86296	07743	25022	97469	27553	84736	66173	18562
	_	_		_	_		_	_	
C170IS	769.29	453.06	316.22	710.92	445.41	265.51	726.61	441.94	284.66
N	1428	58072	56207	97847	892	08647	29166	30621	98545
		_		_				_	
C170S	919 64	547 18	372 46	849 47	538 14	311 32	868 23	534 03	334 19
	66808	2001/	16791	36746	/1771	89035	02354	6939	3296/
1	00000	20014	40734	30740	4771	05055	02554	0555	52504
C171C				- 956.66	- 51772	220 02	- 077 25	- E12.16	265 10
				070.00	217.75	550.95	077.55	00004	0416
IN	NA	INA	NA	8/351	2128	11000	93145	88984	0416
C1 74 C	-	-	407.00	-	-	220.02	-	-	205 40
C1/1n8	932.36	525.35	407.00	856.66	51/./3	338.93	8//.35	512.16	365.19
SN	03192	83726	19466	85531	1946	66071	91325	8/164	0416
		-		-	-		-	-	
C180S		561.24	438.75	933.12	548.37	384.75	957.23	542.52	414.71
Ν	-1000	41365	58636	79041	32582	4646	67149	28569	3858

				-	-		-	-	
C181S				946.26	575.31	370.95	969.23	570.02	399.21
Ν	NA	NA	NA	63921	55979	07942	57924	04942	52982
		-		-	-		-	-	
C181n7		586.96	413.03	946.26	575.31	370.95	969.23	570.02	399.21
SN	-1000	46418	53582	62101	54159	07942	56104	03122	52982
	-	-		-	-		-	-	
C205S	670.61	214.87	455.74	612.34	209.37	402.96	633.82	200.58	433.24
Ν	94738	78036	16702	27944	78131	49812	79817	78014	01803
	-			-			-		
	30.203	50.371	80.574	12.266	51.761	64.028	15.656	52.393	68.049
C50SN	12763	12309	25072	90786	46623	37409	3239	44039	76429
	-			-			-		
	38.026	42.547	80.574	20.090	43.938	64.028	23.479	44.570	68.049
C60ISN	51809	73263	25072	29832	07577	37409	71437	04992	76429
	-			-			-		
	45.543	-1.00E-	45.543	27.607	-1.00E-	27.607	30.997	-1.00E-	30.997
C70ISN	92435	06	92335	70458	06	70358	12063	06	11963
	-	-		-	-		-	-	
	446.23	434.94	11.293	478.36	434.16	44.202	478.52	433.78	44.735
CAT	87709	51364	63447	66774	37416	9358	00326	42101	82252
	-	-		-	-		-	-	
CBL1ab	81.119	23.086	58.032	69.299	19.875	49.423	70.894	18.375	52.518
С	13149	9139	21759	43816	89392	54424	42533	43838	98695
CBLAT	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
	704.09	609.15	94.933	696.38	605.32	91.058	699.91	603.58	96.338
CBPS	02612	70175	24365	18842	33697	51455	93414	08014	53992
	-	-		-	-		-	-	
CDPG4	122.45	87.428	35.030	123.15	86.733	36.420	123.46	86.417	37.052
6D	85694	24206	32737	3741	07049	67051	97281	08341	64466
	-	4 995		-	4 00-		-	4 9 9 7	
CDPME	44.019	-1.00E-	44.019	44.074	-1.00E-	44.074	46.041	-1.00E-	46.041
К	37305	06	37205	84796	06	84696	69034	06	68934
	-	47.070	70.000						
CHOLD	22.182	47.878	/0.060				N1 A		
HI	4915	16325	654/4	NA	NA	NA	NA	NA	NA
CHOLD	4.4944	49.940	45.446						
HZ	41371	55434	11296	NA	NA	NA	NA	NA	NA
CHOLD	4.1887	61.991	57.802						
H3	86113	07516	28905	NA	NA	NA	NA	NA	NA

CHOLD	- 6.6439	63.416	70.060						
H4	24802	72994	65474	NA	NA	NA	NA	NA	NA
CHOLD H5	- 68.743 72903	1.3169 25715	70.060 65474	NA	NA	NA	NA	NA	NA
	-			-			-		
CHOLt4	31.093 01608	32.064 50328	63.157 51936	26.673 68676	33.473 92634	60.147 6131	54.549 36199	16.493 40235	71.042 76434
CHOD	-	-	24.004	-	-		-	-	26.002
м	13306	28.150	34.061	62.907 30463	64258	66205	03.223 29171	27.139	36.083 6362
	-		51051			00205	- 23171		0302
	97.364	52.760	44.603	89.435	50.675	38.759	91.005	49.727	41.278
CHORS	12163	73786	38377	22105	22315	99791	83583	26192	57391
	-	-		-	-		-	-	
	157.40	105.82	51.576	159.15	105.49	53.661	159.94	105.33	54.609
CHRPL	47494	82668	4826	28826	08853	99731	74886	75301	95854
	-	1.005	17 022	-	1 005	21 200	-	1 005	22.050
CKDUA S	101/	-1.00E-	100/	21.388 5/201	-1.00E-	21.388 5/201	15860	-1.00E-	15760
5	1914	00	1904	34391	00	54291	- 13809	00	13703
		17.515	17.515		18.210	18.210	18.526	18.526	37.052
CO2t	0	2	2	0	3	3	3	3	6
COBAL	7.7315	18.343	10.612	6.7456	20.549	13.803	6.2027	21.701	15.498
Tt3	89963	61827	02831	22384	47418	85179	83075	34239	55931
COBAL					13.803	13.803		15.498	15.498
Tt5	0	10.612	10.612	0	9	9	0	6	6
	-	-					-	-	
	56.412	10.966	45.446				60.427	18.179	42.247
LDD	47403	36107	11296	NA	NA	NA	28266	70029	58237
CPPPG	423.05	-	75 707	-	3/13 01	80 623	425.23	3/13 //	81 788
0	92931	18252	46797	58596	22572	60231	13821	29149	46718
CPPPG									
OAN	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
	64.368	12.472	51.895	65.758	18.907	46.851	66.390	17.414	48.975
CS	43256	88192	55063	77569	5316	24409	74985	85504	89481
	-	-	aa -a -	-	-		-	-	
COND	56.614	17.880	38.734	57.292	17.563	39.729	59.667	17.419	42.247
CZIND	95202	33276	01970	46294	45657	00637	00431	42194	58237

	-			-			-		
	22.821	17.515	40.336	23.726	19.595	43.322	24.138	20.663	
CSNt2	2	2	4	9	7	6	7	3	44.802
	-	-	02 4 00	-	-	70.400	-	-	04 477
CTDCO	91.018	8.9084	82.109	83.949	5.7801	/8.169	85.836	4.3582	81.477
CIPSZ	20164	59014	74262	5213	8695	33435	12316	45103	87805
	07 7/9	-	57 1 2 2	- 0E 73/	-	17 760	- גרר דס	-	50 462
CU2+	97.740	40.015	27.132	36008	78667	57/31	61224	26822	30.402
021	10072	94202	24005	30038	78007	57451	01224	20022	54402
СУСРО	430 79	343 22	87 575						
e	5873	00545	81843	NA	NA	NA	NA	NA	NA
-	-	-	01010	-	-		-	-	
	195.80	112.31	83.496	199.30	108.77	90.536	201.15	107.70	93.445
CYOO2	81391	20474	09166	68531	05277	32546	32329	77948	43807
	69.479	189.36	119.88	61.852	182.93	121.07	57.898	185.31	127.41
CYOR7	49492	93119	9817	70997	21936	94836	23121	03403	21091
	-	_		_	_		_	_	
	91.395	21.334	70.060	92.785	19.944	72.841	93.417	19.312	74.105
CYSS	03677	38503	65174	38291	04189	34102	35406	06774	28633
	-	_		-	_		_	_	
	50.513	3.2130	47.300	52.244	2.2009	50.043	55.097	1.7409	53.356
CYSTL	842	17857	82414	31453	70097	34443	47481	48388	52643
CYSTRS	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	_		-	_		-	_	
	56.267	14.227	42.040	59.071	20.746	38.325	60.601	18.952	41.649
CYTBD	9934	45085	54255	5359	11247	42343	92857	0797	84887
	-	-		-	-		-	-	
	49.463	10.728	38.734	50.140	10.411	39.729	52.515	10.267	42.247
CYTD	48694	86768	61926	99786	99149	00637	53923	95686	58237
	-			-			-		
	41.033	11.511	52.545	42.781	11.849	54.631	43.576	12.002	
CYTDH	7	8	5	9	2	1	5	5	55.579
	-	-		-	-		-	-	
CYTDK	54.112	15.662	38.450	54.167	15.103	39.064	56.134	13.959	42.175
1	28381	04553	23828	75872	37852	38019	6011	09545	50565
	-			-			-		
CYTDK	54.112	7.8588	61.971	54.167	9.9444	64.112	56.134	10.892	67.026
2	28281	95294	1781	75772	10003	16772	6001	37123	97133
0.75.1	-	40.00=		-	10.005		-	10.005	
CYTDK	51.871	10.205	62.076	53.261	12.290	65.552	53.893	13.238	67.132
3	00715	37605	3832	35029	89076	24105	32445	85199	17644

	-			-			-		
	22.821	17.515	40.336	23.726	19.595	43.322	24.138	20.663	44.801
CYTDt2	17884	16269	34152	94459	65182	59641	6563	26827	92457
	-			-					
	23.600		23.600	24.351		24.351			
CYTK1	5	0	5	2	0	2	-26.634	0	26.634
	_			_			_		
	33.553	12.881	46.434	33.608	12.744	46.353	35.575		49.148
СҮТК2	3	2	5	8	7	5	7	13.573	7
CampH	_	_			_		_		
vdrolva	30.256	12.325	17.930	30.951	10.577	20.374	31.267	9.7825	21.484
se	1652	24817	91703	33677	115	22178	32385	09008	81484
				-			-		01.01
	25,956		25.956	27,123		27,123	27.653		27.653
Clt	7	0		7	0	7	6	0	6
			-		-		-	-	
	48,475	9,7406	38,734	49,152	9.4237	39,729	51,527	9,2797	42,247
	2617	42445	61926	77262	66255	00637	314	31623	58237
Bridh		12113	01520	-	00233	00037	511	51025	56257
	28 759	17 675	46 434	28 814	17 538	46 353	30 781	18 367	49 148
рарк	20.755	17.073 3		20.014 6	27.550	ч0.555 Д	50.701	10.507	0+1.C+ 6
BRBR				-					0
	22 821	17 515	40 336	23 726	19 595	43 322	24 138	20 663	44 801
2	17884	16269	34152	94459	65182	59641	6563	26827	92457
-		-	51152	51135	03102	55011	-		52157
	48 608	2 1743	46 434				50 631	1 4825	49 148
DAGK	-+0.000 87555	65233	51031	NA	NA	NA	19284	74299	61854
Driek		-	51051	-	_		-	-	01001
	105 60	45 413	60 194	91 240	47 879	43 360	92 174	44 566	47 607
DAHPS	73943	00538	38889	26492	82919	43573	26675	64719	61956
D/ III S	-	-	30005			13373	-	-	01550
	94 489	41 944	52 545	96 238	41 607	54 631	97 032	41 453	55 578
	99734	50329	48906	12552	12176	00376	73351	76651	967
DAIDC	55254	50525	40500	12552	12170	00370		70051	507
				18 888		18 888	19 20/		19 20/
DΔPF	-18 193	0	18 193	10.000	0	10.000	15.204	0	15.204
	10.199		10.195			T			¥
		25 5 22	48 265	75 921	26 938		76 882	25 670	51 202
ΠΔςννι	-73 8/0	2J.J05 E	+0.205 E	, J. 334	20.330 E	18 006	70.00Z	20.079 2	21.202
DAJIN	73.049	J	J	J	J	-0.990	J	2	3
	12/ /0	- חפר כד	51 715	126.24	-	52 201	- 127 02	-	51 710
	124.49 607/9	72.700 21705	82681	120.24 120.24	2.442 82612	36053	127.05 88110	12.209 AQ11Q	22075
DB4PS	124.49 60748	21795	85681	42059	83642	36952	88119	48118	33075

	-			-			-		
	68.335		68.335	56.100		56.100	57.508		57.508
DBTSr	2	0	2	5	0	5	5	0	5
	-	-		-	-		-	-	
	47.654	8.9194	38.734	48.331	8.6026	39.729	50.706	8.4585	42.247
DCYTD	09604	76788	61926	60696	00597	00637	14834	65966	58237
	-			-			-		
	22.821	17.515	40.336	23.726	19.595	43.322	24.138	20.663	44.801
DCYTt2	17884	16269	34152	94459	65182	59641	6563	26827	92457
	-						-		
	34.300		46.434		11.997	46.353	36.322	12.825	49.148
DGK1	5	12.134	5	-34.356	5	5	8	8	6
	-	-		-	-		-	-	
	60.443	25.413	35.030	61.139	24.718	36.420	61.455	24.402	37.052
DHAD1	8502	52283	32737	02177	35126	67051	00884	36418	64466
	-	-		-	-		-	-	
	60.443	25.413	35.030	61.138	24.718	36.420	61.454	24.402	37.052
DHAD2	66364	33627	32737	83521	1647	67051	82229	17762	64466
	-	-		-			-		
DHDPR	47.649	0.1044	47.544	38.849	-1.00E-	38.849	40.621	-1.00E-	40.621
У	22158	422296	77935	80246	06	80146	1871	06	1861
	-	-		-	-		-	-	
	124.11	71.573	52.545	124.45	69.825	54.631	124.60	69.030	55.578
DHDPS	91145	62348	49106	64961	4903	00576	98513	88431	967
	-			-			-		
	60.352			50.857		49.054	52.313	-	52.313
DHFR	3	-7.5333	52.819	7	-1.8033	4	1	0	1
	-			-			-		
	67.401	-1.00E-	67.401	55.166	-1.00E-	55.166	56.574	-1.00E-	56.574
DHFS	23661	06	23561	51348	06	51248	49642	06	49542
	-	-		-	-		-	-	
	144.57	60.396	84.180	149.08	/2.935	/6.149	151.13	/1.834	/9.300
017	/3395	60932	/3022	56537	9/8/8	6/48/	48893	6623	22704
	-			-			-		
	44.795	-1.00E-	44.795	46.544	-1.00E-	46.544	47.338	-1.00E-	47.338
DHNPA	89825	06	89725	03142	06	03042	63741	06	63641
DUGGE	-	-		-	-		-	-	co 075
	191.80	127.00	64.798	183.90	125.40	58.508	185.62	124.67	60.953
2	0005	11376	86/39	91414	02021	93933	64949	25042	99072
DUCCC	-	F7 404	74 00 5	-	F0 705	74 200	-	F0 460	75 202
DHORD	14.089	57.134	/1.224	15.563	58.735	/4.299	16.233	59.463	/5.696
41	58799	50114	08913	/3424	43661	17084	80071	13454	93526

	-	-		-	-		-	-	
DHORD	76.189	4.9653	71.224	77.663	3.3643	74.299	78.333	2.6366	75.696
8	39221	0308	08913	53846	67619	17084	60494	69682	93526
DHORT		18.678	18.678		19.668	19.668			
S	0	6	6	0	2	2	0	20.118	20.118
	_								
DHPPD	4,4721	-1.00F-	4,4721	5,1496	-1.00F-	5,1496	7.5242	-1.00F-	7.5242
A2	68516	06	67516	79434	06	78434	20809	06	19809
	12 277	57 723	45 446					61 738	42 247
DHPRx	7	8	1	20.755	60.484	39,729	19,491	66	6
						001720		-	
	72 272	22 923	49 348	72 911	23 802	49 109	73 202	22 326	50 876
рнрсз	02075	77542	24533	91409	19796	71613	7747	30547	46922
DTH 35	02075	77542	24333		15750	71015	-	50547	40522
пнртр	17 515	17 515	35 030	18 210	18 210	36 / 20	18 526	18 526	37 052
F	17.515	17.515	33.030	10.210	10.210	50.420	10.520	10.520	57.052
	2	Z		5		0	5	5	0
	22 547		22 5/17	- 		22 2/12	22 550		22 550
	22.547	0	22.547	23.242 E	0	ZJ.Z4Z	23.330	0	23.336
DHQDI	3	0	5	5	0	5	4	0	4
	1 6 9 9 2	- 122.25	45 572	161.00	-	20 720	162 57	120.22	42 247
DUOC	108.93	123.35	45.572	101.00	121.27	39.729	102.57	120.32	42.247
DHQS	09128	85206	39223	20122	30059	00637	2627	50446	58237
	-	-	02.040	-	-	C 4 5 5 C	-	-	74.4.00
DKIVIPP	144.23	60.315	83.919	141.48	/6.933	64.556	145.41	/4.251	/1.163
D3	5107	97994	12/1	91848	17348	01133	56997	92162	//812
	-	-	56 9 49	-	-		-	-	50 470
DIAATT	129.29	/3.049	56.249	130.69	/4.404	56.285	131.32	/3.145	58.176
DMATT	96734	89049	78294	00166	84288	17369	19907	55488	43585
	-	-		-	-		-	-	
DMOC	68.691	12.441	56.249	70.081	13.796	56.285	70.713	12.537	58.176
T	57496	79202	78294	9181	74441	17369	89225	4564	43585
	-	-		-	-		-	-	
	88.308	42.862	45.446	79.831	40.102	39.729	81.095	38.847	42.247
DMPPS	40697	294	11296	11943	11307	00637	06774	48537	58237
	-			-			-		
DMQM	27.953	-1.00E-	27.953	21.438	-1.00E-	21.438	23.565	-1.00E-	23.565
Т	64537	06	64437	07805	06	07705	81607	06	81507
DMSO									
R3e	NA	NA	NA	NA	NA	NA	NA	NA	NA
DMSO									
R4e	NA	NA	NA	NA	NA	NA	NA	NA	NA

DNA_S									
YNTHE	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
DNMP	62.753	17.181	45.572	54.824	15.095	39.729	56.395	14.147	42.247
PA	84641	45418	39223	94584	93947	00637	56061	97824	58237
	-	-		-	-		-	-	
DNTPP	86.466	47.732	38.734	88.215	50.140	38.074	89.009	49.359	39.650
A	9899	37064	61926	12307	28464	83844	72906	61555	11352
	-			-			-		
DPCOA	34.328	-1.00E-	34.328	34.384	-1.00E-	34.384	36.350	-1.00E-	36.350
ĸ	26931	06	56831	04422	06	04322	8866	06	8856
	53 360	-1 OOF-	53 360	13 866	-1 00F-	13 866	-	-1 00F-	15 221
DPR	73539	1.001	73439	1447	1.001	1437	54227	1.000	54127
DIR	-	-	75155	-	-	1137	-	-	51127
	51.242	7.0895	44.152	51.983	5.6300	46.353	53.950	4.8017	49.148
DRBK	37905	71757	80729	53693	56266	48066	37931	60767	61854
	-			-			-		
	16.829	-1.00E-	16.829	9.2654	30.463	39.729	11.630	30.616	42.247
DRPA	48172	06	48072	39885	56648	00637	66065	92172	58237
	-			-			-		
	32.372		32.372	32.428		32.428	34.394		34.394
DTMPK	6	0	6	1	0	1	9	0	9
	-	-	16 121	-	-	46 252	-	-	40 1 40
	49.007	5.4526	40.434 50981	49.942	5.5695	40.555	6953	2.7010	49.140 61857
DOMINI	57801	00155	50501		72750	48010	-	70755	01054
		34.476	48.356	17.018	40.920	57.939	18.445	42.328	60.773
DURIPP	-13.88	6	6	5	8	3	1	8	9
	-			-			-		
	22.821	17.515	40.336	23.726	19.595	43.322	24.138	20.663	44.801
DURIt2	17884	16269	34152	94459	65182	59641	6563	26827	92457
	-	-		-	-		-	-	
DUTPD	103.16	64.731	38.429	104.90	67.487	37.421	105.70	66.864	38.839
Р	09062	60175	30449	90394	10153	93789	36454	42597	21943
	- 		E0 022	- 41 227		41 227	42 - 202		42 702
ופסצח	50.832 E	0	50.832 E	41.33/	0	41.33/	42.793	0	42.793
		0				9	-	-	3
	59.008	-1.00F-	59.008	68.330	10.391	57.939	68.962	8.1888	60.773
DXPS	15286	06	15186	73379	39417	33962	70995	05242	9047

	-	-		-	-		-	-	
	53.077	14.730	38.346	62.936	32.121	30.815	64.191	30.857	33.333
E4PD	1	3	8	6	2	4	2	3	9
ECOAH		32.139	35.030			36.420			37.052
2C	-2.8905	8	3	-3.5857	32.835	7	-3.9016	33.151	6
ECOAH			35.030		37.739	36.420		38.055	37.052
9	2.0136	37.044	4	1.3185	1	6	1.0025	1	6
	-			-			-		
	27.098	-1.00E-	27.098	13.944	25.784	39.729	16.309	25.938	42.247
EDA	09057	06	08957	22435	78201	00637	44512	13726	58237
EDTXS5	NA	NA	NA	NA	NA	NA	NA	NA	NA
EDTXS6	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
	21.495	13.534	35.030	12.545		12.545	14.273		14.273
ENO	5	9	4	1	0	1	7	0	7
	-	-		-	-		-	-	
	68.810	23.238	45.572	60.881	21.152	~~ ~~~	62.452	20.204	42.247
EPPP2	5	1	4	6	6	39.729	2	6	6
EX_cpd									
3[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
	NIA	ΝΑ	NIA	NIA	NIA				
_ac[e]	INA	INA	INA	INA	INA	INA	INA	INA	INA
_acga m[e]	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ
FX cpd				1177					
adn[e									
]	NA	NA	NA	NA	NA	NA	NA	NA	NA
, EX cpd									
akg[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX cpd									
_ala-									
D[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_ala-									
L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_asn-									
L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_asp-									
L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA

EX_cpd bgl[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_ca2[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_cbl1[e									
]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd _chitin[
e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_cl[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_co2[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_cobalt									
2[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_cobalt				N I A				N 1 A	N1 A
3[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
ej EV cod	INA	INA	INA	INA	INA	INA	INA	INA	INA
	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ
EX cpd									
cvtd[e									
]	NA	NA	NA	NA	NA	NA	NA	NA	NA
J EX cpd									
dad-									
2[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX cpd									
_damp									
[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
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EX_cpd									
_dcyt[e									
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EX_cpd									
_dgmp									
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EX_cpd									
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EX_cpd									
_dms[e									
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_dna[e									
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_dodca									
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_duri[e									
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EX_cpd									
_etoh[
e]	NA	NA	NA						
EX_cpd									
_fe2[e]	NA	NA	NA						
EX_cpd									
_te3[e]	NA	NA	NA						
EX_cpd									
_for[e]	NA	NA	NA						
EX_cpd									
_fum[e									
	NA	NA	NA						
EX_cpd									
_gal[e]	NA	NA	NA						
EX_cpd									
_galact									
anlej	NA	NA	NA						
EX_CDD									
_gic-									
D[e]	INA	NA	INA						

EX_cpd									
_gln-									
L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
_giu- [[e]	NΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ
EX cnd									
glv-									
asp-									
L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_gly-									
glu-L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_gly[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_glyc-									
K[e]	NA	NA	NA	NA	NA	NA	INA	NA	NA
	NΔ	ΝΔ	NΔ	NΔ	ΝΔ	NΔ	NΔ	NΔ	NΔ
EX cpd									
glyclt[
e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_h2o2[
e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_h2o[e									
	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									ΝΑ
_IIZS[E]	INA	NA	INA	INA	INA	INA	INA	INA	NA
h[e]	NΔ	ΝΔ	NΔ	NΔ	ΝΔ	NΔ	NΔ	NΔ	NΔ
EX cpd									147.1
hdcan									
_ [e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_hxan[
e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_ile-									
L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA

EX_cpd									
[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_ins[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_k[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd _lac-									
D[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd _lac-	NΔ	NΔ	NΔ	NΔ	NΔ	NΔ	NΔ	ΝΔ	ΝΔ
EX cpd		147.		1.17.1					147.1
_lami[e									
]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd _leu-									
L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd _lys- L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd _mal-									
L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd _malt[ΝΑ	ΝΔ	ΝΑ	NA	ΝΑ	ΝΑ	ΝΑ	NIA	NA
ej EV. cod	NA	NA	INA	INA	INA	INA	INA	INA	NA
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FX cnd		147.							147.1
malth									
_ x[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd _maltp									
t[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd _malttr									
[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd _malttt									
r[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA

EX_cpd									
_met-									
L[e]	NA	NA	NA						
_iiigz[e	NΔ	ΝΔ	NΔ	NΔ	NΔ	ΝΔ	NΔ	NΔ	NΔ
FX cnd									
mn2[
el	NA	NA	NA						
EX cpd									
_mn4o									
[e]	NA	NA	NA						
EX_cpd									
_mobd									
[e]	NA	NA	NA						
EX_cpd									
_na1[e									
] EV and	NA	NA	NA	NA	NA	NA	INA	NA	NA
EX_CPO									
]	NΔ	ΝΔ	NΔ	NΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ	ΝΔ
FX cpd									147.1
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EX_cpd									
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EX_cpd									
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EX_cpd									
_ocdca									
n[e]	NA	NA	NA						
_panos e[e]	NA	NA	NA						
EX cpd									
pi[e]	NA	NA	NA						
EX cpd									
_pmco									
a[e]	NA	NA	NA						
EX_cpd									
_ppa[e									
]	NA	NA	NA						

EX_cpd									
_pro-									
L[e]	NA								
EX_cpd									
_ptrc[e									
]	NA								
EX_cpd									
_pyr[e]	NA								
EX_cpd									
_ser-									
L[e]	NA								
EX_cpd									
_so3[e]	NA								
EX_cpd									
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EX_cpd									
_succ[e									
]	NA								
EX_cpd									
_thr-									
L[e]	NA								
EX_cpd									
_tnym[
ej EV. and	NA								
EX_cpa									
_unym d[o]	NIA	NIA	ΝΑ	NIA	ΝΑ	ΝΑ		ΝΑ	ΝΙΑ
	INA								
tmp[o									
	ΝΔ								
J FX cpd									
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_tindo[e]	NA								
EX cnd									
trp-									
L[e]	NA								
EX cod									
tsul[e]	NA								
EX cpd									
ttdca									
n[e]	NA								

EX_cpd									
	NΔ	ΝΔ	NΔ	NΔ	NΔ	ΝΔ	NΔ	ΝΔ	NΔ
EX cpd									
tvr-									
L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX cpd									
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EX_cpd									
_ululo[NA	NA	NA	NA	NA	NA	NA	NA	NA
bac X3									
urea[
e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
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EX_cpd									
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EX_cpd _val-									
L[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
EX_cpd									
_xan[e]	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
	661.34	490.12	171.21	659.54	530.58	128.96	660.38	521.88	138.49
FAO4	92362	96282	96079	12522	06134	06387	38844	63305	75538
	-	-		-	-		-	-	
	780.07	583.80	196.26	779.09	632.03	147.05	779.76	621.76	157.99
FAO5	1212	61372	50748	76132	92383	83749	4697	502	9677
	-	-	221 21	-	-	105 15	-	-	177 50
EAOE	898.79 21070	0/7.48	221.31	20742	733.49	105.15 6111	899.14	27005	12002
FAUU	510/0	20401	05418	39742	78032	0111	55097	57095	10002
		-	228 84		834 05	165.04		- 821 52	178 /17
FAO7	-1000	9155	0845	-1000	64881	35119	-1000	2399	7601
17.07	1000	30 961	30 961	1000	31 984	33113	1000	32 138	32 138
FBA	0	8	8	-7.7441	9	39.729	0	2	2
	-	-		-	-		-	-	
	46.424	10.709	35.714	39.257	8.6238	30.633	40.828	7.6758	33.152
FBP	15307	36098	79209	49399	46272	64772	10876	85041	22372
		ΝΔ	NΔ	NA	NA	NA	NA	NA	NA

	-	-		-	-		-	-	
	112.31	42.256	70.060	113.70	40.866	72.841	114.33	40.234	74.105
FDH10	72064	55362	65274	75485	21148	33702	95237	23632	28733
	-			-			-		
	50.217	19.843	70.060	51.607	21.233	72.841	52.239	21.865	74.105
FDH9	40213	25061	65274	74427	59275	33702	71943	5679	28733
	-	-		-	-		-	-	
	88.202	50.161	38.041	75.810	47.889	27.920	77.128	46.858	30.269
FE2abc	9433	18743	75587	26765	88	38765	31531	56514	75017
	-	-		-	-		-	-	
	59.200	13.855	45.344	60.948	13.518	47.429	61.742	13.365	48.377
FFSD	14374	80847	33527	27692	42694	84998	8829	0717	81121
	-	-		-	-		-	-	
	62.261	14.905	47.356	68.122	14.567	53.554	68.917	14.414	54.502
FGLU	47998	29122	18876	69434	90969	78466	30033	55445	74589
FMETT									
RS	NA	NA	NA	NA	NA	NA	NA	NA	NA
FMNAT	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
	41.288	4.1574	45.446	32.811	6.9176	39.729	34.075	8.1722	42.247
FMNRx	68886	24104	11296	40133	0504	00637	34963	32738	58237
FNOR	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-								
	17.515	17.515	35.030		18.210	18.210		18.526	18.526
FORt	2	2	4	0	3	3	0	3	3
FRD10	NA	NA	NA	NA	NA	NA	NA	NA	NA
FRD11	NA	NA	NA	NA	NA	NA	NA	NA	NA
	_	-		_	-		_	-	
	126.99	70.749	56.249	128.38	72.104	56.285	129.02	70.844	58.176
FRTT	91073	32435	78294	94504	27673	17369	14246	98873	43585
	-	-		_	-		-	-	
	43.694	6.3555	37.339	43.750	6.4920	37.258	45.717	5.6637	40.053
FRUK	73799	86327	15166	2129	91391	12151	05528	95892	25939
	-	-		_	-		-	-	
	67.087	37.040	30.047	59.929	33.585	26.344	61.183	32.014	29.169
FTHFD	38942	36571	0237	33241	01321	3192	96011	39843	56167
	-			-			-		
	35.461	-1.00E-	35.461	26.344	-1.00E-	26.344	29.169	-1.00E-	29.169
FTHFL	07235	06	07135	3202	06	3192	56267	06	56167
ELINA	-3 7711	0	3.7711	-5.5193	0	5.5193	0	15.171	15.171

	-	_		_	_		-	_	
FUMAC	96.036	60.590	35.446	97.784	59.199	38.584	98.578	58.567	40.011
А	25586	17514	08072	38903	832	55703	99502	85785	13717
	-	_		_	_		_	_	
G1PAC	59.162	2.5560	56.606	60.552	8.9907	51.562	61.184	7.4980	53.686
т	42094	53442	3675	76408	03121	06096	73824	26557	71168
	-			_					
	32.555	16.492	49.048	33.946	15.137				
G1PCT	9	8	7	2	8	49.084	NA	NA	NA
	-						-		
G1PTM	29.191	19.857	49.048				31.213	19.761	50.975
Т	09902	52813	62715	NA	NA	NA	41631	86375	28006
	-			_			-		
	26.837	-1.00E-	26.837	27.532	-1.00E-	27.532	27.848	-1.00E-	27.848
G1SATi	00724	06	00624	17881	06	17781	16588	06	16488
	-	-		-	-		-	-	
	58.075	19.341	38.734	59.823	21.749	38.074	60.618	20.968	39.650
G35DP	79575	1765	61926	92893	09049	83844	53492	4214	11352
					46.676	42.935			45.578
G3PD2	5.658	55.476	49.818	3.7412	6	4	2.8699	48.448	1
	-						-		
	5.1746	56.901	62.076				7.1969	59.935	67.132
G3PD4	82239	70096	3832	NA	NA	NA	99533	1769	17644
	-	-					-	-	
	67.274	5.1981	62.076				69.296	2.1646	67.132
G3PD8	48646	03261	3832	NA	NA	NA	80376	2732	17644
	-	-		-	-		-	-	
	75.160	6.8164	68.344	53.733	3.5093	50.224	54.557	2.0060	52.551
G5SD	82754	73634	35391	82885	06552	5223	25226	47787	20448
	-			-			-		
	20.724	-1.00E-	20.724	21.401	-1.00E-	21.401	23.776	-1.00E-	23.776
G6PDA	09751	06	09651	60843	06	60743	1498	06	1488
	-			-			-		
G6PDH	26.875		26.875	28.792		28.792	29.663	15.686	45.350
У	3	0	3	1	0	1	4	7	1
							-	4 9 9 9 7	
GAL1P							44.546	1.2062	45.753
URI	NA	NA	NA	NA	NA	NA	77606	59925	03599
	-		10 10 -	-		40.000	-		40.4.4
CALI	43.789	2 6 4 4 6	46.434	43.845	2 5 2 2 4	46.353	45.811	2 22 2-	49.148
GALKr	6	2.6449	5	1	2.5084	5	9	3.3367	6

	-			-			-		
	25.204		25.204	26.594		26.594	27.226		27.226
GALU	4	0	4	7	0	7	7	0	7
		56.830	55.302						
GAPD	1.5279	4	5	-3.3083	0	3.3083	-5.1949	0	5.1949
	_			_			_		
	43,290		43,290	44,680		44,680	45.312		45.312
GARFT	5	0	5	8	0	8	8	0	8
				-			-		
	61 042	46 835	107 87	48 092	52 605	100 69	49 175	55 229	104 40
GBE7	78936	0.055	77965	40.052	88793	837/1	205/13	01/185	107.40
ODLZ	78550	0071	11505	40010	00755	03741	20343	01403	42203
CCALD	01 074	16 5 20	15 116	01 721		20 720		- 52 7/1	12 217
	91.974	40.520	45.440	94.754	47001	00627	11207	55.741	42.247
ע	30444	19147	11296	48537	47901	00637	11307	5307	58237
	-	-		-	-		-	-	
GGLUG	59.458	1.6565	57.802	61.375	11.151	50.224	62.246	9.6957	52.551
ABDH	88238	93335	28905	70633	18402	5223	99094	86458	20448
	-	-		-	-		-	-	
GGLUG	49.468	2.1125	47.356	55.329	1.7751	53.554	56.124	1.6217	54.502
ABH	6984	09635	18876	91276	28103	78466	51875	72861	74589
	-	-		-	-		-	-	
GGLUP	80.321	12.871	67.450	68.086	5.7095	62.377	69.494	4.5989	64.895
TS	64119	35107	29012	91807	91384	32668	90101	98318	90269
	-	-		-	-		-	-	
	126.99	70.749	56.249	128.38	72.104	56.285	129.02	70.844	58.176
GGTT	91073	32435	78294	94504	27673	17369	14246	98873	43585
					31.358	31.358		31.990	31.990
GHMT	0	29.968	29.968	0	3	3	0	3	3
	_			_			_		
	35.230		35.230	35.285		35.285	37.252		37.252
GK1	2	0	2	7	0	7	5	0	5
GLCGS	99 034	11 / 58	87 575						
D	16713	6/87	818/I3	ΝΛ	ΝΛ	ΝΛ	ΝΛ	ΝΛ	ΝΛ
D	40713	0487	01040	20 770	06 260	75 100	16 500	101 10	01 COC
				20.779	90.200	20654	14001	60000	04.000 72024
GLCP	INA	INA	INA	09025	200/8	59054	14981	00092	15954
	-		120.04	-	-	120.02	-	-	120 77
	1/2./6	40.145	126.61	1/1.25	41.010	129.63	1/8.33	39.558	138.//
GLCS1	09379	4648	54/31	51129	64534	84675	/153	09305	906
	-		_	-			-		
	22.821	17.515	40.336	23.726	19.595	43.322	24.138	20.663	44.801
GLCt2	17884	16269	34152	94459	65182	59641	6563	26827	92457

	-	-		-	-		-	-	
	40.323	8.7903	31.533	41.714	10.840	30.873	42.346	9.8971	32.448
GLGC	78219	18722	46347	12533	44268	68265	09948	41754	95773
	-	-		-	-		-	-	
	66.385	16.450	49.935	54.130	6.9128	47.217	55.529	4.0643	51.464
GLNS	6216	49516	12644	39313	53315	53981	05546	31825	72363
GLNTR									
S	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
	4.9746	34.418	39.393	5.0301	40.067	45.097	6.9969	40.801	47.798
GLU5K	60059	40202	06208	34971	77676	91173	77353	97274	95009
	-	-		-	-		-	-	
GLUCY	90.801	23.351	67.450	78.566	16.189	62.377	79.974	15.078	64.895
SL	32571	03559	29012	60258	2759	32668	58553	68283	90269
		18.040	12.325		23.964	21.388		24.108	22.959
GLUDx	5.7146	5	9	2.5761	7	6	1.1495	7	2
							-	-	
							46.826	5.6549	41.171
GLUN	NA	NA	NA	NA	NA	NA	26691	05646	36126
	-	-		-	-		-	-	
GLUPR	113.76	45.193	68.575	120.32	46.906	73.419	121.43	45.809	75.626
Т	93612	71686	64433	57471	45928	28784	63402	80311	53707
		16.438	16.438		17.134	17.134		17.450	17.450
GLUR	0	9	9	0	1	1	0	1	1
	-	-		-	-		-	-	
	76.463	11.524	64.938	76.141	8.9127	67.228	76.964	7.7254	69.239
GLUSy	6041	75596	84815	26869	60444	50825	6921	88756	20335
GLUTR									
R	NA	NA	NA	NA	NA	NA	NA	NA	NA
GLUTR									
S	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
	17.631	17.515	35.147	22.650	19.595	42.246	23.062	20.663	43.725
GLUt2	87654	16269	03923	72348	65182	3753	43519	26827	70346
	-			-			-		
	22.937	35.030	57.968	22.650	36.420	59.071	49.303	20.663	69.966
GLUt4i	8907	32637	21707	72248	66951	39199	27696	26627	54323
		48.184	54.213		47.339	54.758		48.832	56.449
GLYAT	-6.0288	5	3	-7.4192	7	9	-7.6175	3	8
	-			-			-		
	28.127	35.030	63.157	23.726	36.420	60.147	50.379	20.663	71.042
GLYBt4	2	3	5	9	7	6	5	3	8

	- 26.151	43.672	69.824	۔ 29.985	41.101	71.087	- 31.728	42.509	74.237
GLYCL	90162	35329	25491	5495	76634	31584	11873	74928	86801
GLYCLT DXR	NA	NA	NA	NA	NA	NA	NA	NA	NA
GLYCO GEN_S YNTHE	ΝΑ	NA	NA	NA	NΔ	NA	NΔ	NΔ	NΔ
313		NA		INA	NA		-	NA	INA
GLYCRt							24.138	20.663	
2	NA	NA	NA	NA	NA	NA	7	3	44.802
GLYC T	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	- 18.526 3	18.526 3	37.052 6
	-			-	-		-	-	
	47.341	8.8913	38.450	48.092	9.0278	39.064	50.375	8.1995	42.175
GLYK	60038	61599	23878	24686	66164	38069	07632	71165	50515
	- 69 485	- 16 940	52 545	- 71 233	-	54 631	- 72 028	- 16 449	55 578
GLYOX	62983	13878	49106	76301	75725	00576	369	402	967
GLYTRS	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
	22.537	35.030	57.567	23.726	36.420	60.147	50.379	20.663	71.042
GLYT4	3686	32637	69497	94359	66951	6131	49806	26627	76434
GMHE	77.131	38.396	38.734	78.521	40.446	38.074	79.153	39.503	39.650
PAT	25202	63276	61926	59516	75672	83844	56931	45579	11352
	-	-		-	-		-		
GMHE	37.892	0.4591	37.433	37.947	0.5956	37.352	39.914	-1.00E-	39.914
FN	- 23339	480335	10550	- 7285		0752			30909
GMHE	54.195	8.6234	45.572	46.266	6.5379	39.729	47.837	5.5899	42.247
PPA	84772	55483	39223	94714	40774	00637	56191	79543	58237
	-	-	44564	-	-	47 0 44	-	-	40.005
GPDDA 2	10677	29.858	44.561	/6.863 41152	29.521	47.341	77.974 00459	29.368	48.605 8541
-	- 10077		21332	-		5050	-	-	0341
GPDDA	87.698	43.137	44.561	90.141	42.800	47.341	91.252	42.646	48.605
4	64485	42534	21952	9496	0438	9058	54267	68856	8541
	-	-	FC 242	-	-	FC 205	-	-	F0 470
GRTT	91073	32435	56.249 78294	128.38 94504	27673	50.285 17369	14246	70.844 98873	58.176 43585

	-	- 381 72	58 192						
GSHPO	76093	5301	30829	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
CONK	48.470	2.0356	46.434	48.525	2.1721	46.353	50.492	1.3438	49.148
GSINK	19354	83/22	50981	66845	88286	48016	51083	92287	61854 71 077
GTHRD	-0.5922	2	4	-2.1512	6	8	-2.8599	6	71.077 5
	-			-			-		
GTHRD	35.179	17.365	52.545	36.927	17.703		37.722	17.856	55.578
Н	7	8	5	8	2	54.631	4	5	9
	-	-	<u> </u>	-	-		-	-	<u></u>
стис	94.892	27.634	67.257	82.657	18.380	64.277	84.065	16.714	67.351
	02200	97708	0452	69970	19007	70508	- 0027	50707	57502
	128.37	75.826	52.545	130.12	75.489	54.631	130.91	75.335	55.578
GTPCI	19196	42857	49106	00508	04703	00376	46568	69179	965
	-	-		-	-		-	-	
	149.60	106.39	43.206	152.38	109.15	43.224	155.71	108.54	47.174
GTPCII	08027	40159	78677	42348	97199	51487	6014	16827	33133
OTDDD	-	-	20 724	-	-	20.456	-	-	44 4 2 0
	6/.363		38./34	68.753	29.596	39.156	69.385 E2012	28.256	41.129
ĸ	21204	39338	31 780	22230	32 097	32 097	32012	32 241	32 241
GUAD	0	4	4	0	32.037	32.057	0	32.241	32.241
	_	_		_	_		_	_	
GUAPR	61.114	4.8651	56.249	62.505	6.2200	56.285	63.137	4.9607	58.176
Т	90721	24267	78294	25035	76656	17369	2245	88653	43585
Growth	NA	NA	NA	NA	NA	NA	NA	NA	NA
H2Ot5	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
	10.468	34.977	45.446	13.228	26.500	20 720	14.483	27.764	42.247
HACD8		ð -	1	5	5	39.729		5	0
насоа	224.10	178.66	45.446	226.86	187.13	39.729	228.12	185.87	42.247
Dr	81129	19999	11296	82938	92875	00637	29215	53392	58237
	-	-		-	-		-	-	
HBZOP	126.30	70.052	56.249	127.69	71.407	56.285	128.32	70.147	58.176
Т	19814	19843	78294	23245	15082	17369	42987	86282	43585
HCO3E	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-	56 2 42	-	-	FC 205	-	-	F0 470
HEME	116.28 02075	60.038	56.249	11/.67	61.393	17260	118.31	60.134	58.1/6
05	020/5	50452	/8294	00300	4569	T130A	00048	1093	43385

	-	-		-	-		-	-	
	126.99	70.749	56.249	128.38	72.104	56.285	129.02	70.844	58.176
HEPTT	91073	32435	78294	94504	27673	17369	14246	98873	43585
	-	-		-	-		-	-	
	47.167	7.9337	39.233	47.222	8.0702	39.152	49.189	7.2419	41.947
HEX1	08931	35285	35402	56422	39349	32487	4066	4435	46225
	_	_		_	_		_	_	
	126.99	70,749	56.249	128.38	72.104	56.285	129.02	70.844	58.176
HEXTT	91073	32435	78294	94504	27673	17369	14246	98873	43585
	_	_		_				_	
	66 499	24 211	42 287	68 247	23 178	45 068	69 041	22 709	46 332
HIBHR	06386	0825	98136	19703	5294	66764	80302	18708	61594
	-	0023	30130		5251	00701		10,00	01331
	26 393	12 341	38 734	27 070	12 658	39 729	29 445	12 802	42 247
	08829	53097	61926	59921	40716	00637	14058	44179	58237
IIISDI	00025	55057	01520	55521	40710	00037	14050		50257
	58 / 55	2 5031	55 861	63 280	20 243	13 037	65 173	18 031	17 112
шістр	27700	79522	20256	56720	20.243	2/1777	Q2571	21562	52000
	37709	10333	89830	20739	22317	34222	03371	31303	52008
	-	- 10 057	45 572	- F1 001	-	20 720	-	10 224	42 247
	27200	13.357	45.572	51.001	11.272	39.729	52.572	10.324	42.247
HISTP	37299	98076	39223	4/242	46605	00637	08/19	50482	58237
LUCTRO									
HISTRS	NA	NA	NA	NA	NA	NA	NA	NA	NA
HISTRS	NA -	NA -	NA	NA -	NA -	NA	NA -	NA -	NA
HISTRS	NA - 183.33	NA - 80.942	NA 102.39	NA - 182.88	NA - 78.602	NA 104.28	NA - 190.94	NA - 77.538	NA 113.41
HISTRS HMBS	NA - 183.33 5903	NA - 80.942 91706	NA 102.39 2986	NA - 182.88 70619	NA - 78.602 04219	NA 104.28 50197	NA - 190.94 93706	NA - 77.538 00816	NA 113.41 13625
HISTRS	NA - 183.33 5903 -	NA - 80.942 91706	NA 102.39 2986	NA - 182.88 70619 -	NA - 78.602 04219	NA 104.28 50197	NA - 190.94 93706 -	NA - 77.538 00816	NA 113.41 13625
HISTRS HMBS HMGD	NA - 183.33 5903 - 24.998	NA - 80.942 91706 20.447	NA 102.39 2986 45.446	NA - 182.88 70619 - 27.758	NA 	NA 104.28 50197 39.729	NA 190.94 93706 _ 29.013	NA - 77.538 00816 13.234	NA 113.41 13625 42.247
HISTRS HMBS HMGD x	NA - 183.33 5903 - 24.998 71583	NA 	NA 102.39 2986 45.446 11296	NA - 182.88 70619 - 27.758 89676	NA - 78.602 04219 11.970 1096	NA 104.28 50197 39.729 00637	NA - 190.94 93706 - 29.013 52446	NA - 77.538 00816 13.234 05791	NA 113.41 13625 42.247 58237
HISTRS HMBS HMGD x	NA - 183.33 5903 - 24.998 71583 -	NA 	NA 102.39 2986 45.446 11296	NA - 182.88 70619 - 27.758 89676	NA - 78.602 04219 11.970 1096	NA 104.28 50197 39.729 00637	NA 190.94 93706 - 29.013 52446	NA 77.538 00816 13.234 05791	NA 113.41 13625 42.247 58237
HISTRS HMBS HMGD x	NA - 183.33 5903 - 24.998 71583 - 60.827	NA - 80.942 91706 20.447 39714 - 8.2824	NA 102.39 2986 45.446 11296 52.545	NA - 182.88 70619 - 27.758 89676	NA - 78.602 04219 11.970 1096	NA 104.28 50197 39.729 00637	NA - 190.94 93706 - 29.013 52446	NA - 77.538 00816 13.234 05791	NA 113.41 13625 42.247 58237
HISTRS HMBS HMGD x HMGL	NA - 183.33 5903 - 24.998 71583 - 60.827 91386	NA - 80.942 91706 20.447 39714 - 8.2824 22802	NA 102.39 2986 45.446 11296 52.545 49106	NA - 182.88 70619 - 27.758 89676 NA	NA - 78.602 04219 11.970 1096 NA	NA 104.28 50197 39.729 00637 NA	NA - 190.94 93706 - 29.013 52446 NA	NA - 77.538 00816 13.234 05791 NA	NA 113.41 13625 42.247 58237 NA
HISTRS HMBS HMGD x HMGL	NA - 183.33 5903 - 24.998 71583 - 60.827 91386	NA - 80.942 91706 20.447 39714 - 8.2824 22802	NA 102.39 2986 45.446 11296 52.545 49106	NA - 182.88 70619 - 27.758 89676 NA	NA - 78.602 04219 11.970 1096 NA	NA 104.28 50197 39.729 00637 NA	NA - 190.94 93706 - 29.013 52446 NA	NA - 77.538 00816 13.234 05791 NA	NA 113.41 13625 42.247 58237 NA
HISTRS HMBS HMGD x HMGL	NA - 183.33 5903 - 24.998 71583 - 60.827 91386 - 29.995	NA - 80.942 91706 20.447 39714 - 8.2824 22802 22.550	NA 102.39 2986 45.446 11296 52.545 49106 52.545	NA - 182.88 70619 - 27.758 89676 NA	NA - 78.602 04219 11.970 1096 NA	NA 104.28 50197 39.729 00637 NA	NA - 190.94 93706 - 29.013 52446 NA	NA - 77.538 00816 13.234 05791 NA 25.092	NA 113.41 13625 42.247 58237 NA 55.578
HISTRS HMBS HMGD x HMGL	NA - 183.33 5903 - 24.998 71583 - 60.827 91386 - 29.995 3	NA 80.942 91706 20.447 39714 - 8.2824 22802 22.550 2	NA 102.39 2986 45.446 11296 52.545 49106 52.545 5	NA - 182.88 70619 - 27.758 89676 NA	NA - 78.602 04219 11.970 1096 NA	NA 104.28 50197 39.729 00637 NA	NA - 190.94 93706 - 29.013 52446 NA -30.486	NA - 77.538 00816 13.234 05791 NA 25.092 9	NA 113.41 13625 42.247 58237 NA 55.578 9
HISTRS HMBS HMGD x HMGL HMGSs HOXPR	NA - 183.33 5903 - 24.998 71583 - 60.827 91386 - 29.995 3 11.930	NA - 80.942 91706 20.447 39714 - 8.2824 22802 22.550 2 57.376	NA 102.39 2986 45.446 11296 52.545 49106 52.545 5 45.446	NA - 182.88 70619 - 27.758 89676 NA	NA - 78.602 04219 11.970 1096 NA	NA 104.28 50197 39.729 00637 NA NA	NA - 190.94 93706 - 29.013 52446 NA -30.486	NA - 77.538 00816 13.234 05791 NA 25.092 9	NA 113.41 13625 42.247 58237 NA 55.578 9
HISTRS HMBS HMGD x HMGL HMGSs HOXPR x	NA - 183.33 5903 - 24.998 71583 71583 - 60.827 91386 - 29.995 3 11.930 5	NA - 80.942 91706 20.447 39714 - 8.2824 22802 22.550 2 57.376 6	NA 102.39 2986 45.446 11296 52.545 49106 52.545 5 45.446 1	NA - 182.88 70619 - 27.758 89676 NA NA	NA - 78.602 04219 11.970 1096 NA NA	NA 104.28 50197 39.729 00637 NA NA	NA - 190.94 93706 - 29.013 52446 NA	NA 77.538 00816 13.234 05791 NA 25.092 9 NA	NA 113.41 13625 42.247 58237 NA 55.578 9 NA
HISTRS HMBS HMGD x HMGL HMGSs HOXPR x	NA - 183.33 5903 - 24.998 71583 - 60.827 91386 - 29.995 3 11.930 5	NA - 80.942 91706 20.447 39714 - 8.2824 22802 22.550 2 57.376 6	NA 102.39 2986 45.446 11296 52.545 49106 52.545 5 45.446 1	NA - 182.88 70619 - 27.758 89676 NA NA	NA - 78.602 04219 11.970 1096 NA NA	NA 104.28 50197 39.729 00637 NA NA	NA - 190.94 93706 - 29.013 52446 NA -30.486 NA	NA - 77.538 00816 13.234 05791 NA 25.092 9 NA	NA 113.41 13625 42.247 58237 NA 55.578 9 NA
HISTRS HMBS HMGD x HMGL HMGSs HOXPR x HPPDO	NA - 183.33 5903 - 24.998 71583 71583 - 60.827 91386 - 29.995 3 11.930 5 515.13	NA - 80.942 91706 20.447 39714 - 8.2824 22802 22.550 2 57.376 6 - 456.94	NA 102.39 2986 45.446 11296 52.545 49106 52.545 5 45.446 1 58.192	NA - 182.88 70619 - 27.758 89676 NA NA	NA - 78.602 04219 11.970 1096 NA NA	NA 104.28 50197 39.729 00637 NA NA	NA - 190.94 93706 - 29.013 52446 NA -30.486 NA	NA 77.538 00816 13.234 05791 NA 25.092 9 NA	NA 113.41 13625 42.247 58237 NA 55.578 9 NA
HISTRS HMBS HMGD x HMGL HMGSs HOXPR x HPPDO 1	NA - 183.33 5903 - 24.998 71583 - 60.827 91386 - 29.995 3 11.930 5 515.13 92119	NA 80.942 91706 20.447 39714 - 8.2824 22802 22.550 2 57.376 6 - 456.94 69056	NA 102.39 2986 45.446 11296 52.545 49106 52.545 5 45.446 1 1 58.192 30629	NA - 182.88 70619 - 27.758 89676 NA NA NA	NA - 78.602 04219 11.970 1096 NA NA	NA 104.28 50197 39.729 00637 NA NA NA	NA - 190.94 93706 - 29.013 52446 NA -30.486 NA	NA 77.538 00816 13.234 05791 NA 25.092 9 NA	NA 113.41 13625 42.247 58237 NA 55.578 9 NA
HISTRS HMBS HMGD x HMGL HMGSs HOXPR x HPPDO 1	NA - 183.33 5903 - 24.998 71583 - 60.827 91386 - 29.995 3 11.930 5 515.13 92119	NA - 80.942 91706 20.447 39714 - 8.2824 22802 22.550 2 57.376 6 - 456.94 69056	NA 102.39 2986 45.446 11296 52.545 49106 52.545 5 45.446 1 58.192 30629	NA - 182.88 70619 - 27.758 89676 NA NA NA NA	NA - 78.602 04219 11.970 1096 NA NA NA	NA 104.28 50197 39.729 00637 NA NA NA	NA - 190.94 93706 - 29.013 52446 NA -30.486 NA	NA 77.538 00816 13.234 05791 NA 25.092 9 NA	NA 113.41 13625 42.247 58237 NA 55.578 9 NA NA
HISTRS HMBS HMGD x HMGL HMGSs HOXPR x HPPDO 1	NA - 183.33 5903 - 24.998 71583 - 60.827 91386 - 29.995 3 11.930 5 515.13 92119 - 49.857	NA - 80.942 91706 20.447 39714 - 8.2824 22802 22.550 2 57.376 6 - 456.94 69056 - 11.123	NA 102.39 2986 45.446 11296 52.545 49106 52.545 5 45.446 1 58.192 30629 38.734	NA - 182.88 70619 - 27.758 89676 NA NA NA NA - 51.247	NA - 78.602 04219 11.970 1096 NA NA NA NA - 12.091	NA 104.28 50197 39.729 00637 NA NA NA NA 39.156	NA - 190.94 93706 - 29.013 52446 NA -30.486 NA - 30.486 NA	NA 77.538 00816 13.234 05791 NA 25.092 9 NA NA - 10.750	NA 113.41 13625 42.247 58237 NA 55.578 9 NA NA NA 41.129

	-			-					
HPYRR	55.416		45.446	46.939					42.247
x	4	-9.9703	1	1	-7.2101	39.729	-48.203	-5.9555	5
	_			_			_		
HPYRR	67.466		57.802	57.972		50.224	59.427		52.551
v	9	-9.6646	3	3	-7.7478	5	7	-6.8765	2
-		57.631	57.631		48.137	48.137		49,592	49,592
HSDv	0	8	8	0	3	3	0	7	7
	-	0.0955		_	_		_		
	46.530	533096	46.434	46.585	0.2320	46.353	48,552	-1.00F-	48,552
нѕк	06312	9	50981	53803	57374	48066	38042	06	37942
			30301	-	-	10000			37312
	55 529	13 241	42 287	56 919	11 851	45 068	57 551	11 219	46 332
нсст	34212	36076	98136	68526	01762	66764	65941	04347	61594
11551	54212	50070	50150	00520	01702	00704	05541	04347	01334
	27 244	1.005	27 244	28 625	1 00F	28 625	20 267	1.005	20 267
цстрт	27.244	-1.00L-	27.244	20.033	-1.00L-	20.033	29.207	-1.00L-	29.207
113171	89209	00	89109	23322	00	23422	20938	00	20030
	-	122.20	25 020	1 (9 0 2	-	26 420	100.04	-	27.052
нінвр	107.33	132.30	35.030	168.03	131.60	36.420	108.34	131.29	37.052
D	53885	50611	32/3/	050	98895	67051	65471	39024	64466
	-	-	46 456	-	-	47.000	-	-	40.004
	46.973	0.81/1	46.156	48.721	0.7333	47.988	49.516	0.6952	48.821
HXAD	59908	336373	46544	/3226	305271	40173	33824	382043	10004
	-	-		-	-		-	-	
	53.400	4.0106	49.390	56.856	5.3656	51.490	58.426	4.1063	54.320
НХРКІ	97816	8129	29687	33066	33679	69698	94544	45675	59976
	-	-		-	-		-	-	
	39.571	0.1230	39.448	43.384	2.0507	41.334	45.118	0.9974	44.120
ICDHxi	63894	46588	59235	78148	43829	03765	03009	535719	57652
	-			-					
	39.877		48.482	42.847		42.847			
ICDHy	3	8.6055	8	1	0	1	-44.197	0	44.197
	-			-			-		
ICHORS	16.546	-1.00E-	16.546	17.241	-1.00E-	17.241	17.557	-1.00E-	17.557
i	15623	06	15523	3278	06	3268	31487	06	31387
	-			-			-		
	30.007	-1.00E-	30.007	28.061	-1.00E-	28.061	29.947	15.120	45.068
ICL	64439	06	64339	37378	06	37278	97563	98903	96466
	-	-		-	-		-	-	
	133.92	61.166	72.755	140.47	59.080	81.397	141.58	58.132	83.456
IG3PS	16826	02181	66076	80685	5071	5614	86616	54587	1157

	-	-		-	-		-	-	
	65.438	30.408	35.030	66.133	29.712	36.420	66.449	29.396	37.052
IGPDH	35926	03189	32737	53083	86032	67051	51791	87324	64466
	-	-		-	-		-	-	
	99.075	46.529	52.545	100.82	46.192	54.631	101.61	46.038	55.578
IGPS	02378	53472	48906	3157	15319	00376	77649	79795	967
		39.194	39.194		30.338	30.338		31.430	31.430
ILEDH2	0	5	5	0	9	9	0	9	9
	-			-			-		
	18.040	23.064	41.104	23.964	24.454	48.419	24.108	25.086	49.195
ILETA	5	1	6	7	5	2	7	5	2
ILETRS	NA	NA	NA	NA	NA	NA	NA	NA	NA
	_			_			_		
	28.127	35.030	63.157	23.726	36.420	60.147	50.379	20.663	71.042
ILEt4	19299	32637	51936	94359	66951	6131	49806	26627	76434
		12.531	12.531		16.658	16.658		17.912	17.912
IMPC	0	9	9	0	1	1	0	8	8
	-			_			_		
	10.655	-1.00E-	10.655	13.415	-1.00E-	13.415	14.670	-1.00E-	14.670
IMPD	67861	06	67761	85955	06	85855	48725	06	48625
							-		
								20.000	
INDOLE							24.138	20.663	
t2	NA	NA	NA	NA	NA	NA	24.138 7	20.663	44.802
t2	NA -	NA -	NA	NA -	NA -	NA	24.138 7 -	20.663	44.802
t2	NA - 46.364	NA - 6.7897	NA 39.575	NA - 48.485	NA - 6.9262	NA 41.559	24.138 7 - 51.390	20.663 3 - 6.0979	44.802 45.292
INDOLE t2 INSK	NA - 46.364 77748	NA - 6.7897 53743	NA 39.575 02374	NA - 48.485 26176	NA - 6.9262 57807	NA 41.559 00395	24.138 7 51.390 74476	20.663 3 - 6.0979 62308	44.802 45.292 78246
INDOLE t2 INSK	NA - 46.364 77748 -	NA - 6.7897 53743 -	NA 39.575 02374	NA - 48.485 26176 -	NA - 6.9262 57807 -	NA 41.559 00395	24.138 7 - 51.390 74476	20.663 3 - 6.0979 62308 -	44.802 45.292 78246
INDOLE t2 INSK	NA - 46.364 77748 - 83.706	NA - 6.7897 53743 - 38.260	NA 39.575 02374 45.446	NA - 48.485 26176 - 75.229	NA - 6.9262 57807 - 35.500	NA 41.559 00395 39.729	24.138 7 51.390 74476 - 76.493	20.663 3 - 6.0979 62308 - 34.245	44.802 45.292 78246 42.247
INDOLE t2 INSK IPDPS	NA - 46.364 77748 - 83.706 51924	NA - 6.7897 53743 - 38.260 40628	NA 39.575 02374 45.446 11296	NA - 48.485 26176 - 75.229 23171	NA - 6.9262 57807 - 35.500 22534	NA 41.559 00395 39.729 00637	24.138 7 51.390 74476 - 76.493 18002	20.663 3 - 6.0979 62308 - 34.245 59764	44.802 45.292 78246 42.247 58237
INDOLE t2 INSK IPDPS	NA 46.364 77748 - 83.706 51924	NA - 6.7897 53743 - 38.260 40628	NA 39.575 02374 45.446 11296	NA 48.485 26176 - 75.229 23171	NA - 6.9262 57807 - 35.500 22534	NA 41.559 00395 39.729 00637	24.138 7 51.390 74476 - 76.493 18002	20.663 3 - 6.0979 62308 - 34.245 59764	44.802 45.292 78246 42.247 58237
INDOLE t2 INSK IPDPS	NA - 46.364 77748 - 83.706 51924 - 10.438	NA - 6.7897 53743 - 38.260 40628 -1.00E-	NA 39.575 02374 45.446 11296 10.438	NA 48.485 26176 - 75.229 23171 - 13.198	NA 6.9262 57807 - 35.500 22534 -1.00E-	NA 41.559 00395 39.729 00637 13.198	24.138 7 51.390 74476 - 76.493 18002 - 14.453	20.663 3 - 6.0979 62308 - 34.245 59764 -1.00E-	44.802 45.292 78246 42.247 58237 14.453
INDOLE t2 INSK IPDPS	NA 46.364 77748 - 83.706 51924 - 10.438 66729	NA - 6.7897 53743 - 38.260 40628 -1.00E- 06	NA 39.575 02374 45.446 11296 10.438 66629	NA 48.485 26176 - 75.229 23171 - 13.198 84823	NA - 6.9262 57807 - 35.500 22534 -1.00E- 06	NA 41.559 00395 39.729 00637 13.198 84723	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593	20.663 3 6.0979 62308 - 34.245 59764 -1.00E- 06	44.802 45.292 78246 42.247 58237 14.453 47493
INDOLE t2 INSK IPDPS IPMD IPPMIa	NA 46.364 77748 - 83.706 51924 - 10.438 66729 NA	NA - 6.7897 53743 - 38.260 40628 -1.00E- 06 NA	NA 39.575 02374 45.446 11296 10.438 66629 NA	NA 48.485 26176 - 75.229 23171 - 13.198 84823 NA	NA 6.9262 57807 - 35.500 22534 -1.00E- 06 NA	NA 41.559 00395 39.729 00637 13.198 84723 NA	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593 NA	20.663 3 - 6.0979 62308 - 34.245 59764 -1.00E- 06 NA	44.802 45.292 78246 42.247 58237 14.453 47493 NA
INDOLE t2 INSK IPDPS IPMD IPPMIa	NA 46.364 77748 - 83.706 51924 - 10.438 66729 NA	NA - 6.7897 53743 - 38.260 40628 -1.00E- 06 NA 28.611	NA 39.575 02374 45.446 11296 10.438 66629 NA 28.611	NA 48.485 26176 75.229 23171 13.198 84823 NA	NA 6.9262 57807 - 35.500 22534 -1.00E- 06 NA 29.306	NA 41.559 00395 39.729 00637 13.198 84723 NA 29.306	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593 NA	20.663 3 6.0979 62308 - 34.245 59764 -1.00E- 06 NA 29.622	44.802 45.292 78246 42.247 58237 14.453 47493 NA 29.622
INDOLE t2 INSK IPDPS IPMD IPPMIa IPPMIb	NA - 46.364 77748 - 83.706 51924 - 10.438 66729 NA	NA 6.7897 53743 - 38.260 40628 -1.00E- 06 NA 28.611 2	NA 39.575 02374 45.446 11296 10.438 66629 NA 28.611 2	NA 48.485 26176 - 75.229 23171 - 13.198 84823 NA	NA 6.9262 57807 - 35.500 22534 -1.00E- 06 NA 29.306 4	NA 41.559 00395 39.729 00637 13.198 84723 NA 29.306 4	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593 NA	20.663 3 6.0979 62308 - 34.245 59764 -1.00E- 06 NA 29.622 4	44.802 45.292 78246 42.247 58237 14.453 47493 NA 29.622 4
INDOLE t2 INSK IPDPS IPMD IPPMIa IPPMIb	NA - 46.364 77748 - 83.706 51924 - 10.438 66729 NA 0	NA - 6.7897 53743 - 38.260 40628 -1.00E- 06 NA 28.611 28.611 2	NA 39.575 02374 45.446 11296 10.438 66629 NA 28.611 2	NA 48.485 26176 75.229 23171 13.198 84823 NA 0	NA - 6.9262 57807 - 35.500 22534 -1.00E- 06 NA 29.306 4 -	NA 41.559 00395 39.729 00637 13.198 84723 NA 29.306 4	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593 NA 0 -	20.663 3 - 6.0979 62308 - 34.245 59764 -1.00E- 06 NA 29.622 4 -	44.802 45.292 78246 42.247 58237 14.453 47493 NA 29.622 4
INDOLE t2 INSK IPDPS IPMD IPPMIa IPPMIb	NA - 46.364 77748 - 83.706 51924 - 10.438 66729 NA 0 - 57.474	NA 6.7897 53743 - 38.260 40628 -1.00E- 06 NA 28.611 2 -1.00E-	NA 39.575 02374 45.446 11296 10.438 66629 NA 28.611 2 57.474	NA 48.485 26176 75.229 23171 13.198 84823 NA 0 58.864	NA 6.9262 57807 - 35.500 22534 -1.00E- 06 NA 29.306 4 - 4.1057	NA 41.559 00395 39.729 00637 13.198 84723 NA 29.306 4 54.758	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593 NA 0 - 59.496	20.663 3 6.0979 62308 - 34.245 59764 -1.00E- 06 NA 29.622 4 2.6131	44.802 45.292 78246 42.247 58237 14.453 47493 NA 29.622 4 56.883
INDOLE t2 INSK IPDPS IPMD IPPMIa IPPMIb IPPS	NA - 46.364 77748 - 83.706 51924 - 10.438 66729 NA - 57.474 28678	NA - 6.7897 53743 - 38.260 40628 -1.00E- 06 NA 28.611 2 2 -1.00E- 06	NA 39.575 02374 45.446 11296 10.438 66629 NA 28.611 2 57.474 28578	NA 48.485 26176 75.229 23171 13.198 84823 NA 0 - 58.864 62992	NA 6.9262 57807 - 35.500 22534 -1.00E- 06 NA 29.306 4 - 4.1057 91413	NA 41.559 00395 39.729 00637 13.198 84723 NA 29.306 4 54.758 8385	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593 NA 0 - 59.496 60407	20.663 3 - 6.0979 62308 - 34.245 59764 -1.00E- 06 NA 29.622 4 - 2.6131 14849	44.802 45.292 78246 42.247 58237 14.453 47493 NA 29.622 4 56.883 48922
INDOLE t2 INSK IPDPS IPMD IPPMIa IPPMIb IPPS	NA - 46.364 77748 - 83.706 51924 - 10.438 66729 NA 0 - 57.474 28678 2.7872	NA 6.7897 53743 - 38.260 40628 -1.00E- 06 NA 28.611 2 -1.00E- 06 37.817	NA 39.575 02374 45.446 11296 10.438 66629 NA 28.611 2 57.474 28578 35.030	NA 48.485 26176 - 75.229 23171 - 13.198 84823 NA 0 - 58.864 62992 2.0921	NA 6.9262 57807 - 35.500 22534 -1.00E- 06 NA 29.306 4 - 4.1057 91413 38.512	NA 41.559 00395 39.729 00637 13.198 84723 NA 29.306 4 54.758 8385 36.420	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593 NA 0 - 59.496 60407 1.7761	20.663 3 6.0979 62308 - 34.245 59764 -1.00E- 06 NA 29.622 4 - 2.6131 14849 38.828	44.802 45.292 78246 42.247 58237 14.453 47493 NA 29.622 4 56.883 48922 37.052
INDOLE t2 INSK IPDPS IPMD IPPMIa IPPMIb IPPS IZPN	NA 46.364 77748 83.706 51924 10.438 66729 NA 0 57.474 28678 2.7872 7512	NA 6.7897 53743 - 38.260 40628 -1.00E- 06 NA 28.611 2 -1.00E- 06 37.817 60249	NA 39.575 02374 45.446 11296 10.438 66629 NA 28.611 2 57.474 28578 35.030 32737	NA 48.485 26176 75.229 23171 13.198 84823 NA 0 58.864 62992 2.0921 0355	NA 6.9262 57807 - 35.500 22534 -1.00E- 06 NA 29.306 4 - 4.1057 91413 38.512 77406	NA 41.559 00395 39.729 00637 13.198 84723 NA 29.306 4 54.758 8385 36.420 67051	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593 NA 0 - 59.496 60407 1.7761 16473	20.663 3 - 6.0979 62308 - 34.245 59764 -1.00E- 06 NA 29.622 4 - 2.6131 14849 38.828 76114	44.802 45.292 78246 42.247 58237 14.453 47493 NA 29.622 4 56.883 48922 37.052 64466
INDOLE t2 INSK IPDPS IPMD IPPMIa IPPMIb IPPS IZPN	NA 46.364 77748 - 83.706 51924 - 10.438 66729 NA 0 - 57.474 28678 2.7872 7512	NA 6.7897 53743 - 38.260 40628 -1.00E- 06 NA 28.611 2 -1.00E- 06 37.817 60249	NA 39.575 02374 45.446 11296 10.438 66629 NA 28.611 2 57.474 28578 35.030 32737	NA 48.485 26176 75.229 23171 13.198 84823 NA 0 58.864 62992 2.0921 0355 6	NA 6.9262 57807 - 35.500 22534 -1.00E- 06 NA 29.306 4 - 4.1057 91413 38.512 77406	NA 41.559 00395 39.729 00637 13.198 84723 NA 29.306 4 54.758 8385 36.420 67051	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593 NA 0 - 59.496 60407 1.7761 16473 -	20.663 3 - 6.0979 62308 - 34.245 59764 -1.00E- 06 NA 29.622 4 - 2.6131 14849 38.828 76114	44.802 45.292 78246 42.247 58237 14.453 47493 NA 29.622 4 56.883 48922 37.052 64466
INDOLE t2 INSK IPDPS IPMD IPPMIa IPPMIb IPPS IZPN	NA 46.364 77748 83.706 51924 10.438 66729 NA 0 57.474 28678 2.7872 7512 47.029	NA - 6.7897 53743 - 38.260 40628 -1.00E- 06 NA 28.611 2 -1.00E- 06 37.817 60249 -1.00E-	NA 39.575 02374 45.446 11296 10.438 66629 NA 28.611 2 57.474 28578 35.030 32737 47.029	NA 48.485 26176 75.229 23171 13.198 84823 NA 58.864 62992 2.0921 0355 - 37.534	NA 6.9262 57807 - 35.500 22534 -1.00E- 06 NA 29.306 4 - 4.1057 91413 38.512 77406 -1.00E-	NA 41.559 00395 39.729 00637 13.198 84723 NA 29.306 4 54.758 8385 36.420 67051 37.534	24.138 7 51.390 74476 - 76.493 18002 - 14.453 47593 NA 0 - 59.496 60407 1.7761 16473 - 38.990	20.663 3 - 6.0979 62308 - 34.245 59764 -1.00E- 06 NA 29.622 4 - 2.6131 14849 38.828 76114 -1.00E-	44.802 45.292 78246 42.247 58237 14.453 47493 NA 29.622 4 56.883 48922 37.052 64466 38.990

KAS1553.3411.00e- 6985953.34150.78550.78550.78550.8951.00e- 598450.78550.8951.00e- 598450.78550.8951.00e- 598450.78550.8951.00e- 598450.78550.8951.00e- 3003450.8951.00e- 3003450.8951.00e- 3003450.8951.00e- 3003450.8951.00e- 3003450.1277.8800 300342.2.47 3.8203KDOP55.48510.91345.57548.5578.280130.63748.96583.53532.20951.326MDP99.86236.77455.92928.9011.00E28.90129.34331.00E29.34331.00E29.343K121644360.0627.92928.9011.00E28.90129.3431.00E29.34331.0229.343K12110.61223.52334.1351.03325.88836.92211.22427.09338.344K130293159116284121778040920.217669347.04513.788LDP_Di10.61223.52345.54521.82526.90123.94221.92424.947LEUTANANANANANANANANANALEUTANANANANANANANANANANALEUTANANANANANANANANANANANALEUTANANANA <th></th> <th>-</th> <th></th> <th></th> <th>-</th> <th></th> <th></th> <th>-</th> <th></th> <th></th>		-			-			-		
KAS15698590069759003340000234598400MANAKAS16NANANANANANANANANANANANANAKDOPP56.48510.91345.57248.5078.20010063762.1277.880039.1295.1277.880039.1277.88005.237KDOPP907585153539.2025153530.2015.816131.63648.9658.53532.20251.326KDOPS1500259411555928.50111.07629.34361.5588.260131.63648.96535.53532.20251.326KL2127.92959.106643367.106228.90129.34361.55861.55836.92211.02427.09238.324KL3110.61223.52334.13511.03328.88836.92211.22427.09238.324LDH_D148.5755.129411.02328.98929.79239.79220.669340.9442.247r12.76335.43961.57221.82535.88836.92211.92427.99438.324LDH_D112.76335.43961.57221.82535.89820.92720.669340.94LEUTANANANANANANANANALEUTANANANANANANANANALEUTAS1.7935.03063.157 <td></td> <td>53.341</td> <td>-1.00E-</td> <td>53.341</td> <td>55.785</td> <td>-1.00E-</td> <td>55.785</td> <td>56.895</td> <td>-1.00E-</td> <td>56.895</td>		53.341	-1.00E-	53.341	55.785	-1.00E-	55.785	56.895	-1.00E-	56.895
KAS16NA<	KAS15	69859	06	69759	00334	06	00234	5984	06	5974
NDPPNo.N	KAS16	NA	NA	NA	NA	NA	NA	NA	NA	NA
56.485 10.913 45.572 48.557 8.8280 39.729 50.127 7.8800 42.247 KDOPP 90758 51535 39223 00701 00641 00637 62178 3941 58237 KDOPS 1002 59411 55592 85315 11779 73536 83.535 32.209 51.326 KDOPS 27.929 -1.00E 27.929 27.929 27.929 34.135 11.035 28.901 28.901 21.00E 27.939 61.338 066 61238 K121 64436 006 64336 37106 006 37006 61358 0.00E 27.939 38.324 K131 23.523 34.135 11.032 25.888 36.922 11.224 27.099 38.324 K131 48.575 -3.1294 1 22 58.48 36.923 37.05 36.15 37.05 LDH_DI 48.575 -3.1294 1 22 8.54 2 28.98		-	-		-	-		-	-	
KDOPP90758515353922300701006410063762178394158237KDOPS35.0725559285.0131.63648.96583.53532.20951.326KDOPS1500259115559228.9111.00E28.90129.3431.00E-29.343K12i6443600664336371060637006613580.00E29.343K12i0.061223.52334.13511.03325.88836.92211.22427.09938.324K13i0293159916284121.77780409021776669347.045137.88LDH_Di48.575-3.129412-0.369239.72920.885442.247r48.575-3.129412-0.369239.72923.39636.61560.111LEUTA11228.54857.80923.99636.61560.111LEUTA12.76334.59363.15723.62636.42061.14750.37920.66371.424LEUTANANANANANANANANANANANALEUTA1929932.63751.93663.15723.64661.14750.37920.66371.424LEUTANANANANANANANANANANANALEUTANANANANANANANANANA7		56.485	10.913	45.572	48.557	8.8280	39.729	50.127	7.8800	42.247
NDM KDDPSNDM SS592NDM <br< td=""><td>KDOPP</td><td>90758</td><td>51535</td><td>39223</td><td>00701</td><td>00641</td><td>00637</td><td>62178</td><td>3941</td><td>58237</td></br<>	KDOPP	90758	51535	39223	00701	00641	00637	62178	3941	58237
99.86236.77463.08782.60133.63648.96583.53532.20951.326KDOPS150025941155592853151177973536855485376531783K12i644360066433637106-1.00E-28.90129.343-1.00E-29.343-1.378-1.378LDH_Di48.575-3.12941102-0.369239.72902.176669347.04542.247-1.378LDH_Di48.575-3.12941102-0.369235.78023.39636.61560.11460.144 <td></td> <td>-</td> <td>-</td> <td></td> <td>-</td> <td>-</td> <td></td> <td>-</td> <td>-</td> <td></td>		-	-		-	-		-	-	
KDOPS 15002 59411 55592 85315 11779 73536 85548 53765 31783 K12i 64436 0.00 64336 37106 1.00E- 28.901 37006 61338 0.06 61238 K12i 64436 0.0612 23.523 34.135 11.033 25.888 36.922 11.224 27.099 38.324 K13 02931 5991 62841 21767 80409 02177 66693 47045 13738 LDH_0i 48.575 -3.1294 1 2 -0.3692 39.729 2 0.8854 6 LEUTA 12.763 34.593 47.356 21.825 35.983 57.809 23.396 36.615 60.111 LEUTR NA <		99.862	36.774	63.087	82.601	33.636	48.965	83.535	32.209	51.326
27.929 4436 -1.006 6436 27.929 6436 28.901 37106 28.901 37006 29.343 61358 -1.006 61358 29.343 61358 $K12$ 10.612 23.923 23.523 5991 34.135 62841 11.037 21767 25.888 80409 36.922 211224 11.224 66693 27.099 47.045 38.324 47.045 LDH_{D1} r 48.575 5 -3.1294 45.446 10 40.098 2 -3.692 20.3692 39.729 20.277 20.8854 42.247 66693 LDH_{D1} r 48.575 5 -3.1294 47.356 10.224 21.825 21.825 35.983 51.929 57.809 23.396 36.615 23.396 60.611 40.44 42.247 60.44 $LEUTR$ $LEUTRNANANANANANANANALEUTRS1929934.59363.15723.62623.4966695160.147613150.3794980620.66320.663771.04220.663LIPIDASYNTHESISNANANANANANANANANANANANANANALIPIDASS1.577450.77350.77357.25050.77357.46050.77357.46050.77371.04221.3789LIPIDASS2.777450.77350.77457.47650.77357.46050.77357.46050.77357.46050.77357.46050.774LIPIDASLISO$	KDOPS	15002	59411	55592	85315	11779	73536	85548	53765	31783
27.929-1.00E-27.92928.901-1.00E-28.90129.343-1.00E-29.343Kt2i64436066433637106063700661358066125810.61223.52334.13511.03325.88836.92211.22427.09938.324Kt302931599162841217678040902177666934704513738LDH_Di48.575-3.1294120.369239.72920.885460.011r12.76334.59347.35621.82535.98357.80923.39636.61560.011LEUTRNANANANANANANANANALEUTRSNANANANANANANANANALIPID_S35.03063.15723.72636.42060.14750.37920.66371.042LEUTRNANANANANANANANANANALIPID_S35.03063.15723.72636.42060.14750.37920.66371.042LEUTRNANANANANANANANANANALIPID_S35.72735.03063.15723.72636.42060.14750.37920.66371.042LEUTRNANANANANANANANANANANASISNANANANA </td <td></td> <td>-</td> <td></td> <td></td> <td>-</td> <td></td> <td></td> <td>-</td> <td></td> <td></td>		-			-			-		
Kt2i 64436 0.6 64336 37106 0.6 37006 61358 0.6 61258 10.612 23.523 34.135 11.033 25.888 36.922 11.224 27.099 38.324 Kt3 02931 5991 62841 21767 80409 02177 66693 47045 13738 LDH_Di 48.575 -3.1294 45.446 40.098 -0.3692 39.729 22 0.8854 60.011 LEUTA 12.763 34.593 47.355 21.825 35.983 57.809 23.396 36.615 60.011 LEUTR NA		27.929	-1.00E-	27.929	28.901	-1.00E-	28.901	29.343	-1.00E-	29.343
NA23.52334.13511.03325.88836.92211.22427.09938.324LDH_D148.575599145.44140.09820177666934704513738LDH_D148.575-3.129445.44140.09820.369239.72020202012.67634.59347.35621.82535.98357.80923.39636.61260.011LEUTA12.76334.59347.35621.82535.98357.80923.39636.61560.11LEUTANANANANANANANANANALEUTA12.67335.03063.15723.72636.42060.14750.37920.66371.042LEUTA28.12735.03051.93623.72636.42060.14750.37920.66371.042LEUTA19.29932.63751.93623.72636.42060.14750.37920.66371.042LEUTANANANANANANANANANANALEUTAS1.27451.93651.93624.7236.42061.91750.37920.66371.042LEUTANANANANANANANANANANALEUTAS1.27451.93637.25037.25037.25037.25037.25037.25037.25037.25038.64070.9939.72037.25039.27239.272LPADSNA	Kt2i	64436	06	64336	37106	06	37006	61358	06	61258
10.61223.52334.13511.03325.88836.92211.22427.09938.324Kt302931599162841217678040902177666934704513738LDH_Di48.57545.44640.098-39.729200.885466r12.76334.59347.35621.82535.98357.80923.39636.61560.011LEUTA11228.8535.98357.80923.39636.61560.011LEUTANANANANANANANANANALEUTRSNANANANANANANANANALEUTRNANANANANANANANANANALEUTRNANANANANANANANANANALEUTRNANANANANANANANANANALEUTRNANANANANANANANANANALIPID_S SYNTHENANANANANANANANANANALIPID_S SYNTHENANANANANANANANANANALIPID_S SYNTHENANANANANANANANANANANANALIPID_S LIPASSY NTHESNANA		-			-			-		
Kt3 02931 5991 62841 21767 80409 02177 66693 47045 13738 LDH_Di 48.575 -3.1294 45.446 40.098 39.729 39.729 2 0.8854 6 r 12.763 34.593 47.356 21.825 35.983 57.809 23.396 36.615 60.011 LEUTA NA		10.612	23.523	34.135	11.033	25.888	36.922	11.224	27.099	38.324
LDH_DI rA8.575A5.446A0.098A0.098A9.269A9.729A1.362A9.827A2.247r12.76334.59347.35621.82535.98357.80923.39636.61560.011LEUTA111221.82535.98357.80923.39636.61560.011LEUTSNANANANANANANANANALEUTS192935.03063.15723.72636.42060.14750.37920.66371.042LEUT41929932637519369435936.42060.14750.37920.66371.042LEUT41929932637519369435936.42060.14750.37920.66371.042LEUT41929932637519369435936.42060.14750.37920.66371.042LEUT41929932637519369435936.42060.91449.8062602776.44LIPID_SNANANANANANANANANANALEUT45.27745121.3899939.7290.71239920.66339.272LEUT45.2774537.25037.25038.64039.27271.00239.272LPADS45.0850679399607929976.81470.0639.272LPADSA5NANANANANANANANA </td <td>Kt3</td> <td>02931</td> <td>5991</td> <td>62841</td> <td>21767</td> <td>80409</td> <td>02177</td> <td>66693</td> <td>47045</td> <td>13738</td>	Kt3	02931	5991	62841	21767	80409	02177	66693	47045	13738
LDH_Di48.57545.44640.098-41.36241.36242.247r5-3.129412-0.369239.72920.8854612.76334.59347.35621.82535.98357.80923.39636.61560.011LEUTA11220.8235.98357.80923.39636.61560.011LEUTRNANANANANANANANANA28.12735.03063.15723.72636.42060.14750.37920.66371.042LEUt41929326375193623.72636.42060.14750.37920.66371.042LEUt41929326375193623.72636.42060.14750.37920.66371.042LEUt41929326375193623.72636.42060.14750.37920.66371.042LEUt41929326375193623.72636.42060.14750.37920.66371.042LIPID_SNANANANANANANANANALEUt45.277450.72345.44640.8993.7290.712396JLEUTA5.277450.72345.44640.8639.27276.8439.27276.714LEUTA5.277450.72345.446793950.6639.27276.1439.272LPADSS450850644.985793966		-			-			-		
r100-3.129411100-0.369239.72910010010010012.76334.59347.35621.82535.98357.80923.39636.61560.011LEUTRNANANANANANANANANA28.12735.03063.15723.72636.42060.14750.37920.66371.042LEUTA19299326375193694359669516131498062662776434LIPID_S35.0305193694359669516131498062662776434LIPID_SNANANANANANANANANASISNANANANANANANANANALEUTA50.77450.17345.44619.8939.7250.712342.95942.247LEUDT5.277450.17337.25038.64079.9939.7290.712396LEUTA5.277450.72345.44621.389939.7250.712396LEUTA5.277450.7337.25038.64079.9939.72576.81442.95939.272LPADSS45.985NANANANANANANANANALPADSSNANANANANANANANANANALPADSSNANANANANANAN	LDH_Di	48.575		45.446	40.098			41.362		42.247
LEUTA12.76334.59347.35621.82535.98357.80923.39636.61560.011LEUTRSNANANANANANANANANANALEUTRSNANANANANANANANANANALEUTRSNANANANANANANANANANALEUTA28.12735.03063.15723.72636.42060.14750.37920.66371.042LEUt419299326375193694359669516131498062062776434LIPID_S YNTHENANANANANANANANANALIEUTANANANANANANANANANALIPID_S YNTHENANANANANANANANALIEUTA5.277450.72345.44641.86739.7290.712396LIEUTA5.277450.7637.25038.64039.7290.712396LPADSS45.0850637.25038.64039.2727.00639.2721.00639.272LPADS45.085NANANANANANANANALPSSYN NTHESINANANANANANANANASNANANANANANANANANANA <td>r</td> <td>5</td> <td>-3.1294</td> <td>1</td> <td>2</td> <td>-0.3692</td> <td>39.729</td> <td>2</td> <td>0.8854</td> <td>6</td>	r	5	-3.1294	1	2	-0.3692	39.729	2	0.8854	6
12.763 34.593 47.356 21.825 35.983 57.809 23.396 36.615 60.011 LEUTA 1 2 8 4 2 4 4 8 LEUTRS NA NA NA NA NA NA NA NA NA LEUTRS NA NA NA NA NA NA NA NA NA LEUt4 19299 32637 51936 63.157 23.726 36.420 60.147 50.379 20.663 71.042 LEUt4 19299 32637 51936 94359 66951 6131 49806 26627 76434 LIPID_S NA NA NA NA NA NA NA NA Sis NA 12.247 35.250 20.663 71.042 20.663 71.042 20.663 71.042 20.663 71.042 20.663 71.042 20.663 71.73 9 6 <td></td> <td>-</td> <td></td> <td></td> <td>-</td> <td></td> <td></td> <td>-</td> <td></td> <td></td>		-			-			-		
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LEUTRSNANANANANANANANANANANALEUTA28.12735.03063.15723.72636.42060.14750.37920.66371.042LEUT419299326375193694359669516131498062662776434LIPID_S YNTHE19299326375193694359669516131498062662776434SISNANANANANANANANANANALLEUTO5.277450.72345.446NANANANANANALLEUTO5.277450.72345.4462.138993.72939.7290.712342.95942.247LPADSS37.25045.94638.6407939950.72938.64039.2727681460.14739.272LPADSS450850637.25038.640792997681460.6139.27276714LPSSYN _coreNANANANANANANANANANALPSSYN NTHESINANANANANANANANANANANALPS_SYN 	LEUTA	1	1	2	8	4	2	4	4	8
$1 \\ 28,127$ $35,030$ $63,157$ $23,726$ $36,420$ $60,147$ $50,379$ $20,663$ $71,042$ $LEUt4$ 19299 32637 51936 94359 66951 6131 49806 26627 76434 $LIPID_S$ YNTHE SISNANANANANANANANA $LIPID_S$ YNTHE SISNANANANANANANA $LIPLD_S$ SISNANANANANANANANA $LIEUDr5.277450.72345.4461.05521.138941.8671.05639.7290.712342.95942.2471.0026LIEUDr5.277450.72345.4461.05621.138941.8671.05639.7290.712310.02639.272LIEUDr5.277450.72345.4461.05638.6407939939.72939.7271.002639.272LPADSS45.08537.2504508537.2504498538.6404498539.27239.27276.141LPSSYN.coreNANANANANANANANALPSSYNNTHESINANANANANANALPSSYNNTHESINANANANANANALPSSYNNTHESINANANANANANALSSYNNTHESINANANANANANA$	LEUTRS	NA	NA	NA	NA	NA	NA	NA	NA	NA
28.127 35.030 63.157 23.726 36.420 60.147 50.379 20.663 71.042 LEUt4 19299 32637 51936 94359 66951 6131 49806 26627 76434 LIPID_S YNTHE Image: Sige state st		-			-			-		
LEUt419299326375193694359669516131498062662776434LIPID_S YNTHE		28.127	35.030	63.157	23.726	36.420	60.147	50.379	20.663	71.042
LIPID_S YNTHE SISNANANANANANANANANASISNANANANANANANANANANANALLEUDr5.277450.72345.446 52.138941.867 539.7290.712342.95942.247LLEUDr5.277450.72345.446 52.1389939.7290.712396LLEUDr5.2774-1.00E- 450837.25038.640 4498539.27239.2721.00E- 7939939.27239.2721.00E- 7681439.272LPADSS450850637.250 4498538.640 7939938.640 7929939.2721.00E- 7681439.272LPSSYN _coreNANANANANANANANALPSSYS _roreNANANANANANANANALPS_SY NTHESINANANANANANANANALPS_SY NTHESINANANANANANANANANALPS_SY NTHESINANANANANANANANANALPS_SY NTHESINANANANANANANANANALPS_SY NTHESINANANANANANANANANALYSTPSNANANANANANANANANA	LEUt4	19299	32637	51936	94359	66951	6131	49806	26627	76434
YNTHEIndicationIndicationIndicationIndicationIndicationIndicationSISNANANANANANANANANALIEUDr5.277450.72345.44641.86739.7290.712342.95942.247LIEUDr5.277450102.13899990.71239637.25071.000-37.25037.25038.6401.000-38.64039.2721.000-39.272LPADSS450850637.25038.640793990679299768140.000-39.272LPSSYNNANANANANANANANANALPS_SYNNANANANANANANANALPS_SYNNANANANANANANANASNANANANANANANANALYSTESNANANANANANANANA	LIPID_S									
SISNA <td>YNTHE</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>	YNTHE									
LLEUDr 5.2774 5 1 2.1389 9 39.729 0.7123 9 6 LLEUDr 5.2774 5 1 2.1389 9 39.729 0.7123 9 6 37.250 45085 -1.00E- 37.250 38.640 -1.00E- 38.640 39.272 1.00E- 39.272 LPADSS 45085 06 37.250 37.250 38.640 79399 06 79299 76814 06 76714 LPSSYN A NA NA <t< td=""><td>CIC</td><td>NIA</td><td></td><td>N1.0</td><td></td><td></td><td>N1 A</td><td>N I A</td><td>N A</td><td></td></t<>	CIC	NIA		N1.0			N1 A	N I A	N A	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	SIS	NA	NA	NA	NA	NA	NA	NA	NA	NA
LPADSS37.250-1.00E-37.25038.640-1.00E-38.64039.272-1.00E-39.272LPADSS450850644985793990679299768140676714LPSSYN _coreNANANANANANANANANALPS_SYN NTHESINANANANANANANANALPS_SYN NTHESINANANANANANANALYSTESNANANANANANANA	SIS	NA	NA 50.723	NA 45.446	NA	NA 41.867	NA 20 720	NA	NA 42.959	NA 42.247
S7.250 -1.00E- S7.250 -1.00E- S8.640 -1.00E- S8.640 S9.272 -1.00E- S9.272 LPADSS 45085 06 44985 79399 06 79299 76814 06 76714 LPSSYN	SIS LLEUDr	NA 5.2774	NA 50.723 5	NA 45.446 1	NA 2.1389	NA 41.867 9	NA 39.729	NA 0.7123	NA 42.959 9	NA 42.247 6
LPAD33430830004498379393000792937081400070714LPSSYN _coreNANANANANANANANANANALPS_SY NTHESINANANANANANANANANANASNANANANANANANANANANALYSTESNANANANANANANANA	SIS LLEUDr	NA 5.2774 -	NA 50.723 5	NA 45.446 1	NA 2.1389 -	NA 41.867 9	NA 39.729	NA 0.7123 -	NA 42.959 9	NA 42.247 6
LFSSTNNANANANANANANA_coreNANANANANANANANALPS_SY NTHESINANANANANANANASNANANANANANANANALYSTRSNANANANANANANA	SIS	NA 5.2774 - 37.250	NA 50.723 5 -1.00E-	NA 45.446 1 37.250	NA 2.1389 - 38.640	NA 41.867 9 -1.00E-	NA 39.729 38.640	NA 0.7123 - 39.272 76814	NA 42.959 9 -1.00E-	NA 42.247 6 39.272
LPS_SY NTHESI S NA NA LYSTRS NA NA NA NA NA NA NA NA NA	SIS LLEUDr LPADSS	NA 5.2774 - 37.250 45085	NA 50.723 5 -1.00E- 06	NA 45.446 1 37.250 44985	NA 2.1389 - 38.640 79399	NA 41.867 9 -1.00E- 06	NA 39.729 38.640 79299	NA 0.7123 - 39.272 76814	NA 42.959 9 -1.00E- 06	NA 42.247 6 39.272 76714
NTHESI S NA	SIS LLEUDr LPADSS LPSSYN	NA 5.2774 - 37.250 45085	NA 50.723 5 -1.00E- 06	NA 45.446 1 37.250 44985	NA 2.1389 - 38.640 79399	NA 41.867 9 -1.00E- 06	NA 39.729 38.640 79299	NA 0.7123 - 39.272 76814	NA 42.959 9 -1.00E- 06	NA 42.247 6 39.272 76714
S NA	SIS LLEUDr LPADSS LPSSYN _core	NA 5.2774 - 37.250 45085 NA	NA 50.723 5 -1.00E- 06 NA	NA 45.446 1 37.250 44985 NA	NA 2.1389 - 38.640 79399 NA	NA 41.867 9 -1.00E- 06 NA	NA 39.729 38.640 79299 NA	NA 0.7123 - 39.272 76814 NA	NA 42.959 9 -1.00E- 06 NA	NA 42.247 6 39.272 76714 NA
	SIS LLEUDr LPADSS LPSSYN _core LPS_SY NTHFSI	NA 5.2774 37.250 45085 NA	NA 50.723 5 -1.00E- 06 NA	NA 45.446 1 37.250 44985 NA	NA 2.1389 - 38.640 79399 NA	NA 41.867 9 -1.00E- 06 NA	NA 39.729 38.640 79299 NA	NA 0.7123 - 39.272 76814 NA	NA 42.959 9 -1.00E- 06 NA	NA 42.247 6 39.272 76714 NA
	SIS LLEUDr LPADSS LPSSYN _core LPS_SY NTHESI S	NA 5.2774 - 37.250 45085 NA	NA 50.723 5 -1.00E- 06 NA	NA 45.446 1 37.250 44985 NA	NA 2.1389 - 38.640 79399 NA	NA 41.867 9 -1.00E- 06 NA	NA 39.729 38.640 79299 NA	NA 0.7123 - 39.272 76814 NA	NA 42.959 9 -1.00E- 06 NA	NA 42.247 6 39.272 76714 NA
	SIS LLEUDr LPADSS LPSSYN _core LPS_SY NTHESI S	NA 5.2774 37.250 45085 NA NA	NA 50.723 5 -1.00E- 06 NA NA	NA 45.446 1 37.250 44985 NA NA	NA 2.1389 - 38.640 79399 NA NA	NA 41.867 9 -1.00E- 06 NA NA	NA 39.729 38.640 79299 NA NA	NA 0.7123 - 39.272 76814 NA NA	NA 42.959 9 -1.00E- 06 NA NA	NA 42.247 6 39.272 76714 NA NA
23 726 10 505 43 322	SIS LLEUDr LPADSS LPSSYN _core LPS_SY NTHESI S LYSTRS	NA 5.2774 37.250 45085 NA NA	NA 50.723 5 -1.00E- 06 NA NA	NA 45.446 1 37.250 44985 NA NA	NA 2.1389 - 38.640 79399 NA NA	NA 41.867 9 -1.00E- 06 NA NA	NA 39.729 38.640 79299 NA NA	NA 0.7123 - 39.272 76814 NA NA	NA 42.959 9 -1.00E- 06 NA NA	NA 42.247 6 39.272 76714 NA NA
IYSt3 NA NA NA 94359 65182 59541 NA NA NA	SIS LLEUDr LPADSS LPSSYN _core LPS_SY NTHESI S LYSTRS	NA 5.2774 37.250 45085 NA NA NA	NA 50.723 5 -1.00E- 06 NA NA NA	NA 45.446 1 37.250 44985 NA NA NA	NA 2.1389 - 38.640 79399 NA NA NA	NA 41.867 9 -1.00E- 06 NA NA NA	NA 39.729 38.640 79299 NA NA NA	NA 0.7123 - 39.272 76814 NA NA	NA 42.959 9 -1.00E- 06 NA NA	NA 42.247 6 39.272 76714 NA NA

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	62.610	15.718	46.891	64.358	18.540	45.818	65.153	15.629	49.523
MACPD	51106	99772	51335	64424	6054	03884	25223	81027	44196
	-	_		-	-		-	-	
	64.267	18.208	46.059	65.658	23.830	41.827	62.934	9.4065	53.528
MALS	68347	57817	1053	02661	69808	32853	62817	11546	11662
	-			-			-		
MAN1P	27.501	35.586	63.087	19.214	38.724	57.939	20.622	40.151	60.773
Т2	50076	05515	55592	81015	53147	34162	79309	11161	9047
	-	-					-		
	35.139	0.1096	35.030				36.151	0.9015	37.052
MCITD	98591	585406	32737	NA	NA	NA	14456	001062	64466
	-	-		-	-		-	-	
	78.026	18.223	59.803	79.416	16.137	63.279	80.048	15.189	64.858
MCITS	32856	18351	14504	6717	66881	00289	64585	70757	93828
	-			-			-		
MCOA	36.831		36.831	38.221		38.221	38.853		38.853
ТА	1	0	1	4	0	4	4	0	4
	21.665		31.702	17.852	44.890			42.799	38.892
MDH	9	53.368	1	7	7	27.038	3.907	2	2
	-	-		-	-		-	-	
MDRP	68.826	33.795	35.030	69.521	33.100	36.420	69.837	32.784	37.052
D	02993	70256	32737	2015	53099	67051	18858	54392	64466
	-			-			-		
	26.549	-1.00E-	26.549	30.572	-1.00E-	30.572	44.613	23.109	67.722
ME2	3618	06	3608	10896	06	10796	09262	06159	15421
MEAM	-			-			-		
P1_GL	36.416	10.028	46.444	41.638	10.365	52.003	43.983	10.518	54.502
U-ASP	6	1	7	1	5	6	9	8	7
MEAM	-			-			-		
P1_GLY	32.410		46.044	39.108	13.971	53.079	41.454	14.124	
-ASP	2	13.634	2	4	4	8	2	8	55.579
MEAM	-			-			-		
P1_GLY	34.590		41.766	46.041		53.554	46.836		54.502
-GLU	9	7.1755	4	9	7.5129	8	5	7.6662	7
MECDP									
DH	NA	NA	NA	NA	NA	NA	NA	NA	NA
MECDP									
S	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
	81.745	25.495	56.249	83.135	26.850	56.285	83.767	25.591	58.176
MEPCT	48876	70582	78294	8319	6582	17369	80605	3702	43585

	-	-		-	-		-	-	
MET-	83.043	34.684	48.359	63.237	32.072	31.165	66.378	30.885	35.493
LABC	50293	29585	20708	66926	30033	36893	89881	03015	86867
	_			_			_		
	10.542	-1.00E-	10.542	3.3083	-1.00E-	3.3083	5.1949	-1.00E-	5.1949
METAT	06586	06	06486	36855	06	35855	38708	06	37708
	130.81	180.09	49.276				126.23	173.67	47.442
METGL	51361	18202	68412	NA	NA	NA	15033	40233	52008
	_	_		_	_		_	_	
	197.78	151.82	45.959	192.29	146.61	45.676	194.97	144.81	50.160
METS	08822	18591	02306	52863	83734	91291	64942	62381	25603
METTR									
S	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-								
	6.3890	28.641	35.030						
MGCH	72136	25523	32737	NA	NA	NA	NA	NA	NA
	6.5572	25.246	18.689	6.2703	27.726	21.456	6.1421	29.002	22.860
MGt3	78194	74965	47146	6433	58876	22443	43179	99512	85194
		11.583	11.583		12.316	12.316		12.649	12.649
MGt5	0	5	5	0	8	8	0	1	1
	-	-		-	-		-	-	
	78.934	33.361	45.572	71.005	31.276	39.729	72.576	30.328	42.247
MI1PP	34857	95634	39223	448	44163	00637	06277	4804	58237
				-			-		
	0.1083	35.138	35.030	0.5867	35.833	36.420	0.9027	36.149	37.052
MICITH	910332	7184	32737	805365	88997	67051	676136	87705	64466
	-			-			-		
	29.886	22.658	52.545	27.940	22.996	50.936	29.827	23.149	52.976
MICITL	7	7	4	5	1	6	1	5	6
	-								
	17.515	17.515	35.030						
MLACI	16369	16369	32737	NA	NA	NA	NA	NA	NA
MLTS	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
	58.711	6.1660	52.545	60.459	5.8286	54.631	61.254	5.6753	55.578
MLTSp	55731	66258	49106	69049	84725	00576	29648	29483	967
MMSD	156.52	226.74	70.218	152.37	218.95	66.587	150.48	220.53	70.053
Hir	28115	17401	92864	22874	96241	33675	56835	95595	87598
	-	-	<u></u>	-	-		-	-	
N 4 N 1	100.62	34.684	65.944	89.172	29.301	59.871	90.934	26.611	64.323
MNabc	86311	29785	33321	88633	66721	21912	95037	13776	8126
MOAT3	NA	NA	NA	NA	NA	NA	NA	NA	NA

	-	-		-	-		-	-	
MOBD	83.114	41.586	41.528	70.963	39.248	31.715	72.409	38.185	34.224
abc	62422	27238	35184	75376	21423	53953	85155	46053	39102
	-			-			-		
монм	34.493	-1.00E-	34.493	35.883	-1.00E-	35.883	36.515	-1.00E-	36.515
т	07503	06	07403	41817	06	41717	39232	06	39132
	-			_			-		
	50.436	-1.00E-	50.436	52.184	-1.00E-	52.184	52.979	-1.00E-	52.979
MTAN	36613	06	36513	49931	06	49831	1053	06	1043
		10.513	10.513		11.208	11.208		11.524	11.524
MTHFC	0	1	1	0	2	2	0	2	2
		37.867	37.867		28.372	28.372		29.828	29.828
MTHFD	0	5	5	0	9	9	0	3	3
	_	_		_	_		_	_	
MTHFR	65.784	20.338	45.446	57.307	17.578	39.729	58.571	16.323	42.247
2	56131	44834	11296	27377	26741	00637	22208	63971	58237
	_	_							
МТНРТ	217.73	166.78	50.942						
GHM	08218	84951	32673	NA	NA	NA	NA	NA	NA
	_								
	18.736		18.736						
MTRI	9	0	9	-19.432	0	19.432	-19.748	0	19.748
					_				
	-			-	0.0338		-		
	46.331	-1.00E-	46.331	46.387	778907	46.353	48.354	-1.00E-	48.354
MTRK	88364	06	88264	35855	5	48066	20093	06	19993
NADH1									
1	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	_		_	_		_	_	
NADH1	199.26	160.24	39.020	181.42	157.48	23.938	183.73	156.22	27.504
2	45687	36775	89122	22714	34966	77485	35067	88689	63783
NADH1									
3	NA	NA	NA	NA	NA	NA	NA	NA	NA
NADH1									
4	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			_			_		
	21.554	23.891	45.446	13.076	26.652	39.729	14.340	27.906	42.247
NADH4	15177	9612	11296	86423	14213	00637	81254	76983	58237
	-			-	-		-		
	30.171	-1.00E-	30.171	31.597	0.4317	31.165	34.186	-1.00E-	34.186
NADK	85515	06	85415	16786	989278	36893	66378	06	66278

	-			-			-		
	3.7042	-1.00E-	3.7042	3.3083	-1.00E-	3.3083	5.1949	-1.00E-	5.1949
NADS1	92886	06	91886	36855	06	35855	38708	06	37708
	-	-	40 420						
	90.016	41.587	48.429	ΝΑ	ΝΑ	ΝΑ	ΝΑ	ΝΑ	ΝΑ
0	00075	43025	17052		INA	INA	INA	INA	INA
	22,821	5.3060	28,127	23.726	-1.00F-	23,726	2.00F-	33,990	33,990
NAt3	17784	14153	19199	94359	06	94259	06	12167	11967
	-			_			_		
	28.127	-1.00E-	28.127	29.243	1.3853	30.628	5.6123	36.127	41.739
NAt3_2	19299	06	19199	55293	1556	86849	31964	06762	39958
		47.476	47.476		49.453	49.453		33.990	33.990
NAt9	0	8	8	0	7	7	0	1	1
	-			-			-		
	34.925		34.925	34.980		34.980	36.947		36.947
NDPK1	1	0	1	6	0	6	4	0	4
	-		27.042	-		27.000			
באססוא	37.942	0	37.942	37.998	0	37.998	20.005	0	20.005
NDPK2	D	0	0	1	0	L	-39.905	0	39.905
	2/1 822		24 822	2/1 877		24 877	26.844		26 844
	24.022 Д	0	24.022 A	24.877	0	24.877	20.844	0	20.844
			•				-		
	24.304		24.304	24.360		24.360	26.327		26.327
NDPK4	9	0	9	4	0	4	2	0	2
	-			-					
	34.047	12.386	46.434	34.103	12.250	46.353		13.078	49.148
NDPK5	6	9	5	1	4	5	-36.07	7	7
	-			-					
	27.728	18.705	46.434	27.784	18.569	46.353		19.397	49.148
NDPK6	7	8	5	1	3	4	-29.751	6	6
	-	24.424	16 10 1	-		46 959	-		40.4.40
דאססוא	25.303	21.131	46.434	25.358	20.994	46.353	27.325	21 022	49.148
NDPK/	5	Ζ	5	0	/	5	/	21.825	/
	26 655	19 778	46 434	- 26 711	19 642	46 352	28 678	20 470	49 148
NDPK8	20.055	8		20.711	3	-0.555	20.070	20.470	43.140 7
	,	16.998	16.998		17.673	17.673		17.979	17.979
NH4t	0	5	5	0	2	2	0	9	9
				_			-		
			28.326	10.654	20.547	31.202	10.958	21.699	32.657
NIt3	-9.9848	18.342	8	7	8	5	1	7	8

	-	-		-	-		-	-	
	63.602	38.678	24.923	63.901	40.728	23.172	66.104	39.785	26.318
NNAT	32926	5818	74746	5448	70576	83904	13373	40484	72889
	-	-		-	-		-	-	
	74.618	0.8531	73.764	77.061	2.5658	74.495	78.172	1.4692	76.702
NNDPR	10095	563203	94463	40569	98746	50695	00076	42578	75818
	-	-		-			-		
	98.242	6.4727	91.770	87.811	3.9025	91.714	88.236	6.4304	94.666
NODOx	81995	4515	0748	64724	60225	20746	16992	12824	58275
	-	-		-			-		
	110.29	6.1670	104.12	98.844	3.3648	102.20	99.460	5.5093	104.97
NODOy	33408	89891	62509	86491	5849	97234	83685	68002	02049
	-	-		-	-		-	-	
	102.53	60.242	42.287	104.27	59.210	45.068	105.07	58.740	46.332
NPHS	07822	8008	98136	89153	2477	66764	35213	90538	61594
	-	-		-	-		-	-	
	57.644	12.071	45.572	49.062	9.9864	39.076	50.475	9.0385	41.436
NTD1	38743	9952	39223	5868	80489	10631	20804	19257	68878
	-			-			-		
	28.337	-1.00E-	28.337	31.096	-1.00E-	31.096	33.605	-1.00E-	33.605
NTD10	51391	06	51291	03594	06	03494	29134	06	29034
	-	-		-	-		-	-	
	54.307	15.594	38./12	46.378	11.444	34.934	47.949	9.5574	38.391
NID11	50188	59572	90616	6013	0/165	52966	21608	69794	74629
	-	-	45 530						
	/1./36	26.164	45.572						
NIDIZ	9	6	3	NA	NA	NA	NA	NA	NA
	-	-	45 573	-	-	20 720	-	-	42 247
	59.029	13.457	45.572	51.100	11.3/1	39.729	52.6/1	10.423	42.247
NIDZ	78001	38//8	39223	87944	8/30/	00637	49421	91184	58237
NID3	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
NID3_	61.308	9.6572	51.650	58.895	9.3554	49.540	60.562	9.2182	51.343
Р	09679	91259	80553	80455	19485	38507	14396	05043	93891
	45 425	-	27 500	-	-	22 420	-	-	25 274
	45.435	1.8470	37.588	38.201	5.7615	32.439	40.088	4.8130	35.274
NTD4	21009	89399	12069	48109	7469	9064	08294	13459	40948
INT D5	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-	F4 650	-	-	40 5 40	-	-	F4 0 40
	54.240	2.5894	51.650	51.827	2.28/6	49.540	53.494	2.1503	51.343
۲	28367	/814	80553	99143	06366	38507	33084	91924	93891
NTD6	NA	NA	NA	NA	NA	NA	NA	NA	NA

	-	-		-	-		-	-	
NTD6_	59.541	7.8903	51.650	57.128	7.5885	49.540	58.795	7.4513	51.343
Р	20535	99819	80553	91311	28046	38507	25252	13604	93891
	-	-		-	-		-	-	
	46.259	29.932	16.327	37.220	26.793	10.426	38.474	25.367	13.107
NTD7	98817	23547	7527	16268	75916	40353	79038	17901	61137
NTD8	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		_	_		_	_	
NTD8	72.109	20.458	51.650	69.696	20.156	49.540	71.363	20.019	51.343
P _	05483	2493	80553	76259	37752	38507	10199	16308	93891
	-	_		_	_		_	_	
	59.061	13.489	45.572	51.132	11.403	39.729	52.703	10.455	42.247
NTD9	5719	17967	39223	67133	66496	00637	2861	70373	58237
	-	-					_	_	
NTPP1	92.385	53.650	38.734				94.927	55.277	39.650
0	23199	61273	61926	NA	NA	NA	97116	85764	11352
	-	_					_	_	
NTPP1	92.402	64.231	28.170				94.945	61.748	33.196
1	47724	63595	8413	NA	NA	NA	21641	40783	80858
	-	-					-	-	
	68.197	36.321	31.875				73.743	37.949	35.794
NTPP9	02115	88797	13318	NA	NA	NA	41031	13288	27743
	-	-		-	-		-	-	
	217.77	147.71	70.060	219.16	146.32	72.841	219.79	145.69	74.105
NTR4	50121	43574	65474	53553	40143	34102	73294	20401	28933
	-	-		-	-		-	-	
	155.67	85.614	70.060	157.06	84.224	72.841	157.69	83.592	74.105
NTR5	52079	55317	65474	55511	21003	34102	75252	23588	28933
O2t	-5.6468	0	5.6468	-7.7823	0	7.7823	-7.6832	0	7.6832
	-	-		-	-		-	-	
	65.424	24.371	41.053	67.172	22.511	44.661	67.967	12.388	55.578
OAADC	74893	62348	12545	88211	0298	85231	4901	5231	967
	-			_			-		
	38.005	-1.00E-	38.005	40.091	-1.00E-	40.091	41.039	-1.00E-	41.039
OBTFL	77141	06	77041	28412	06	28312	24535	06	24435
	-			-			-		
	60.148		60.148	51.862		51.862	53.270		53.270
OCBT	8	0	8	1	0	1	1	0	1
	-			-			-		
OHPBA	12.325		12.325	20.815	36.993	57.809	21.447	38.564	60.011
Т	9	0	9	6	6	2	6	2	8
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ОНРН	27.937	-1.00E-	27.937	22.451	-1.00E-	22.451	25.133	-1.00E-	25.133
M	56381	06	56281	96798	06	96698	17582	06	17482
	_			_					
	59 685	-1 00F-	59 685	60 902	-1 00F-	60 902	62 123	-1 00F-	62 123
	69521	1.001	69/21	56903	1.001	56803	208/13	1.000	297/13
OIVDI	05521	00	03421	30303	00	50005	23043	00	23743
	-	10 200	70.240	-	0 4275		-	10.007	70.052
	54.009	16.209	/0.218	58.159	8.4275	00.587	60.046	10.007	/0.053
OIVD2	22691	/01/3	92864	/5099	85761	33675	35484	52115	87598
	-			-			-		
	54.009	16.209	70.218	58.159	8.4277	66.587	60.046	10.007	70.053
OIVD3	08072	84792	92864	60479	31951	33675	20865	66734	87598
	-			-			-		
OMBZL	15.912	-1.00E-	15.911	10.426	-1.00E-	10.426	13.107	-1.00E-	13.107
М	00035	06	99935	40453	06	40353	61237	06	61137
	-	-		-	-		-	-	
OMCD	47.734	2.2655	45.468	51.547	1.9281	49.619	53.280	1.7748	51.506
С	5582	66537	99166	70074	85005	51574	94935	29763	11959
	_	_		_	_		_	_	
OMMB	220 30	184 05	36 250	214 15	181 62	32 527	216 54	181 07	35 475
інх	37822	32105	57166	59222	80507	87143	82768	27542	52263
	57022	52105	57100	55222	00507	07145	02700	27542	52205
	1/0 70	61 210	91 11C	120.22	69 001	E1 720	126.25		60 274
	140.79	04.540	04.440	01806	71025	47027	120.55	202.905	00.574
LITXAN	49854	0/9/	9057	01890	/1935	47027	92935	20382	08900
	-	4 9 9 5		-	4 9 9 5		-	4 995	
OMPD	40.848	-1.00E-	40.848	42.596	-1.00E-	42.596	43.391	-1.00E-	43.391
С	56599	06	56499	69916	06	69816	30715	06	30615
	-	-		-	-		-	-	
OMPH	220.30	184.05	36.250	214.15	181.62	32.527	216.54	181.07	35.475
HX	45561	39844	57166	66961	88246	87143	90507	35281	52263
	-	-		-	-		-	-	
OMPH	148.79	64.348	84.446	120.23	68.992	51.238	126.36	65.985	60.374
HXAN	57593	85358	9057	09635	49323	47027	00674	9787	08866
OMP		17.515	17.515		18.210	18.210		18.526	18.526
AC	0	2	2	0	3	3	0	3	3
OMP	-								
ACGA	14,320		14,320				15,147		15,147
M	- 1.525	0	- 1.520	-14 889	Ω	14 889	/ 	0	/
	/		/	14.005	0	14.005		0	
	- 17 515	17 515	25 020	10 210	10 210	26 120			
	с 17.212	CTC./T	55.050	10.210	10.210	50.420			
ADN	<u> </u>	2	4	3	3	6	NA	INA	INA

OMP_ 17.515 17.515 35.030 18.210 18.210 36.420 18.526 18.526 18.526 ALA-D 2 2 4 3 3 6 0 3 3 OMP_ 17.515 17.515 35.030 18.210 18.210 36.420 18.526 18.526 37.0 OMP_ 17.515 17.515 35.030 18.210 18.210 36.420 18.526 18.526 37.0 ALA-L 2 2 4 3 3 6 3 3 3	526 3 052 6 052 6
ALA-D 2 2 4 3 3 6 0 3 OMP_ 17.515 17.515 35.030 18.210 18.210 36.420 18.526 18.526 37.0 ALA-L 2 2 4 3 3 6 3 3 3	3 052 6 052 6
OMP_ 17.515 17.515 35.030 18.210 18.210 36.420 18.526 18.526 37.0 ALA-L 2 2 4 3 3 6 3 3 3	052 6 052 6
OMP_ 17.515 17.515 35.030 18.210 18.210 36.420 18.526 18.526 37.0 ALA-L 2 2 4 3 3 6 3 3 3	052 6 052 6
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UMP_C 17.515 17.515 35.030 18.210 18.210 36.420 18.526 18.526 37.0	J52
HITOB 2 2 4 3 3 6 3 3	6
OMP_C 17.515 17.515 35.030 18.210 18.210 36.420 18.526 18.526 37.0)52
HOL 2 2 4 3 3 6 3 3	6
OMP_C 17.515 17.515 35.030 18.210 18.210 36.420 18.526 18.526 37.0)52
IT 2 2 4 3 3 6 3 3	6
OMP_C 25.956 25.956 27.123 27.123 27.653 27.6	653
L 7 0 7 7 0 7 6 0	6
OMP_C 17.515 17.515 18.210 18.210 18.526 18.526 37.0)52
02 0 2 2 0 3 3 3 3	6
OMP_C	
OBALT 11.033 11.033 11.224 11.2	224
2 -10.612 0 10.612 2 0 2 7 0	7
OMP C 17.515 17.515 18.210 18.210 18.526 18.5	526
U2 2 0 2 3 0 3 3 0	3
OMP C 17.515 17.515 35.030 18.210 18.210 36.420	
YTD 2 2 4 3 3 6 NA NA NA	
OMP 17.515 17.515 35.030 18.210 18.210 36.420	
DAD-2 2 2 4 3 3 6 NA NA NA	

OMP_ DAMP	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	NA	NA	NA
OMP_ DCMP	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	NA	NA	NA
OMP_ DCYT	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	NA	NA	NA
OMP_ DGMP	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	NA	NA	NA
OMP_ DGSN	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	NA	NA	NA
OMP_ DMS	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	- 18.526 3	18.526 3	37.052 6
OMP_ DMSO	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	- 18.526 3	18.526 3	37.052 6
OMP_ DODCA	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	- 18.526 3	18.526 3	37.052 6
OMP_ DTMP	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	NA	NA	NA
OMP_ DURI	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	NA	NA	NA
OMP_F E2	-7.9699	0	7.9699	-8.2862	0	8.2862	-8.43	0	8.43
OMP_F OR	- 17.515 2	17.515 2	35.030 4	0	18.210 3	18.210 3	0	18.526 3	18.526 3
OMP_F UM	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	- 18.526 3	18.526 3	37.052 6
OMP_ GLU-L	- 17.515 2	17.515 2	35.030 4	- 18.210 3	18.210 3	36.420 6	- 18.526 3	18.526 3	37.052 6

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OMP_	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
GLY	2	2	4	3	3	6	3	3	6
OMP	-			_			_		
GLY-	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
ASP-I	2	2	4	3	3	6	3	3	6
			•						
	17515	17 515	25 020	10 210	10 210	26 120	10 576	10 526	27 052
	17.515	17.515	55.050	10.210	10.210	50.420	10.520	10.520	57.052
GLU-L	Z	Ζ	4	3	3	b	3	3	b
	-			-			-		
OMP_	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
GLYB	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
GLYCLT	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
GTHRD	2	2	4	3	3	6	3	3	6
OMP									
н	NA	NA	NA	NA	NA	NA	NA	NA	NA
				-					
	17 5 1 5	17 515	35 030	18 210	18 210	36 120	18 526	18 526	37 052
	27.515	17.515 2	33.030	10.210	10.210	50.420	10.520	10.520	57.052
	2	Z	4	3	J	0	3	3	0
		NIA	NIA	NIA	NIA	NIA	NLA	NIA	
1120	INA	NA	NA	NA	NA	NA	NA	NA	NA
	- -	NA	NA	NA -	NA	NA	NA -	NA	NA
OMP_	- 17.515	NA 17.515	NA 35.030	NA - 18.210	NA 18.210	NA 36.420	NA - 18.526	NA 18.526	NA 37.052
OMP_ H2O2	- 17.515 2	NA 17.515 2	NA 35.030 4	NA - 18.210 3	NA 18.210 3	NA 36.420 6	NA - 18.526 3	NA 18.526 3	NA 37.052 6
OMP_ H2O2	17.515 2	NA 17.515 2	NA 35.030 4	NA - 18.210 3 -	NA 18.210 3	NA 36.420 6	NA - 18.526 3 -	NA 18.526 3	NA 37.052 6
OMP_ H2O2 OMP_	17.515 2 17.515	NA 17.515 2 17.515	NA 35.030 4 35.030	NA - 18.210 3 - 18.210	NA 18.210 3 18.210	NA 36.420 6 36.420	NA - 18.526 3 - 18.526	NA 18.526 3 18.526	NA 37.052 6 37.052
OMP_ H2O2 OMP_ H2S	17.515 2 17.515 2 17.515 2	NA 17.515 2 17.515 2	NA 35.030 4 35.030 4	NA - 18.210 3 - 18.210 3	NA 18.210 3 18.210 3	NA 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3	NA 18.526 3 18.526 3	NA 37.052 6 37.052 6
OMP_ H2O2 OMP_ H2S	17.515 2 17.515 2 17.515 2	NA 17.515 2 17.515 2	NA 35.030 4 35.030 4	NA - 18.210 3 - 18.210 3 -	NA 18.210 3 18.210 3	NA 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3 -	NA 18.526 3 18.526 3	NA 37.052 6 37.052 6
OMP_ H2O2 OMP_ H2S OMP_	17.515 2 17.515 2 17.515 2 17.515	NA 17.515 2 17.515 2 17.515	NA 35.030 4 35.030 4 35.030	NA 18.210 3 - 18.210 3 - 18.210	NA 18.210 3 18.210 3 18.210	NA 36.420 6 36.420 6 36.420	NA - 18.526 3 - 18.526 3 - 18.526	NA 18.526 3 18.526 3 18.526	NA 37.052 6 37.052 6 37.052
OMP_ H2O2 OMP_ H2S OMP_ HDCA	17.515 2 17.515 2 17.515 2 17.515 2	NA 17.515 2 17.515 2 17.515 2	NA 35.030 4 35.030 4 35.030 4	NA - 18.210 3 - 18.210 3 - 18.210 3	NA 18.210 3 18.210 3 18.210 3	NA 36.420 6 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3 - 18.526 3	NA 18.526 3 18.526 3 18.526 3	NA 37.052 6 37.052 6 37.052 6
OMP_ H2O2 OMP_ H2S OMP_ HDCA	17.515 2 17.515 2 17.515 2 17.515 2	NA 17.515 2 17.515 2 17.515 2	NA 35.030 4 35.030 4 35.030 4	NA - 18.210 3 - 18.210 3 - 18.210 3 -	NA 18.210 3 18.210 3 18.210 3	NA 36.420 6 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3 - 18.526 3 -	NA 18.526 3 18.526 3 18.526 3	NA 37.052 6 37.052 6 37.052 6
OMP_ H2O2 OMP_ H2S OMP_ HDCA	17.515 2 17.515 2 17.515 2 17.515 2 - 17.515	NA 17.515 2 17.515 2 17.515 2 17.515	NA 35.030 4 35.030 4 35.030 4 35.030	NA 18.210 3 - 18.210 3 - 18.210 3 - 18.210 - 18.210	NA 18.210 3 18.210 3 18.210 3 18.210	NA 36.420 6 36.420 6 36.420 6 36.420	NA - 18.526 3 - 18.526 3 - 18.526 3 - 18.526	NA 18.526 3 18.526 3 18.526 3 18.526	NA 37.052 6 37.052 6 37.052 6 37.052
OMP_ H2O2 OMP_ H2S OMP_ HDCA OMP_I LE-I	17.515 2 17.515 2 17.515 2 17.515 2 17.515 2	NA 17.515 2 17.515 2 17.515 2 17.515 2	NA 35.030 4 35.030 4 35.030 4 35.030 4	NA - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3	NA 18.210 3 18.210 3 18.210 3 18.210 3	NA 36.420 6 36.420 6 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3 - 18.526 3	NA 18.526 3 18.526 3 18.526 3 18.526 3	NA 37.052 6 37.052 6 37.052 6 37.052 6
OMP_ H2O2 OMP_ H2S OMP_ HDCA OMP_I LE-L	17.515 2 17.515 2 17.515 2 17.515 2 17.515 2	NA 17.515 2 17.515 2 17.515 2 17.515 2	NA 35.030 4 35.030 4 35.030 4 35.030 4	NA 18.210 3 18.210 3 18.210 3 18.210 3 18.210 3	NA 18.210 3 18.210 3 18.210 3 18.210 3	NA 36.420 6 36.420 6 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3 - 18.526 3 - 18.526 3	NA 18.526 3 18.526 3 18.526 3 18.526 3	NA 37.052 6 37.052 6 37.052 6 37.052 6
OMP_ H2O2 OMP_ H2S OMP_ HDCA OMP_I LE-L	17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515	NA 17.515 2 17.515 2 17.515 2 17.515 2 17.515	NA 35.030 4 35.030 4 35.030 4 35.030 4 35.030	NA - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210	NA 18.210 3 18.210 3 18.210 3 18.210 3 18.210	NA 36.420 6 36.420 6 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3 - 18.526 3 - 18.526 3 - 18.526	NA 18.526 3 18.526 3 18.526 3 18.526 3	NA 37.052 6 37.052 6 37.052 6 37.052 6
OMP_ H2O2 OMP_ H2S OMP_ HDCA OMP_I LE-L OMP_I	17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515	NA 17.515 2 17.515 2 17.515 2 17.515 2 17.515	NA 35.030 4 35.030 4 35.030 4 35.030 4	NA - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210	NA 18.210 3 18.210 3 18.210 3 18.210 3 18.210 3 18.210 3	NA 36.420 6 36.420 6 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3 - 18.526 3 - 18.526 3	NA 18.526 3 18.526 3 18.526 3 18.526 3	NA 37.052 6 37.052 6 37.052 6 37.052 6 37.052
OMP_ H2O2 OMP_ H2S OMP_ HDCA OMP_I LE-L OMP_I NDOLE	17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2	NA 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2	NA 35.030 4 35.030 4 35.030 4 35.030 4 35.030 4	NA 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - - - - - - - - - - - - -	NA 18.210 3 18.210 3 18.210 3 18.210 3	NA 36.420 6 36.420 6 36.420 6 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3 - 18.526 3 - 18.526 3	NA 18.526 3 18.526 3 18.526 3 18.526 3	NA 37.052 6 37.052 6 37.052 6 37.052 6 37.052 6
OMP_ H2O2 OMP_ H2S OMP_ HDCA OMP_I LE-L OMP_I NDOLE	17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2	NA 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2	NA 35.030 4 35.030 4 35.030 4 35.030 4 35.030 4	NA - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 - 18.210 - 18.210	NA 18.210 3 18.210 3 18.210 3 18.210 3 18.210 3 18.210 3 18.210 3	NA 36.420 6 36.420 6 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3 - 18.526 3 - 18.526 3 - 18.526 3 -	NA 18.526 3 18.526 3 18.526 3 18.526 3 18.526 3	NA 37.052 6 37.052 6 37.052 6 37.052 6
OMP_ H2O2 OMP_ H2S OMP_ HDCA OMP_I LE-L OMP_I NDOLE OMP_I	- 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515	NA 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515 2 17.515	NA 35.030 4 35.030 4 35.030 4 35.030 4 35.030 4 35.030	NA - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210 3 - 18.210	NA 18.210 3 18.210 3 18.210 3 18.210 3 18.210 3 18.210 3 18.210 3	NA 36.420 6 36.420 6 36.420 6 36.420 6 36.420 6	NA - 18.526 3 - 18.526 3 - 18.526 3 - 18.526 3 - 18.526 3 - 18.526	NA 18.526 3 18.526 3 18.526 3 18.526 3 18.526 3 18.526	NA 37.052 6 37.052 6 37.052 6 37.052 6 37.052 6

OMP_I	-			-			-		
NOSPP	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
1	2	2	4	3	3	6	3	3	6
	-						-		
	19.657		19.657				20.792		20.792
OMP_K	8	0	8	-20.438	0	20.438	7	0	7
	-			-			-		
OMP_L	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
AC-D	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_L	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
AC-L	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_L	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
EU-L	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_L	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
YS-L	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
MAL-L	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
MET-L	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_	11.583		11.583	12.316		12.316	12.649		12.649
MG2	5	0	5	8	0	8	1	0	1
	-			-			-		
OMP_	17.515		17.515	18.210		18.210	18.526		18.526
MN2	2	0	2	3	0	3	3	0	3
	-			-			-		
OMP_	10.613		10.613	11.034		11.034	11.225		11.225
MOBD	2	0	2	4	0	4	9	0	9
OMP		16.998	16.998		17.673	17.673		17.979	17.979
NH4	0	5	5	0	2	2	0	9	9
	_			_			_		
OMP	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
NMN	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
NO2	2	2	4	3	3	6	3	3	6

	-			-			-		
OMP	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
NO3	2	2	4	3	3	6	3	3	6
OMP									
02	-5 6468	0	5 6468	-7 7823	0	7 7823	-7 6832	0	7 6832
	-		510 100			///020	-		,10002
	17 515	17 515	35 030	18 210	18 210	36 420	18 526	18 526	37 052
	17.515	17.515	JJ.050 A	10.210	10.210	50.420	10.520	10.520	57.052
UCDCA	Z	۷	4		5	0			0
	16 620		16 620	12 110		12 110	1/1 201		14 201
	10.020	0	10.020	15.119	0	15.119	14.291	0	14.291
1	5	0	5	/	0	/	5	0	5
	- 17 5 1 5		17 515	-		10 210	- 10 5 2 C		10 5 26
	17.515	0	17.515	18.210	0	18.210	18.526	0	18.526
IVICUA	Ζ	0	Z	3	0	3	3	0	3
0145 B	-	47 545	25 020	-	40.040	26.420	-	40 500	27.052
OMP_P	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
РА	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_P	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
RO-L	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_P	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
TRC	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_P	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
YR	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_S	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
ER-L	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_S	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
03	2	2	4	3	3	6	3	3	6
	_			_			_		
OMP S	25.219		25.219	26.220		26.220	26.675		26.675
04	3	0	3	2	0	2	2	0	2
	-								
OMP S	17,515	17,515	35,030	18,210	18,210	36.420		18,526	18,526
	27.515	27.515	JJ.050 ⊿	10.210 2	10.210 2	50.420 6	Ω	10.520 2	10.520 2
	Z	2				0	0		
	- 17 515	17 515	32 030	-	18 210	36 420	- 18 526	18 526	37 052
	с.,тт СтС.,тт С	د ديد. بي	55.050 A	10.210	10.210	50.420 6	10.520	10.520	220.72 م
	Z	2	4	3	3	0	3	3	0

OMP_T	- 17.515	17.515	35.030	- 18.210	18.210	36.420			
HYMD	2	2	4	3	3	6	NA	NA	NA
	-			-			-		
OMP_T	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
MA	2	2	4	3	3	6	3	3	6
014D T	-	47 545	25 020	-	10.240	26 420	-	40 500	27 052
	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
MAU	Z	Z	4	3	3	6	3	3	0
	- 17515	17 515	35 030	- 18 210	18 210	36 420	18 526	18 526	37 052
RP-I	17.515	17.515	33.030 4	10.210	10.210	50.420	10.520	10.520	57.052
	-	2		-	5	0			0
омр т	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
SUL	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_T	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
TDCA	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_T	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
TTNT	2	2	4	3	3	6	3	3	6
	-			-			-		
OMP_T	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
YR-L	2	2	4	3	3	6	3	3	6
	-			-			-	10 500	
OMP_	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
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	0	17.515	17.515	0	18.210 c	18.210	0	18.520	18.520
UREA	0	Z	Z	0	5	5	0	5	5
OMP	- 17 515	17 515	35 030	18 210	18 210	36 420			
	2	2	33.030 4	10.210	3	50.420 6	NA	NA	NA
			· · ·	-			_		
OMP V	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	37.052
AL-L	2	2	4	3	3	6	3	3	6
	-			-					
OMP_X	17.515	17.515	35.030	18.210	18.210	36.420			
AN	2	2	4	3	3	6	NA	NA	NA
	-			-			-		
OMP_n	28.890	28.890	57.781	30.037	30.037	60.074	30.558	30.558	61.117
a1	7	7	4	4	4	8	6	6	2

	-	-		-	-		-	-	
OPHBD	55.203	2.6582	52.545	56.951	2.3208	54.631	57.746	2.1674	55.578
С	70214	13084	48906	83532	31552	00376	44331	7631	967
	_	_		_	_		_	_	
	221.91	184.05	37.853	221.94	181.63	40.311	221.97	181.07	40.894
орннх	27433	90074	73599	56507	38476	80316	27846	8551	23359
		_		_	_			_	
ОРННХ	150 40	64 353	86.050	128 01	68 997	59 022	131 78	65 991	65 792
ΔΝ	39466	87653	07003	99182	51618	402	38013	00065	80062
	33400	0/035	07003	55102	51010	402	50015	00005	00002
		10 257	20 721	- 	10.040		61 1 1 1	10 006	12 217
	56.092	19.557	50.754	56.709	19.040	20 720	01.144	10.090	42.247
URINCD	34,000	/	56.240	0	00 4 4 2	59.729	4	00.075	0
	31.803	88.053	56.249	33.158	89.443	56.285	31.899	90.075	58.176
ORPT	6	4	8	5	/	2	2	/	5
	-			-			-		
OXGDC	56.345	-1.00E-	56.345	62.924	-1.00E-	62.924	63.556	-1.00E-	63.556
2	18573	06	18473	83116	06	83016	80732	06	80632
	-	-		-	-		-	-	
	51.604	11.347	40.256	58.477	19.824	38.652	59.732	18.560	41.171
P5CD	28013	46946	81067	54225	757	78526	16995	80869	36126
	-	-		-	-		-	-	
	85.318	27.516	57.802	75.824	25.599	50.224	77.279	24.728	52.551
P5CR	78708	49803	28905	19639	67409	5223	59395	38948	20448
	-	-		-	-		-	_	
	109.75	60.413	49.345	112.25	62.060	50.189	113.38	61.029	52.353
PANTS	90089	22778	78112	00295	93213	09738	23116	20259	109
	_			_	_		_	_	
	58 922	13 350	45 572	50 993	11 264	39 729	52 564	10 317	42 247
ΡΔΡ	88989	49766	39223	98931	98295	00637	60409	02172	58237
		13700	35223		56255	00007		02172	30237
DADDT	22 686	-1 00F-	22 686	24 076	-1 00F-	24 076	2/1 708	-1 00F-	2/1 708
2	56852	1.000	56752	01166	1.000	01066	24.700	1.000	24.700
	50052						00001		00401
PAPSR	INA	INA	INA	INA	INA	INA	NA	INA	INA
PASYN									
_WP2	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-	-		-	-	
	59.399	0.1164	59.515	60.864	5.9784	54.885	61.530	4.3984	57.131
PDH	09981	649096	56472	40586	08323	99754	45607	72937	98313
PDX5P					56.342	62.413		56.974	63.262
0	-5.6468	0	5.6468	-6.0704	8	2	-6.2873	8	1
	-	-		-	-		-	-	
PDX5P	293.60	219.64	73.960	305.49	226.03	79.458	308.31	223.82	84.495
S	12177	03632	85445	01468	21361	01073	53913	02265	16474

PEPTID									
OXe	NA	NA	NA	NA	NA	NA	NA	NA	NA
PEPTID									
O SYN									
THESIS	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-						-		
	10.415		10.415				14.430		42.247
PERD	8	0	8	-13.176	26.553	39.729	6	27.817	6
	_			_			_		
	46.851		46.851	40.416		40.416	41.909		41.909
PFL	3	0	3	7	0	7	4	0	4
		14.318	14.318		15.013	15.013		15.329	15.329
PGAMT	0	4	4	0	6	6	0	5	5
	12.402	57.848	45.446	13.925	44.008	30.083	11.257	45.272	34.014
PGCD	7505	86346	11296	07738	50305	42567	82844	45136	62291
	_			_			_		
	40.836	19.913	60.750	43.806	-1.00E-	43.806	45.156	25.091	70.247
PGDH	74873	3052	05393	53428	06	53328	4398	45276	89256
		_		_	_			_	
	58.780	23.750	35.030	59.475	23.054	36.420	59.791	22.739	37.052
PGDHY	49256	16519	32737	66413	99362	67051	65121	00655	64466
					13.553	13.553		13.869	13.869
PGI	0	12.858	12.858	0	1	1	0	1	1
	-						-		
	30,334	16,100	46.434				10,293		10,293
PGK	4	1	5	-8.5648	0	8.5648	4	0	4
				_					
	40.325	5.2953	35.030	41.020	4.6002	36.420	41.336	4.2842	37.052
PGL	7264	99029	32737	89797	27459	67051	88505	40382	64466
	_	_		_			_	_	
PGLYC	83,446	37.874	45.572	75.517	35.788	39,729	77.088	34,840	42,247
P	80607	41383	39223	90549	89912	00637	52027	93789	58237
	-						-		
	12.152	22.878	35.030				10.293		10.293
PGM	1	2	3	-8.5648	0	8.5648	4	0	4
					11.009	11.009		11.325	11.325
PGMT	0	10.314	10.314	0	2	2	0	2	2
	-			-	-		-	-	
	48.497	10.909	37.588	41.263	8.8238	32.439	43.150	7.8759	35.274
PGPPH	52343	40273	12069	79442	88025	9064	39627	26794	46948
				-					
				10.921		10.921	11.553		11.553
PGSA	-9.5309	0	9.5309	2	0	2	2	0	2

	-	-							
PHE4M	459.46	383.75	75.707						
0	31406	56686	47197	NA	NA	NA	NA	NA	NA
	-	4 7556	20 724	-	- 0705	20 720	-	E 946E	40.047
	33.978	4.7556	38.734	34.656	5.0725	39.729	37.031	5.2165	42.247
PHEAL	97042	48838	61926	48134	25029	00637	02271	5966	58237
	-	-	FF 222	- 70 120	-	46.067			
	90.010	24.004	20.552	70.159	52.072	40.007	ΝΑ	ΝΑ	ΝΑ
	0	5		/	35 962	35 962		36 594	36 594
1	0	34.572	34.572	0	4	4	0	4	4
PHETR									
S	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-							
	89.121	46.893	42.228						
Plabc	91623	44588	47035	NA	NA	NA	NA	NA	NA
	-			-			-		
	21.926		21.926	13.119		13.119	14.291		14.291
PIt6	5	0	5	7	0	7	3	0	3
	-						-		
PMAN	23.276	11.753	35.030				24.287	12.764	37.052
Μ	8	5	3	NA	NA	NA	9	7	6
PMCO		17.515	17.515		18.210	18.210		18.526	18.526
At	0	2	2	0	3	3	0	3	3
	-	-	45 530	-	-	20 720	-	-	42.247
	58.662	13.090	45.572	50.733	11.004	39.729	52.304	10.056	42.247
	20928	1//35	39223	009	00204	00637	28378	70141	58237
	35 304	-1 00F-	35 304	34 680	-1 00F-	34 680	36 338	-1 00F-	36 338
ΡΝΤΚ	79657	-1.00L-	79557	74784	06	74684	71584	06	71484
	-		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			74004			71404
	42,990	18.202	24.788	20.985	14.368	6.6166	23.015	12.625	10.389
РРА	57045	14884	42161	17266	50095	71711	80915	93373	87542
	_			_			_		
	28.127	35.030	63.157	23.726	36.420	60.147	50.379	20.663	71.042
PPAtNa	2	3	5	9	7	6	5	3	8
	_	_		_	_		_	_	
PPBNG	115.25	62.705	52.545	115.58	60.957	54.631	115.74	60.163	55.578
S	12853	7942	49106	86668	66102	00576	2022	05503	967
	-			-	-		-	-	
	70.733	7.6455	63.087	53.472	4.5070	48.965	54.406	3.0804	51.326
PPC	09089	36974	55392	79402	60658	73336	79685	78514	31833

	-	-		-	-		-	-	
	59.454	6.9090	52.545	61.202	6.5716	54.631	61.997	6.4182	55.578
PPCDC	51867	29611	48906	65184	48078	00376	25983	92836	967
	-			-			-		
	54.313	9.6358	63.949	55.422	2.1082	57.530	57.867	3.5161	61.383
РРСК	83623	35268	6715	27275	15672	48842	73604	98612	93466
								10.062	10.062
PPM	0	9.0513	9.0513	0	9.7465	9.7465	0	5	5
					14.478	36.420		14.794	37.052
PPM2	-16.926	0	16.926	-21.942	7	7	-22.258	7	7
	_	_		_	_		_	_	
	99.046	11.136	87.909	86.812	7.3031	79.508	88.220	5.5605	82.659
PPNCL	76434	77554	9888	04122	27656	91356	02416	60436	46372
	_	_		_	_		_	_	
	129.56	66.602	62.961	133.37	75.437	57.939	135.10	74.335	60.773
PPND	34442	16957	27465	65868	24714	33962	98354	93067	9047
	_	_		_	_		_	_	
	132.79	80.249	52.545	134.54	79.912	54.631	135.33	79.758	55.578
PPNDH	49456	45658	48906	30788	07505	00376	76868	71981	967
	_	_		_	_		_	_	
PPPGF	156.24	67.423	88.823	151.10	64.642	86.460	157.07	63.378	93.699
UM	66059	52747	07846	29657	84119	12447	87583	89289	86541
	_			_			_		
PPPGM	3.0796	137.04	140.12	5.8603	139.82	145.68	7.1243	141.08	148.21
EN	9886	16106	13095	85138	22969	2682	33447	62452	05787
	_	_		_	-		_	_	
PPPGN	551.31	411.19	140.12	554.09	408.41	145.68	555.35	407.14	148.21
03	37532	24437	13095	44394	17574	2682	83877	78091	05787
	-	-		-	-		-	_	
	619.19	575.69	43.500	617.90	569.81	48.094	617.35	568.78	48.577
PPPGO	96191	90659	55322	79981	39297	06845	74257	00142	41145
	-	-		-	-		-	-	
	59.801	13.813	45.988	52.567	17.422	35.145	54.454	14.980	39.474
PPS	61405	46847	14558	88504	20532	67972	48689	30693	17996
PPTGS									
e	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
	126.99	70.749	56.249	128.38	72.104	56.285	129.02	70.844	58.176
PPTT	91073	32435	78294	94504	27673	17369	14246	98873	43585
	-	_		-	-		-	-	
	87.372	20.115	67.257	75.138	10.860	64.277	76.546	9.1946	67.351
PRAGS	95473	30953	6452	2316	52852	70308	21454	38421	57612

	-	-		-	-		-	-	
	104.25	48.919	55.332	92.375	46.307	46.067	93.945	45.120	48.825
PRAIS	21281	82223	3059	19505	82672	36833	80982	55603	25379
	-			-			-		
	22.886	-1.00E-	22.886	23.581	-1.00E-	23.581	23.897	-1.00E-	23.897
PRAli	55267	06	55167	72424	06	72324	71132	06	71032
PRAMP									
С	NA	NA	NA	NA	NA	NA	NA	NA	NA
	_	_			_		_	_	
	86.567	34.022	52.545		30.884	44.501	77.272	29.457	47.815
PRASCS	8	6	2	-75.386	1	9	6	5	1
	_	_		_	_		_	_	
PRATP	88.200	49.466	38.734	89.948	51.873	38.074	90.743	51.093	39.650
Р	68033	06107	61926	8135	97507	83844	41949	30598	11352
	_			_			_		
	52.610	-1.00E-	52.610	45.541	-1.00E-	45.541	47.428	-1.00E-	47.428
PRFGS	41779	06	41679	73746	06	73646	33931	06	33831
	-	_		-			-		
	49 4 39	3 8348	45 604	49 495	3 9713	45 523	51 462	3 1430	48 318
PRKIN	70088	2531	87557	17579	29374	84641	01817	33875	98429
	-	2001	0/33/	-	25571	01011	-	33673	50125
PRMICI	22 860	-1 00F-	22 860	23 555	-1 00F-	23 555	23 871	-1 00F-	23 871
i	47664	06	47564	64821	06	64721	63529	06	63429
		-			-	0.722	-	_	00.25
	161 02	97 391	63 635	153.05	96 000	57 051	154 73	95 368	59 362
PRO1a	66299	19687	433	19632	85373	1095	12244	87957	34479
PROTR	00200	1000/		10001	00070	1000		0,007	01170
s	NA	NA	NA	NA	NA	NA	NA	NA	NA
	147.		1473			1473			
SYNTH									
FSIS	NA	NA	NA	NA	NA	NA	NA	NA	NA
20.0	_			_			_		
	28 127	35 030	63 157	23 726	36 420	60 147	50 379	20 663	71 042
PROt4	19299	32637	51936	94359	66951	6131	49806	26627	76434
······		-	51550	5 1000	00001	0101			, , , , , , , , , , , , , , , , , , , ,
	41 373	11 102	30 270					10 730	32 665
PRPPS	6	8	80.270	-42,764	-12.071	30,693	-43,396	4	6
	-				12.071	22.055	-		5
	71,191		63,087	53,931		48,965	54,865		51,326
PSCVT	7	-8,1042	55.007	4	-4.9657	7	4	-3.5391	3
	_			-			-		
	61 690	9,1448	52 545	63 438	8,8074	54 631	64 233	8,6540	55 578
PSD	31672	2766	48906	44989	46127	00376	05788	90885	967
	31072	2,00	.0000	1,505		00070	00700	50005	507

	-			-			-		
	45.462	1.8941	47.356	46.852	10.956	57.809	47.484	12.527	60.011
PSERT	06064	28123	18876	40378	80964	21342	37793	42442	80235
	-	-		-	-		-	-	
	53.127	7.5553	45.572	45.198	5.4697	39.729	46.769	4.5218	42.247
PSP_L	70627	14036	39223	80569	99327	00637	42047	38096	58237
				-			-		
				28.421		28.421	29.053		29.053
PSSA	-27.031	0	27.031	4	0	4	3	0	3
	-			-			-		
	42.678	1.4030	44.081	43.016	3.1511	46.167	43.169	3.9457	47.115
PSUDS	64851	2139	6699	03004	54566	1846	38528	60556	14584
				-			-		
		35.317	35.317	20.651		20.651	22.077		22.077
PTAr	0	3	3	2	0	2	8	0	8
	-	-		-	-		-	-	
	97.296	58.569	38.727	98.694	60.619	38.074	99.326	59.676	39.650
PTPATi	65296	46198	19098	42437	58594	83844	39853	28501	11352
		34.348	34.348		26.220	26.220		27.628	27.628
PUNP1	0	6	6	0	5	5	0	5	5
	-			-			-		
	13.326	35.584	48.910	16.464	41.474	57.939	17.891	42.882	60.773
PUNP2	3	1	4	7	6	3	3	6	9
		36.498	36.498		31.620	31.620		33.028	33.028
PUNP3	0	7	7	0	6	6	0	6	6
				-			-		
		41.840	48.910	10.208	47.731	57.939	11.634	49.139	60.773
PUNP4	-7.0697	7	4	1	2	3	7	2	9
				-					
		34.140	54.465	23.463	26.012	49.475		27.420	52.310
PUNP5	-20.325	2	2	5	1	6	-24.89	1	1
	-			-					
	17.090	31.819	48.910	20.229		57.939			
PUNP6	9	5	4	4	37.71	4	-21.656	39.118	60.774
	-			-			-		
	19.434		19.434	22.573		22.573	23.999		23.999
PUNP7	8	0	8	3	0	3	9	0	9
	-			-			-		
PYAM5	2.4998	24.366	26.866	2.9058	62.815	65.721	5.1812	63.275	68.457
PO	74861	39794	2728	19012	7879	60691	7295	80961	08256
	-	-		-	-		-	-	
PYDXL5	357.57	296.11	61.465	365.23	295.31	69.917	366.94	292.00	74.941
PSYN	978	4616	16398	25915	46211	97046	28958	14391	45672

	-			-			-		
	40.030	6.4042	46.434	32.860	-1.00E-	32.860	34.431	-1.00E-	34.431
РҮК	25933	50982	51031	42927	06	42827	04405	06	04305
	-	22 1 1 0		-	22.001	40 475	-	25 200	52.240
	22.345	32.119	54.405	25.484	23.991	49.475	20.910	25.399	52.310
FTINF Z	/	4			3	J	0	3	⊥
	22,821	17.515	40.336	23.726	19,595	43.322	24,138	20.663	
PYRt2	2	2	4	9	7	6	7	3	44.802
	_	-		_	_		-	-	
	255.88	197.31	58.561	252.12	194.18	57.939	253.52	192.75	60.773
QULNS	11691	91823	9868	00476	0706	34162	80306	41259	9047
RBFK	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
	170.03	106.94	63.087	161.74	103.80	57.939	163.15	102.38	60.773
RBFSa	49388	73829	55592	82482	89065	34162	62311	23264	9047
	-	1 005	CE 100	-	1 005	CC 400	-	1 005	67 4 2 0
DDCCh	65.108	-1.00E-	65.108	66.499	-1.00E-	66.499	67.130	-1.00E-	67.130
КВГЗО	00714	00	00014	01028	00	00928	98443	00	98343
	53 635	15 664	37 970	53 690	15 800	37 889	55 657	14 972	40 684
RBK	05168	36303	68865	52659	86709	6595	36898	5716	79738
	-	-		-	-		-	-	
	59.096	15.499	43.596	60.844	14.109	46.735	61.639	13.477	48.161
RHCCE	36411	83186	53226	49729	48872	00857	10328	51456	58872
							-		
							79.710		48.825
RIBabc	NA	NA	NA	NA	NA	NA	3	-30.885	3
RNA_S									
YNTHE									
SIS	NA	NA	NA	NA	NA	NA	NA	NA	NA
RNDR1	NA	NA	NA	NA	NA	NA	NA	NA	NA
RNDR2	NA	NA	NA	NA	NA	NA	NA	NA	NA
RNDR3	NA	NA	NA	NA	NA	NA	NA	NA	NA
RNDR4	NA	NA	NA	NA	NA	NA	NA	NA	NA
RNTR1	NA	NA	NA	NA	NA	NA	NA	NA	NA
RNTR2	NA	NA	NA	NA	NA	NA	NA	NA	NA
RNTR3	NA	NA	NA	NA	NA	NA	NA	NA	NA
RNTR4	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
	19.080	-	19.080	19.775		19.775	20.091		20.091
RPE	1	0	1	3	0	3	3	0	3

	-			-			-		
	16.685		16.685	17.380		17.380	17.696		17.696
RPI	5	0	5	7	0	7	7	0	7
S7PI	-8.5138	0	8.5138	-9.2089	0	9.2089	-9.5249	0	9.5249
	-	-		-	-		-	-	
	153.38	93.434	59.954	155.10	93.853	61.247	160.01	94.043	65.968
SADH	82467	17386	07283	10586	38309	67548	27752	93274	84241
	-			-			-		
	73.583	-1.00E-	73.583	62.707	-1.00E-	62.707	64.732	-1.00E-	64.732
SADT2	30992	06	30892	32181	06	32081	91158	06	91058
	-			-			-		
	28.143	-1.00E-	28.143	25.956	-1.00E-	25.956	27.843	-1.00E-	27.843
SDPDS	70013	06	69913	65717	06	65617	25903	06	25803
					25.956	25.956		27.565	27.565
SDPTA	0	24.532	24.532	0	7	7	0	5	5
SELNPS	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
	41.822		41.822	43.212		43.212	43.844		43.844
SERAT	3	0	3	6	0	6	6	0	6
	-	-		-	-		-	-	
	64.092	25.358	38.734	64.770	25.041	39.729	67.144	24.897	42.247
SERD_L	92616	3069	61926	43708	43071	00637	97545	39608	57937
	-			-			-		
SERGLY	28.194	36.276	64.470	30.112	37.666		30.744	38.298	
Х	7	2	9	5	5	67.779	5	5	69.043
SERTRS	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			-			-		
	28.127	35.030	63.157	23.726	36.420	60.147	50.379	20.663	71.042
SERt4	19299	32637	51936	94359	66951	6131	49806	26627	76434
	-			-			-		
	22.821	17.515	40.336	23.726	19.595	43.322	24.138	20.663	44.801
SERt6	1/884	16269	34152	94459	65182	59641	6563	26827	92457
	-	-	F2 F4F	-	-		-	-	
CECTU	67.502	14.957	52.545	69.251	14.620	F4 C21	70.045	14.466	
SFGIH	9	4	5	1		54.631	/	/	55.579
	- 104	10.074	47 250	-	10 400	10 960	- 41 777	10 562	E1 000
SCDS	57.284	10.071	47.330	39.451	10.409	49.800	41.337	27052	22706
2002	55502	03374	199/0	30259	01258	3808/	90744	37052	33/90
	- 61 E00	-		64 240	-	20 720		-	12 247
SCEAD	50763	10.143	45.440	04.349 76057	24.020	53.129	20607	23.330	42.24/
JUACDC	50/03	4/40/	11730	10057	1022	00057	33027	0123	50257

	-	-		-	-		-	-	
SHCHC	124.53	37.928	86.606	126.97	36.895	90.082	128.08	36.426	91.662
S2	53267	51671	80997	86314	96361	66782	92245	62129	6032
	-			-			-		
SHCHD	33.013	-1.00E-	33.013	35.773	-1.00E-	35.773	37.028	-1.00E-	37.028
2	55822	06	55722	73916	06	73816	36686	06	36586
SHCHF	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-			-	
	78.801	20.998	57.802	69.306	19.082	50.224		18.210	52.551
SHK3D	2	9	3	6	1	5	-70.762	8	2
	-			-			-		
.	38.023	-1.00E-	38.023	38.079	-1.00E-	38.079	40.046	-1.00E-	40.046
SHKK	/459/	06	/449/	22088	06	21988	06326	06	06226
	-	-	70.000	-	-	CO 14C	-	-	74 500
	100.46	30.400	/0.060	98.157	29.010	69.146	99.881	28.378	/1.502
SHSLI	11910	53689	65474	13098	19375	93723	101	2196	8814
	-	-	70.000	-		72 0 4 1	-	- 	74 105
	5/0.20	600.14	/0.060	0/1.59	598.75	72.841	0/2.22	598.12	74.105
SLCTSS	/1914	05597	05174	/55/0	01900	54102	95117	42224	20955
	20 5 25	1 005	20 525	-	1 005	21 726	- דסר רכ	1 005	22 202
SO/1+2	30.323 27707	-1.00E-	27607	21.750 8171 <i>/</i>	-1.00E-	\$1.750 \$1617	51676	-1.00E-	51576
30412	66 3 27	112 65	16 3 23	62 530	12/ 0/	62 / 13	61 808	125 16	63 262
SOD	36294	132/18	9618/	02.330	3276	27106	01.030	01757	1//85
300		13240	50104		5270	27100		01/5/	14403
	17 915	29 440	47 356	26 977	30 831	57 809	28 548	31 463	60 011
SOTA	25647	9323	18876	93798	27544	21342	55276	24959	80235
		5625	20070	-	2/011	21012		2.000	00200
	28.194	38.471	66.666	30.112	39.862	69.974	30.744	40.493	71.238
SPA	67666	65977	33643	48516	00291	48807	45931	97707	43638
SPMS	NA	NA	NA	NA	NA	NA	NA	NA	NA
							350.63	424.74	74.105
SPRS	NA	NA	NA	NA	NA	NA	92923	45816	28933
	-	-		_	_		_	_	
	63.001	17.555	45.446	62.067	26.032	36.034	64.413	24.768	39.645
SSALx	36985	25689	11296	147	54442	60258	77056	59611	17445
	-	-		-	-		-	-	
	67.560	21.568	45.992	70.341	22.536	47.804	71.605	21.195	50.409
SUCBZL	51098	23773	27324	19726	41843	77882	14556	81451	33105
	-	-		-	-		-	-	
SUCBZ	72.425	37.395	35.030	73.120	36.700	36.420	73.436	36.384	37.052
S	55304	22567	32737	72461	0541	67051	71169	06702	64466

	-			-			-		
SUCCte	22.821	17.515	40.336	23.726	14.247	37.974	24.138	-1.00E-	24.138
x	17884	16269	34152	94459	0801	02469	6553	06	6543
	-	-		-	-		-	-	
	144.58	98.049	46.536	136.61	99.300	37.310	138.29	97.098	41.192
SUCD7	56983	67566	02266	10317	7747	25698	02928	18577	10704
	-			-			-		
SUCOA	26.750		26.750	14.515		14.515	15.923		15.923
S	7	0	7	9	0	9	9	0	9
	-			-			-		
	27.062		55.886	30.200	20.537	50.738	31.627	21.945	53.572
SUCP	4	28.824	4	9	3	2	5	3	8
	_	_		_	_		_	_	
SUCRP	89.751	19.690	70.060	85.476	18.300	67.176	87.520	17.668	69.852
тs	24022	58548	65474	31296	24234	07062	90885	26819	64066
SULR	NA	NA	NA	NA	NA	NA	NA	NA	NA
		16.839	16.839					14,807	14.807
TAL	0	6	6	0	12.605	12.605	0	6	6
				-			-		
TDP3A	1.3723	45,983	47.356	2,7626	55.046	57,809	3,3946	56.617	60.011
AAT	05984	88278	18876	49124	5643	21342	23278	17907	80235
	_								
TDPDR	17.515	17.515	35.030	18,210	18,210	36.420	18,526	18,526	37.052
F	271010	271010	4	3	3	6	3	3	6
							-		
TDPDR	10,169	47.633	57,802	12.085	38,138	50.224	12,957		52,551
R	1	2	3	9	6	5	22.007	39,594	2
					-			-	
TDPGD	97.649	62,619	35.030	98.345	61,924	36.420	98,661	61.608	37.052
H	96124	63387	32737	13281	4623	67051	11989	47522	64466
		ΝΔ	ΝΔ		NΔ	ΝΔ	ΝΔ	NΔ	ΝΔ
TESK				-			-		
	21 222	22 466	43 799	13 803	-1 00F-	13 803	15 498	-1 00F-	15 498
тнр2	47116	30442	77558	85279	1.000	85179	56081	1.000	55981
	47110	30442	//550		00	03175	50001	00	55501
	22 466	10 721	22 187	11 033	2 7706	13 803	11 22/	1 2738	15 / 98
тнр5	30642	10.721	7/727	21767	3/121	85179	66693	97885	55981
	50042	005	, 7, 2,	21/0/	34121	0.5175	00055	52005	55501
	7 2576	-1 005-	7 2576	8 6/70	-1 005-	8 6/70	- ۵ 27۵۵	-1 005-	9 2700
	5/027	-100L-	53087	98126	1.000	97126	7779	-100L- 06	7179
	54507	00	55507	20120	00	57120	1220	00	/ 120
тнил+	- 22 221	17 515	10 336	23 726	10 505	13 200	- 2/1 1 2 2	20 662	11 QO1
2	17001	16260	2/152	23.720 Q//EQ	65100	506/1	6563	20.005	44.001 02/57
2	1/004	10703	54152	54459	03195	55041	0303	2002/	92437

				-			-		
		11.925	11.925	42.368	12.262		43.162		50.780
THRA	0	3	3	3	7	54.631	9	7.6175	4
	-			-			_		
	4.1231	35.733	39.856	12.473	27.255	39.729	13.727	28.519	42.247
THRD	01346	18723	28857	10667	89969	00637	73437	848	58237
	-	-		-	-		-	-	
THRD_	56.314	23.169	33.144	62.582	22.853	39.729	64.956	22.709	42.247
L	73489	94003	79487	0702	06384	00637	61158	02921	58237
				-					
				23.726	19.595	43.322		20.663	20.663
THRHT	NA	NA	NA	9	7	6	0	3	3
	_			_			_		
THRLA	19.849		29.440	44.702			45.497	10.081	55.578
D	6	9.5909	5	7	9.9283	54.631	3	6	9
	_	_		_	_		_	_	
	65.132	25.149	39.982	57.203	17.474	39.729	58.313	16.526	41.787
THRS	46849	90065	56784	56791	56155	00637	65878	60031	05846
THRTR									
S	NA	NA							
	_						_		
	17.231	17.515	34.746				24.138	4.2738	28.412
THRt3	35445	16269	51713	NA	NA	NA	6563	90885	54718
	-			_			_		
	28.127	29.440	57.567	23.726	36.420	60.147	33.990	-1.00E-	33.990
THRt4	19299	50198	69497	94359	66951	6131	12067	06	11967
	_	_		_	_		_	_	
THZPS	361.78	235.62	126.16	366.67	236.61	130.06	368.89	235.28	133.61
N	55687	31543	24144	21782	17435	04347	33663	04161	29502
		19.774	19.774		24.909	24.909		25.541	25.541
TKT1	0	7	7	0	4	4	0	3	3
		16.839	16.839					18.861	18.861
ткт2	0	6	6	0	18.23	18.23	0	9	9
ΤΜΑΟ									
R3e	NA	NA							
	_	_		_	_		_	_	
	53.291	6.8569	46.434	53.346	6.9934	46.353	55.313	6.1651	49.148
TMDK1	48176	7195	50981	95668	76015	48066	79906	80516	61854
	-			-			-		
	14.911	33.999	48.910	18.049	39.889	57.939	19.476	41.297	60.773
TMDPP	1	3	4	6	8	4	1	8	9

	-	-		-	-		-	-	
	89.147	19.086	70.060	90.537	17.696	72.841	91.169	17.064	74.105
TMDS	13157	47683	65474	47471	13369	34102	44887	15954	28933
	-			-					
	29.946		29.946	30.002		30.002			
TMPKr	7	0	7	2	0	2	-31.969	0	31.969
	-			-	-		-		
	55.714	-1.00E-	55.714	57.105	0.8198	56.285	57.737	-1.00E-	57.737
TMPPP	68461	06	68361	02775	540538	17369	0019	06	0009
		23.435	23.435			21.518			23.721
TPI	0	2	2	3.2973	24.816	7	1.4107	25.132	3
TRACE									
_ELEM									
ENTS	NA	NA	NA	NA	NA	NA	NA	NA	NA
TRDR	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
	59.941	14.368	45.572	52.012	12.283	39.729	53.582	11.335	42.247
TRE6PP	2375	84527	39223	33692	33056	00637	9517	36933	58237
	-			-			-		
	50.264	2.2811	52.545	52.012	2.6185	54.631	52.807	2.7718	55.578
TREH	36007	30988	49106	49324	1252	00576	09923	67762	967
	-	-		-	-		-	-	
TREHte	79.709	9.6488	70.060	75.434	8.2584	67.176	77.479	7.6265	69.852
х	47919	2445	65474	55193	8131	07062	14782	07156	64066
	-	-		-	-		-	-	
	430.27	328.60	101.66	430.45	322.70	107.74	430.55	321.11	109.44
TRPOR	18187	76962	41225	16761	4415	72611	72329	5203	20299
	-	-		-	-		-	-	
	63.028	10.482	52.545	63.365	8.7344	54.631	63.518	7.9398	55.578
TRPS2	05512	56406	49106	43665	30887	00576	79189	24898	967
	-	-		-	-		-	-	
	71.398	19.538	51.859	58.244	18.515	39.729	60.609	18.361	42.247
TRPS3	00248	19439	80809	13625	12989	00637	35702	77465	58237
TRPTRS	NA	NA	NA	NA	NA	NA	NA	NA	NA
				-			-		
				23.726	19.595	43.322	24.138	20.663	
TRPt6	NA	NA	NA	9	7	6	7	3	44.802
	14.716	84.776	70.060				12.693	86.799	74.105
TSULST	28894	94368	65474	NA	NA	NA	97165	26097	28933
TYRTA	NA	NA	NA	NA	NA	NA	NA	NA	NA
TYRTRS	NA	NA	NA	NA	NA	NA	NA	NA	NA

				-			-		
				23.726	19.595	43.322	24.138	20.663	
TYRt6	NA	NA	NA	9	7	6	7	3	44.802
	-	-		-	-		-	-	
U23GA	287.93	217.87	70.060	289.32	216.48	72.841	289.95	215.85	74.105
AT	37952	31405	65474	41384	27973	34102	61125	08232	28933
	-	-		-	-		-	-	
UAAGD	91.094	18.247	72.847	78.860	14.582	64.277	80.268	12.916	67.351
S	8136	34401	46959	09048	38689	70358	07342	4973	57612
	-	-		-	-		-	-	
UAGAA	280.09	210.03	70.060	281.48	208.64	72.841	282.11	208.01	74.105
Т	32	26	6	36	22	4	55	02	3
	-	-		-	-		-	-	
UAGCV	79.065	15.978	63.087	61.805	12.839	48.965	62.739	11.413	51.326
Т	63659	08068	55592	34022	60436	73586	34255	02422	31833
	-	-		-	-		-	-	
	66.131	9.8821	56.249	67.522	11.237	56.285	68.154	9.9778	58.176
UAGDP	9392	56259	78294	28234	10865	17369	25649	20644	43585
	-			-			-		
UAGPT	39.988	-1.00E-	39.988	41.378	-1.00E-	41.378	42.010	-1.00E-	42.010
3	23527	06	23427	57841	06	57741	55256	06	55156
	-	-		-	-		-	-	
UAMA	86.459	14.688	71.771	74.224	11.023	63.201	75.632	9.3574	66.275
GS	56788	3194	24848	84476	36228	48247	8277	72685	35501
	-	-		-	-		-	-	
UAMA	87.618	14.918	72.699	75.383	11.254	64.129	76.791	9.5881	67.203
S	43941	9911	44831	71628	03448	6818	69922	44379	55484
	-	-		-	-		-	-	
	88.034	30.232	57.802	78.540	28.315	50.224	79.995	27.444	52.551
UAPGR	93344	64439	28905	34275	82045	5223	74032	53584	20448
	-	-		-	-		-	-	
UDCPD	75.713	30.141	45.572	67.784	28.055	39.729	69.355	27.107	42.247
Р	51687	12464	39223	61629	60993	00637	23107	6487	58237
	-	-		-	-		-	-	
UDCPD	893.38	688.60	204.78	899.64	704.30	195.33	902.48	696.44	206.04
PS	67125	07406	59719	32566	65607	6696	71403	41662	29742
	-			-			-		
UDPG4	14.186		14.186	14.881		14.881	15.197		15.197
E	7	0	7	9	0	9	9	0	9
							-		
UDPHE							43.843	1.2062	45.049
XURI	NA	NA	NA	NA	NA	NA	12839	60925	38932

	-	-		-	-		-	-	
UGMD	90.869	18.021	72.847	78.634	14.356	64.277	80.042	12.690	67.351
DS	17248	70289	46959	44936	74578	70358	4323	85618	57612
	-			-			-		
UHGAD	48.002	-1.00E-	48.002	49.750	-1.00E-	49.750	50.545	-1.00E-	50.544
A	25786	06	25686	39404	06	39304	00003	06	99903
	-			-			-		
	30.786		30.786	30.841		30.841	32.808		32.808
UMPK	1	0	1	6	0	6	4	0	4
	-	-		-	-		-	-	
	184.41	144.02	40.383	177.87	134.96	42.907	180.07	133.39	46.680
UNK3	16122	85222	08994	30547	58407	21402	56437	5226	41773
UPP3M									
<u> </u>	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-	-		-	-		-	-	
	260.02	224.99	35.030	260.72	224.30	36.420	261.03	223.98	37.052
02232	67694	6442	32/3/	19409	12704	67051	/928	52834	64466
	-	-	405.00	-	-	100.20	472.20	-	444 45
UPPDC	166.12	61.031	105.09	1/1.02	61./6/	109.26	1/3.26	62.102	111.15
1	2969	99492	09741	9987	9835	20035	04578	52376	7934
	- 	2 7222	FC 240	-	1 2772	FC 20F	-	2 6266	F0 17C
	53.517	2.7323	50.249	54.907	1.3773	17260	55.539 סדדד		58.170 12505
UPPRI	4603	2204	78294	80344	70251	1/309	///0	58254	43585
	-	-	05 275	-	- 1/6/15	71 202	100 00	-	02 024
	Z34.Z9 //20/1	06180	33.273 27521	217.04	02700	66003	730/6	21252	08100
UQUN	40541	50185	27521	25555	02755	00005	73540	51552	00105
	22 821	17 515	40 336	23 726	19 595	43 322	24 138	20 663	
URA†6	22.021	2	40.000	9	7		24.130	20.003	44 802
010.00			•		,		_		11.002
	23.364	11.665	35.030	24.059	12.361	36.420	24.375	12.677	37.052
URCN	41684	91053	32737	58841	0821	67051	57549	06917	64466
	_	_		_	_		_	_	
URHYD	365.08	313.99	51.092	355.28	307.77	47.511	355.97	306.04	49.930
ROX	67	38	9	49	36	3	12	04	8
					18.925	18.925		19.753	19.753
URIDK2	0	19.062	19.062	0	5	5	0	8	8
	-			-			-		
	48.185		52.545	49.933			50.727		55.578
URIH	2	4.3603	5	3	4.6977	54.631	9	4.851	9
	-	-		-	-		-	-	
	48.501	2.0674	46.434	48.557	2.2039	46.353	50.524	1.3756	49.148
URIK1	98542	7511	51031	46033	79674	48066	30272	84174	61854

	-			-			-		
	48.501	21.453	69.955	48.557	22.843	71.401	50.524	23.475	74.000
URIK2	98442	46521	44964	45933	80835	26769	30172	78251	08422
	-			-			-		
	46.260	23.799	70.060	47.651	25.190	72.841	48.283	25.822	74.105
URIK3	70877	94597	65474	05191	28911	34102	02607	26326	28933
	-			_			_		
	22.821	17.515	40.336	23.726	19.595	43.322	24.138	20.663	44.801
URIt2	17884	16269	34152	94459	65182	59641	6563	26827	92457
	-			_			_		
	47.238	-1.00E-	47.238	48.986	-1.00E-	48.986	49.780	-1.00E-	49.780
USHD	01136	06	01036	14454	06	14354	75052	06	74952
	-			_			_		
UreaEx	17.515		17.515	18.210		18.210	18.526		18.526
q	2	0	2	3	0	3	3	0	3
-	-			_			_		
VALAL	37.183	29.482	66.666	41.820	30.873	72.693	42.452	31.505	73.957
АМОВ	4	9	3	1	2	3	1	2	3
VALDH		46.106	45.446		37.250	37.250		38.342	38.342
r	0.6602	3	1	0	7	7	0	7	7
	-			-			-		
	17.380	29.975	47.356	23.964	31.366		24.108	31.998	56.106
VALTA	3	9	2	7	3	55.331	7	2	9
VALTRS	NA	NA	NA	NA	NA	NA	NA	NA	NA
	-			_			_		
	30.467	38.896	69.363	26.296	41.871	68.168	50.590	26.970	77.560
VALt4	38506	11935	50441	80976	45504	2648	72322	07614	79936
	-	-		-	-		-		
WO4ab	90.016	34.684	55.332	78.139	32.072	46.067	79.710		48.825
с	6	3	3	7	3	4	3	-30.885	3
	-			-	-		-	-	
	71.429		45.446	74.189	34.460		75.443	33.196	42.247
XAND	1	-25.983	1	3	3	39.729	9	3	6
	-			_			_		
	1				40.240	26 420	10 520	40 500	27 052
	17.515	17.515	35.030	18.210	18.210	36.420	18.526	18.526	57.052
XANt	17.515 2	17.515 2	35.030 4	18.210 3	18.210	36.420	18.526	18.526	57.052
XANt	17.515 2 -	17.515 2 -	35.030 4	18.210 3 -	18.210	36.420 6	18.526	18.526	6
XANt	17.515 2 - 75.081	17.515 2 - 34.636	35.030 4 40.444	18.210 3 - 70.169	18.210 3 - 32.659	36.420 6 37.509	18.526 3 - 72.537	18.526 3 - 32.027	40.510

	4C	4C	15C	15C	20C	20C
	Normaliz	Normaliz	Normaliz	Normaliz	Normaliz	Normaliz
	ed Lower	ed Upper	ed Lower	ed Upper	ed Lower	ed Upper
Reaction ID	Bound	Bound	Bound	Bound	Bound	Bound
	-	-	-	-	-	-
2MAHMP	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
4HBASink	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
4HBTE	0	0	NA	NA	0	0
5DOAN	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06
5DRIB_Sink	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06
5HPUDICDCr	0	0	0	0	0	0
5HPUDICDCs	0	0	NA	NA	NA	NA
A5PISO	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
AACPS10	0	0	NA	NA	0	0
AACPS11	0	0	NA	NA	0	0
AACPS12	0	0	NA	NA	0	0
AACPS13	0	0	NA	NA	0	0
AACPS14	0	0	NA	NA	0	0
AACPS15	0	0	NA	NA	0	0
AACPS16	0	0	NA	NA	0	0
AACPS3	0	0	NA	NA	0	0
AACPS4	0	0	NA	NA	0	0
AACPS5	0	0	NA	NA	0	0
AACPS6	0	0	NA	NA	0	0
AACPS7	0	0	NA	NA	0	0
AACPS8	0	0	NA	NA	0	0
AACPS9	0	0	NA	NA	0	0
AACPSFA130OH	0	0	NA	NA	0	0
AACPSFA1718	0	0	NA	NA	0	0
AACPSFA1817	0	0	NA	NA	0	0
ABTA	0	0	0	0	0	0
ACACCB	0	0	0	0	0	0
ACACCT	0	0	0	0	0	0
ACACT10R	0	0	0	0	0	0
ACALDi	0	0	0	0	0	0.990343
ACBIPGT	0	0	NA	NA	NA	NA
ACCOAC	5.068387	5.068387	5.068387	5.068387	5.068387	5.068387
	45.16035	45.16035	19.62897	19.62897	53.54705	53.54705
ACGAMK	9	9	4	4	3	3

Data S2 Table C Reaction Fluxes Normalized by the biomass flux in each simulation

	45.16035	45.16035	19.62897	19.62897	53.54705	53.54705
ACGAt2	9	9	4	4	3	3
ACGK	0.376736	0.376736	0.376736	0.376736	0.376737	0.376737
ACGS	0.376736	0.376736	0.376736	0.376736	0.376737	0.376737
ACHBS	0.268394	0.268394	0.268394	0.268394	0.268394	0.268394
	111.5002	111.5002	31.88904	31.88904	122.3640	122.3640
ACKr	03	03	6	6	24	24
ACLS	0.799812	0.799812	0.799812	0.799812	0.799812	0.799812
ACMAT1	0	0.661538	0	0.661538	0	0.661538
ACNAMS	0	0	0	0	0	0
ACOAD10	0	0	0	0	0	0
ACOAD8	NA	NA	NA	NA	0	0
ACOAD9	0	0	0	0	0	0
ACOATA	0	0.661538	0	0.661538	0	0.661538
ACODA	0.376736	0.376736	0.376736	0.376736	0.376737	0.376737
ACONT	2.336425	2.336425	1.832539	1.832539	0.842196	0.842196
	-	_	_	_	_	-
ACOTA	0.376736	0.376736	0.376736	0.376736	0.376737	0.376737
ACPS1	0	0	0	0	0	0
ACPSc	0	0	0	0	0	0
ACS	0	0	0	0	0	0
	-	-			-	-
	157.2119	157.2119	-	-	176.4624	176.4624
ACt6	01	01	52.06936	52.06936	18	18
ADA	0	0	0	0	0	0
ADCL	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
ADCOBAK	0	0	NA	NA	NA	NA
ADCS	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
ADHMCYSSYN	0.001514	0.001514	0.001514	0.001514	0.001514	0.001514
		18.86626		13.85229		13.85229
ADK1	0	1	0	4	0	4
		10.27661				
ADK3	-8.58965	1	-8.58965	5.262644	-8.58965	5.262644
	-					
ADK4	0.503885	0	0	0	0	0
ADMDC	0.007633	0.007633	0.007633	0.007633	0.007633	0.007633
ADNCYC	0	0	0	0	0	0
ADNK1	0.00915	0.513035	0.00915	0.00915	0.00915	0.00915
ADNt2	0	0	0	0	0	0
ADPT	0	0	0	0	0	0
ADSK	0.150736	0.150736	0.150736	0.150736	0.150736	0.150736

ADSL1r	0.16639	0.16639	0.16639	0.16639	0.16639	0.16639
ADSL2r	0.150541	0.150541	0.150541	0.150541	0.150541	0.150541
ADSS	0.16639	0.16639	0.16639	0.16639	0.16639	0.16639
	45.16035	45.16035	19.62897	19.62897	53.54705	53.54705
AGDC	9	9	4	4	3	3
AGMAHYD	0.045289	0.045289	0.045289	0.045289	0.045289	0.045289
	-	-	-	-	-	-
AGPR	0.376736	0.376736	0.376736	0.376736	0.376737	0.376737
AHAI	0.799812	0.799812	0.799812	0.799812	0.799812	0.799812
AHCYSNS	0	0	0	0	0	0
AICART	0.238914	0.238914	0.238914	0.238914	0.238914	0.238914
AIRC2	0.150541	0.150541	0.150541	0.150541	0.150541	0.150541
	-	-	-	-	-	-
AIRC3	0.150541	0.150541	0.150541	0.150541	0.150541	0.150541
AKGD	0	0	0	0	0	0
ALAALA	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
ALAD_L	0	0	0	0	0	0
ALAGLYX	1.494481	1.494481	0.990595	0.990595	0.000252	0.000252
ALAR	0.02772	0.02772	0.02772	0.02772	0.05544	0.05544
ALATA_D2	0	0	0	0	0	0
	-		-		-	
ALATA_L	2.168105	4.01504	1.664219	4.518673	0.701596	5.509016
ALATA_L2	0	0	0	0	0	0
ALATRS	0.346091	0.346091	0.346091	0.346091	0.346091	0.346091
ALA_Dt4	0.02772	0.02772	0.02772	0.02772	0	0
ALAt4	0	0	0	0	0	0
ALCD2x	0	0	0	0	0	0
ALDD2x	0	0	0	0	NA	NA
ALLNRAC	0	0	0	0	0	0
ALLTC	0	0	NA	NA	NA	NA
ALLTN	0	0	0	0	0	0
AMAA	0	0	0	0	0	0
AMALT1	0	0	0	0	0	0
AMALT2	0	0	0	0	0	0
AMALT3	0	0	0	0	0	0
AMALT4	0	0	0	0	0	0
AMAOT	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06
AMMQT7 2	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
AMOR Sink			a aa= ac	2 005 00	2 005 00	2 005 06
AIVIOD SIIIK	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06
AMPMS2	2.00E-06 0.000252	2.00E-06 0.000252	2.00E-06 0.000252	0.000252	0.000252	0.000252

AMPTASEPG	0	0	NA	NA	0	0
ANPRT	0.049387	0.049387	0.049387	0.049387	0.049387	0.049387
ANS1	0.049387	0.049387	0.049387	0.049387	0.049387	0.049387
AOXS	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06
APRAUR	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505
ARBABC	NA	NA	NA	NA	0	0
ARGDC	0.045289	0.045289	0.045289	0.045289	0.045289	0.045289
ARGSL	0.221268	0.221268	0.221268	0.221268	0.221268	0.221268
ARGSS	0.221268	0.221268	0.221268	0.221268	0.221268	0.221268
ARGTRS	0.175979	0.175979	0.175979	0.175979	0.175979	0.175979
			-	-	-	-
ASAD	-0.35446	-0.35446	0.858345	0.858345	1.848688	1.848688
ASNN	0	0	NA	NA	0	0
ASNS1	0.175627	0.175627	0.175627	0.175627	0.175627	0.175627
ASNTRS	0.175627	0.175627	0.175627	0.175627	0.175627	0.175627
ASP1DC	0.000615	0.000615	0.000615	0.000615	0.000615	0.000615
ASPCT	0.141483	0.141483	0.141482	0.141482	0.141482	0.141482
ASPK	0.35446	0.35446	0.858345	0.858345	1.848688	1.848688
ASPO3	0	0.002579	0	0.002579	0	0.002579
ASPO5	0	0.002579	0	0.002579	0	0.002579
ASPO6	0	0	0	0	0	0
ASPO8	0	0	0	0	0	0
ASPO9	0	0	0	0.002579	0	0.002579
	-	-	-	-	-	-
ASPTA1	1.445588	1.445588	1.949474	1.949474	2.939817	2.939817
ASPTA4	0	0	0	0	0	0
ASPTRS	0.232626	0.232626	0.232626	0.232626	0.232626	0.232626
ASPt2	0	0	0	0	0	0
AST	0	0	0	0	0	0
	25.17332	25.17332			84.46862	84.46862
ATPM	8	8	3.877508	3.877508	3	3
ATPPRT	0.088373	0.088373	0.088373	0.088373	0.088373	0.088373
				-		
ATPS4r	0	0	-7.40024	7.398726	0	0
BPNT	0.150736	0.150736	0.150736	0.150736	0.150736	0.150736
BTS4	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06
BUTSUCCCOA	0	0	0	0	0	0
Biomass_WP2	1	1	1	1	1	1
C120SN	0.101504	0.101504	0.101504	0.101504	0.101504	0.101504
C130ISN	0.051761	0.051761	0.051761	0.051761	0.051761	0.051761
C1300HISN	0.012763	0.012763	0.012763	0.012763	0.012763	0.012763

C140ISN	0	0	0	0	0	0
C140SN	0.067949	0.067949	0.067949	0.067949	0.067949	0.067949
C150ISN	0.028362	0.028362	0.028362	0.028362	0.028362	0.028362
C150SN	0	0	0	0	0	0
C151SN	NA	NA	0	0	0	0
C160ISN	0	0	0	0	0	0
C160SN	0.09005	0.09005	0.09005	0.09005	0.09005	0.09005
C161SN	0.27086	0.27086	0.27086	0.27086	0.27086	0.27086
C170ISN	0	0	0	0	0	0
C170SN	0	0	0	0	0	0
C171SN	NA	NA	0	0	0	0
C171n8SN	0.011345	0.011345	0.011345	0.011345	0.011345	0.011345
C180SN	0.014181	0.014181	0.014181	0.014181	0.014181	0.014181
C181SN	NA	NA	0	0	0	0
C181n7SN	0.066651	0.066651	0.066651	0.066651	0.066651	0.066651
C205SN	0.050343	0.050343	0.050343	0.050343	0.050343	0.050343
C50SN	0	0	0	0	0	0
C60ISN	0	0	0	0	0	0
C70ISN	0.092886	0.092886	0.092886	0.092886	0.092886	0.092886
CAT	0.000126	0.000126	0	0	0	0
CBL1abc	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
CBLAT	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
CBPS	0.362751	0.362751	0.362751	0.362751	0.362751	0.362751
CDPG46D	0	0	0	0	0	0
CDPMEK	0.004471	0.004471	0.004471	0.004471	0.004471	0.004471
CHOLDH1	0	0	NA	NA	NA	NA
CHOLDH2	0	0	NA	NA	NA	NA
CHOLDH3	0	0	NA	NA	NA	NA
CHOLDH4	0	0	NA	NA	NA	NA
CHOLDH5	0	0	NA	NA	NA	NA
CHOLt4	0	0	0	0	0	0
CHORM	0.29381	0.29381	0.29381	0.29381	0.29381	0.29381
CHORS	0.344207	0.344207	0.344207	0.344207	0.344207	0.344207
CHRPL	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
CKDOAS	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
	-	-	-	-		
CO2t	6.406695	6.406695	0.753705	0.753705	0	0
COBALTt3	0	0	0	0	0	0
COBALTt5	-2.70E-05	-2.70E-05	-2.70E-05	-2.70E-05	-2.70E-05	-2.70E-05
CONFALDD	0	0	NA	NA	0	0
CPPPGO	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252

CS 2.336425 2.336425 1.832539 1.832539 0.842196 0.842196 CSND 0 0 0 0 0 0 0 0 0 CSNt2 0.067309 0.067309 0.067308 0.067308 0.067309 0.067309 0.067308 0.00763 0.000763
CSND 0 0 0 0 0 0 CSNt2 0<
CSNt2 0 0 0 0 0 0 CTPS2 0.067309 0.067309 0.067308 0.067308 0.067309 0.067309 CU2t 0.000763 0.000763 0.000763 0.000763 0.000763 0.000763
CTPS2 0.067309 0.067309 0.067308 0.067308 0.067309 0.067309 CU2t 0.000763 0.000763 0.000763 0.000763 0.000763 0.000763
CU2t 0.000763 0.000763 0.000763 0.000763 0.000763 0.000763
CYCPUe U U NA NA NA NA
CYOO2 0 0 0 0 0 0
CYOR7 0 0 0 0 0 0
CYSS 0.150736 0.150736 0.150736 0.150736 0.150736 0.150736
CYSTL 0.108051 0.108051 0.108051 0.108051 0.108051 0.108051
CYSTRS 0.041816 0.041816 0.041815 0.041815 0.041816 0.041816
CYTBD 1.63818 1.638937 2.020205 2.020962 5.008139 5.008139
CYTD 0 0 0 0 0 0
CYTDH 0 0 0 0 0 0
CYTDK1 0 0 0 0 0 0
CYTDK2 0 0 0 0 0 0 0
CYTDK3 0 0 0 0 0 0 0
CYTDt2 0 0 0 0 0 0
CYTK1 0.090071 0.090071 0.090071 0.090071 0.090071 0.090071
CYTK2 0 0 0 0 0 0 0
CampHydrolyase 0 0 0 0 0 0
Clt 0.005605 0.005605 0.005605 0.005605 0.005605 0.005605
DADA 0 0 0 0 0 0
DADK 0.503885 0 0 0 0 0
DADNt2 0 0 0 0 0 0
DAGK 0 0 NA NA 0 0
DAHPS 0.344207 0.344207 0.344207 0.344207 0.344207 0.344207
DAPDC 0.218689 0.218689 0.218689 0.218689 0.218689 0.218689
DAPE 0.246409 0.246409 0.246409 0.246409 0.246409 0.246409
DASYN 0.073667 0.073667 0.073667 0.073667 0.073667 0.073667
DB4PS 0.00101 0.00101 0.00101 0.00101 0.00101 0.00101
DBTSr 2.00E-06 2.00E-06 2.00E-06 2.00E-06 2.00E-06 2.00E-06
DCYTD 0 0 0 0 0 0
DCYTt2 0 0 0 0 0 0
- DGK1 0.503885 0 0 0 0 0 0
DHAD1 0.799812 0.799812 0.799812 0.799812 0.799812 0.799812
DHAD2 0.268394 0.268394 0.268394 0.268394 0.268394 0.268394 0.268394
DHDPRy 0.246409 0.246409 0.246409 0.246409 0.246409 0.246409 0.246409

DHDPS	0.246409	0.246409	0.246409	0.246409	0.246409	0.246409
DHFR	0.022996	0.022996	0.022996	0.022996	0.022996	0.022996
DHFS	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
DHNAOT7	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
DHNPA	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
DHORD2	0	0.141483	0	0.141482	0	0.141482
DHORD4i	0	0.141483	0	0.141482	0	0.141482
DHORD8	0	0	0	0.141482	0	0.141482
	-	-	-	-	-	-
DHORTS	0.141483	0.141483	0.141482	0.141482	0.141482	0.141482
DHPPDA2	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505
DHPRx	0	0	0	0	0	0
DHPS3	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
DHPTPE	0	0	0	0	0	0
DHQD1	0.344207	0.344207	0.344207	0.344207	0.344207	0.344207
DHQS	0.344207	0.344207	0.344207	0.344207	0.344207	0.344207
DKMPPD3	0.007633	0.007633	0.007633	0.007633	0.007633	0.007633
DMATT	0.000567	0.000567	0.000567	0.000567	0.000567	0.000567
DMOCT	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
DMPPS	0.000567	0.000567	0.000567	0.000567	0.000567	0.000567
DMQMT	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
DMSOR3e	0	0	0	0	0	0
DMSOR4e	0	0	0	0	0	0
DNA_SYNTHESIS	0.05	0.05	0.05	0.05	0.05	0.05
DNMPPA	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
DNTPPA	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
DPCOAK	0.000615	0.000615	0.000615	0.000615	0.000615	0.000615
DPR	0.000615	0.000615	0.000615	0.000615	0.000615	0.000615
DRBK	0	0	0	0	0	0
DRPA	0.503885	0.503885	0	0	0	0
DTMPK	0.022744	0.022744	0.022744	0.022744	0.022744	0.022744
DURIK1	0	0	0	0	0	0
DURIPP	0	0.503885	0	0	0	0
DURIt2	0	0	0	0	0	0
DUTPDP	0	0	0	0	0	0
DXPRI	0.004471	0.004471	0.004471	0.004471	0.004471	0.004471
DXPS	0.004975	0.004975	0.004723	0.004723	0.004723	0.004723
E4PD	0.000252	0.000252	0	0	0	0
ECOAH2C	0	0	0	0	0	0
ECOAH9	0	0	0	0	0	0
EDA	5.898494	11.21305	0	0	0	0

EDTXS5	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
EDTXS6	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
			18.08912	18.08912	30.24969	30.24969
ENO	0	0	4	4	7	7
EPPP2	0	0	0	0	0	0
EX_cpd_CrOH3[e]	0	0	0	0	0	0
	157.2119	157.2119			176.4624	176.4624
EX_cpd_ac[e]	01	01	52.06936	52.06936	18	18
	-	-	-	-	-	-
	45.16035	45.16035	19.62897	19.62897	53.54705	53.54705
EX_cpd_acgam[e]	9	9	4	4	3	3
EX_cpd_adn[e]	0	0	0	0	0	0
EX_cpd_akg[e]	0	0	0	0	0	0
EX_cpd_ala-D[e]	0	0	0	0	0.02772	0.02772
EX_cpd_ala-L[e]	0	0	0	0	0	0
EX_cpd_asn-L[e]	0	0	0	0	0	0
EX_cpd_asp-L[e]	0	0	0	0	0	0
EX_cpd_bgl[e]	0	0	0	0	0	0
	-	-	-	-	-	-
EX_cpd_ca2[e]	0.005605	0.005605	0.005605	0.005605	0.005605	0.005605
	-	-	-	-	-	-
EX_cpd_cbl1[e]	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
EX_cpd_cnitin[e]	0	0	0	0	0	0
EV and al[a]						
EX_cpd_ci[e]	0.005005	0.005005	0.005005	0.005005	0.005005	0.005005
EX_cpd_co2[e]	0.400095	2 705 05	2 705 05	0.755705 2 70E 0E		2 705 05
EX_cpd_cobalt2[e]	-2.70L-03	-2.701-03	-2.701-03	-2.70L-05	-2.701-03	-2.70L-05
EX_cpd_cobaltS[e]	0	0	0	0	0	0
	0	U	0	U	U	0
FX and cu2[e]	0 000763	0 000763	0 000762	0 000762	0 000763	0 000763
EX_cpd_cu2[c]	0.000705					
EX_cpd_cytd[c]	0	0.0007.05	0.000703	0.000703	0.000703	0.000705
FX CDD DAD-7161	0	0	0.000703	0.000703	0	0
EX_cpd_dad-2[e]	0	0	0.000703	0.000703	0	0
EX_cpd_dad-2[e] EX_cpd_damp[e]	0 0 0 0	000000000000000000000000000000000000000	0.000703	0.000703	0	0
EX_cpd_dad-2[e] EX_cpd_damp[e] EX_cpd_dcmp[e] EX_cpd_dcvt[e]	0 0 0 0	000000000000000000000000000000000000000	0.000703	0.000703	000703	0000703
EX_cpd_dad-2[e] EX_cpd_damp[e] EX_cpd_dcmp[e] EX_cpd_dcyt[e] EX_cpd_dgmp[e]	0 0 0 0 0	000700	0.000703	0.000703	000703	000703
EX_cpd_dad-2[e] EX_cpd_damp[e] EX_cpd_dcmp[e] EX_cpd_dcyt[e] EX_cpd_dgmp[e] EX_cpd_dgmp[e]	0 0 0 0 0 0	0 0 0 0 0 0 0 0	0.000703	0.000703	0007003	000703
EX_cpd_dad-2[e] EX_cpd_damp[e] EX_cpd_dcmp[e] EX_cpd_dcyt[e] EX_cpd_dgmp[e] EX_cpd_dgsn[e] EX_cpd_dgsn[e]	0 0 0 0 0 0	0 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0
EX_cpd_dad-2[e] EX_cpd_damp[e] EX_cpd_dcmp[e] EX_cpd_dcyt[e] EX_cpd_dgmp[e] EX_cpd_dgsn[e] EX_cpd_dms[e] EX_cpd_dmso[e]	0 0 0 0 0 0 0 0	0.0007003 0 0 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0 0
EX_cpd_dad-2[e] EX_cpd_damp[e] EX_cpd_dcmp[e] EX_cpd_dcyt[e] EX_cpd_dgmp[e] EX_cpd_dgsn[e] EX_cpd_dms[e] EX_cpd_dmso[e] EX_cpd_dmso[e]	0 0 0 0 0 0 0 0 0	0.0007003 0 0 0 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0 0 0 0	0.000703 0 0 0 0 0 0 0 0 0 0 0

EX_cpd_	_dodcan[e]	0	0	0	0	0	0
EX_cpd_	_dtmp[e]	0	0	0	0	0	0
EX_cpd_	_duri[e]	0	0	0	0	0	0
EX_cpd_	_etoh[e]	0	0	0	0	0	0
		-	-	-	-	-	-
EX_cpd_	fe2[e]	0.007735	0.007735	0.007735	0.007735	0.007735	0.007735
EX_cpd_	fe3[e]	0	0	0	0	0	0
				11.68699	11.68699		
EX_cpd_	_for[e]	0	0	6	6	9.937768	9.937768
EX_cpd_	_fum[e]	0	0	0	0	0	0
EX_cpd_	gal[e]	0	0	0	0	0	0
EX_cpd_	galactan[e						
]		0	0	0	0	0	0
EX_cpd_	_glc-D[e]	0	0	0	0	0	0
EX_cpd_	_gln-L[e]	0	0	0	0	0	0
EX_cpd_	_glu-L[e]	0	0	0	0	0	0
EX_cpd_	_gly-asp-						
L[e]		0	0	0	0	0	0
EX_cpd_	_gly-glu-						
L[e]		0	0	0	0	0	0
EX_cpd_	gly[e]	0	0	0	0	0	0
EX_cpd_	_glyc-R[e]	0	0	0	0	0	0
EX_cpd_	_glyc[e]	0	0	0	0	0	0
EX_cpd_	glyclt[e]	0	0	0	0	0	0
EX_cpd_	_h2o2[e]	0	0	0	0	0	0
		-	-	-	-	-	-
	h2a[a]	65.60584 2	65.60584 2	20.19606	20.19606	82.51363	82.51363
EX_cpd_	nzo[e]	3	3	4	4	4	4
ЕХ_сра_	nzslej		105 5110	U 27 50775	0 27 59775	120 0202	120 0202
EV and	h[o]	105.5119	105.5119	57.58775	37.38773	138.8303	138.8303
EX cpd	hdcan[e]	10	10	0	0	0	0
EX cpd	hvan[e]	0	0	0	0	0	0
EX_cpd		0	0	0	0	0	0
EX_cpd		0	0	0	0	0	0
EX cpd		0	0	0	0	0	0
EX and	 k[]	U 	U 	U _0 21017	U 	U 71017 D	U 71017 D
EX and		-0.21017	-0.21017	-0.21017	-0.21017	0.21017	0.21017
		0	0	0	0	0	0
	_iac-L[e]	0	0	0	0	0	0
		0	0	0	0	0	0
EX_CDQ	_ieu-L[e]	0	0	0	0	0	0

EX_cpd_lys-L[e]	0	0	0	0	0	0
EX_cpd_mal-L[e]	0	0	0	0	0	0
EX_cpd_malt[e]	0	0	0	0	0	0
EX_cpd_malthp[e]	0	0	0	0	0	0
EX_cpd_malthx[e]	0	0	0	0	0	0
EX_cpd_maltpt[e]	0	0	0	0	0	0
EX_cpd_malttr[e]	0	0	0	0	0	0
EX_cpd_maltttr[e]	0	0	0	0	0	0
EX_cpd_met-L[e]	0	0	0	0	0	0
	-	-	-	-	-	-
EX_cpd_mg2[e]	0.009341	0.009341	0.009341	0.009341	0.009341	0.009341
	-	-	-	-	-	-
EX_cpd_mn2[e]	0.000745	0.000745	0.000745	0.000745	0.000745	0.000745
EX_cpd_mn4o[e]	0	0	0	0	0	0
EX_cpd_mobd[e]	-8.00E-06	-8.00E-06	-8.00E-06	-8.00E-06	-8.00E-06	-8.00E-06
EX_cpd_na1[e]	0	0	0	0	0	0
	38.12459	38.12459	12.59320	12.59320	46.48356	46.48356
EX_cpd_nh4[e]	3	3	8	8	7	7
EX_cpd_no2[e]	0	0	0	0	0	0
EX_cpd_no3[e]	0	0	0	0	0	0
	-	-	-	-		
EX_cpd_o2[e]	0.820226	0.820226	1.010734	1.010734	-2.5047	-2.5047
EX_cpd_ocdcan[e]	0	0	0	0	0	0
EX_cpd_panose[e]	0	0	0	0	0	0
	-	-	-	-	-	-
EX_cpd_pi[e]	0.421062	0.421062	0.421062	0.421062	0.421062	0.421062
EX_cpd_pmcoa[e]	-2.00E-06	-2.00E-06	-2.00E-06	-2.00E-06	-2.00E-06	-2.00E-06
EX_cpd_ppa[e]	0	0	0	0	0	0
EX_cpd_pro-L[e]	0	0	0	0	0	0
EX_cpd_ptrc[e]	0	0	0	0	0	0
EX_cpd_pyr[e]			U	•	-	
	0	0	0	0	0	0
EX_cpd_ser-L[e]	0	0	0	0	0	0 0
EX_cpd_ser-L[e] EX_cpd_so3[e]	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0
EX_cpd_ser-L[e] EX_cpd_so3[e]	0 0 0	0 0 0 -	0 0 0 -	0 0 0 -	0 0 0 -	0 0 0
EX_cpd_ser-L[e] EX_cpd_so3[e] EX_cpd_so4[e]	0 0 0 0.155406	0 0 0 - 0.155406	0 0 0 0.155406	0 0 0 0.155406	0 0 0 0.155406	0 0 0 0.155406
EX_cpd_ser-L[e] EX_cpd_so3[e] EX_cpd_so4[e] EX_cpd_succ[e]	0 0 0 0.155406 0	0 0 0 0.155406 0	0 0 0 0.155406 0	0 0 0 0.155406 0	0 0 0 0.155406 6.244573	0 0 0 0.155406 6.244573
EX_cpd_ser-L[e] EX_cpd_so3[e] EX_cpd_so4[e] EX_cpd_succ[e] EX_cpd_thr-L[e]	0 0 0 0.155406 0 0	0 0 0 0.155406 0 0	0 0 0 0.155406 0 0	0 0 0 0.155406 0 0	0 0 0 0.155406 6.244573 0	0 0 0 0.155406 6.244573 0
EX_cpd_ser-L[e] EX_cpd_so3[e] EX_cpd_so4[e] EX_cpd_succ[e] EX_cpd_thr-L[e] EX_cpd_thym[e]	0 0 0 0.155406 0 0 0 0	0 0 0 0.155406 0 0 0	0 0 0 0.155406 0 0 0 0	0 0 0 0.155406 0 0 0 0	0 0 0 0.155406 6.244573 0 0	0 0 0 0.155406 6.244573 0 0
EX_cpd_ser-L[e] EX_cpd_so3[e] EX_cpd_so4[e] EX_cpd_succ[e] EX_cpd_thr-L[e] EX_cpd_thym[e] EX_cpd_thymd[e]	0 0 0.155406 0 0 0 0 0 0	0 0 0 0.155406 0 0 0 0 0	0 0 0 0.155406 0 0 0 0 0 0 0	0 0 0 0.155406 0 0 0 0 0 0	0 0 0 0.155406 6.244573 0 0 0	0 0 0.155406 6.244573 0 0 0
EX_cpd_ser-L[e] EX_cpd_so3[e] EX_cpd_so4[e] EX_cpd_succ[e] EX_cpd_thr-L[e] EX_cpd_thym[e] EX_cpd_thymd[e] EX_cpd_tma[e]	0 0 0 0.155406 0 0 0 0 0 0 0 0 0 0	0 0 0 0.155406 0 0 0 0 0 0 0 0	0 0 0 0.155406 0 0 0 0 0 0 0 0 0 0	0 0 0 0.155406 0 0 0 0 0 0 0 0 0 0	0 0 0 0.155406 6.244573 0 0 0 0 0	0 0 0.155406 6.244573 0 0 0 0

	1					
EX_cpd_trp-L[e]	0	0	0	0	0	0
EX_cpd_tsul[e]	0	0	0	0	0	0
EX_cpd_ttdcan[e]	0	0	0	0	0	0
EX_cpd_tttnt[e]	0	0	0	0	0	0
EX_cpd_tyr-L[e]	0	0	0	0	0	0
EX_cpd_ura[e]	0	0	0	0	0	0
EX_cpd_urdio[e]	0	0	0	0	0	0
EX_cpd_urea[e]	0.045289	0.045289	0.045289	0.045289	0.045289	0.045289
EX_cpd_uri[e]	0	0	0	0	0	0
EX_cpd_urnyl[e]	0	0	0	0	0	0
EX_cpd_val-L[e]	0	0	0	0	0	0
EX_cpd_xan[e]	0	0	0	0	0	0
FAO4	0	0	0	0	0	0
FAO5	0	0	0	0	0	0
FAO6	0	0	0	0	0	0
FAO7	0	0	0	0	0	0
	-	-			-	-
	43.62050	43.62050			21.75750	21.75750
FBA	8	8	0	0	6	6
	43.62050	43.62050			21.75750	21.75750
FBP	8	8	0	0	6	6
FCLT	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
FDH10	0	0	0	0	0	0
FDH9	0	0	0	0	0	0
FE2abc	0.007735	0.007735	0.007735	0.007735	0.007735	0.007735
FFSD	0	0	0	0	0	0
FGLU	0	0	0	0	0	0
FMETTRS	0	0	0	0	0	0
FMNAT	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
FMNRx	0	0	0	0	0	0
FNOR	0	0	0	0	0	0
			-	-		
FOR	0	0	11.68699	11.68699	-	-
FORT	0	0	6	6	9.937768	9.937768
	0	0 1 4 2 2 4	0	1 020151		11.25024
		U.14224	0	1.028151	208660.0	0 144062
				0.144062		0.144062
	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505
	0	0.000505	0	0	0	0
	U	U	1.070404	U	U	U
FIMFL	1.079494	1.079494	1.079494	1.079494	1.079494	1.079494

					-	-
FUM	2.032317	2.032317	1.528431	1.528431	5.706485	5.706485
FUMACA	0	0	0	0	0	0
G1PACT	0.079308	0.079308	0.079308	0.079308	0.079308	0.079308
G1PCT	0	0	0	0	NA	NA
G1PTMT	0	0	NA	NA	0	0
G1SATi	0.004038	0.004038	0.004038	0.004038	0.004038	0.004038
G35DP	0	0	0	0	0	0
G3PD2	-0.19153	-0.19153	-0.19153	-0.19153	-0.19153	-0.19153
G3PD4	0	0	NA	NA	0	0
G3PD8	0	0	NA	NA	0	0
G5SD	0	0	0	0	0	0
	45.08105	45.08105	19.54966	19.54966	53.46774	53.46774
G6PDA	1	1	6	6	5	5
G6PDHy	11.21305	11.21305	0.165955	0.165955	0	0
GAL1PURI	NA	NA	NA	NA	0	0
GALKr	0	0	0	0	0	0
GALU	0.039197	0.039197	0.039197	0.039197	0.039197	0.039197
			18.08912	18.08912	30.24969	30.24969
GAPD	0	0	4	4	7	7
GARFT	0.150793	0.150793	0.150793	0.150793	0.150793	0.150793
GBEZ	0	0	0	0	0	0
GCALDD	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
GGLUGABDH	0	0	0	0	0	0
GGLUGABH	0	0	0	0	0	0
GGLUPTS	0	0	0	0	0	0
GGTT	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505
	-	-	-	-	-	-
GHMT	0.556611	0.556611	0.556611	0.556611	0.556611	0.556611
GK1	0.072524	0.576409	0.072524	0.072524	0.072524	0.072524
GLCGSD	0	0	NA	NA	NA	NA
GLCP	NA	NA	0	0	0	0
GLCS1	0.115515	0.115515	0.115515	0.115515	0.115515	0.115515
GLCt2	0	0	0	0	0	0
GLGC	0.46206	0.46206	0.46206	0.46206	0.46206	0.46206
GLNS	1.229981	1.229981	1.230233	1.230233	1.230233	1.230233
GLNTRS	0.184695	0.184695	0.184695	0.184695	0.184695	0.184695
GLU5K	0	0	0	0	0	0
GLUCYSL	0	0	0	0	0	0
	-		_		-	
GLUDx	6.183145	0	6.182892	0	6.210613	0

GLUN	NA	NA	NA	NA	0	0
GLUPRT	0.150793	0.150793	0.150793	0.150793	0.150793	0.150793
GLUR	-0.02772	-0.02772	-0.02772	-0.02772	-0.02772	-0.02772
GLUSy	0	0	0	0	0	0
GLUTRR	0.004038	0.004038	0.004038	0.004038	0.004038	0.004038
GLUTRS	0.252539	0.252539	0.252539	0.252539	0.252539	0.252539
GLUt2	0	0	0	0	0	0
GLUt4i	0	0	0	0	0	0
					-	
GLYAT	0	0	0	0	0.990343	0
GLYBt4	0	0	0	0	0	0
GLYCL	0	0	0	0	0	0
GLYCLTDXR	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
GLYCOGEN_SYNTH						
ESIS	0.077	0.077	0.077	0.077	0.077	0.077
GLYCRt2	NA	NA	NA	NA	0	0
GLYC_T	0	0	0	0	0	0
GLYK	0	0	0	0	0	0
GLYOX	0	0	0	0	0	0
GLYTRS	0.283191	0.283191	0.283191	0.283191	0.283191	0.283191
GLYt4	0	0	0	0	0	0
GMHEPAT	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
GMHEPK	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
GMHEPPA	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
GPDDA2	0	0	0	0	0	0
GPDDA4	0	0	0	0	0	0
GRTT	0.000567	0.000567	0.000567	0.000567	0.000567	0.000567
GSHPO	0	0	NA	NA	NA	NA
GSNK	0.072524	0.576409	0.072524	0.072524	0.072524	0.072524
GTHRD	0	0	0	0	0	0
GTHRDH	0	0	0	0	0	0
GTHS	0	0	0	0	0	0
GTPCI	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
GTPCII	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505
GTPDPK	0	0	0	0	0	0
	-	-	-	-	-	-
GUAD	0.072524	0.072524	0.072524	0.072524	0.072524	0.072524
GUAPRT	0	0	0	0	0	0
Growth	1	1	1	1	1	1
	65.60584	65.60584	20.19606	20.19606	82.51363	82.51363
H2Ot5	3	3	4	4	4	4

HACD8	0	0	0	0	0	0
HACOADr	0	0	0	0	0	0
HBZOPT	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
HCO3E	5.581679	5.581679	5.581679	5.581679	5.581679	5.581679
HEMEOS	0	0	0	0	0	0
HEPTT	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
HEX1	0	0	0	0	0	0
HEXTT	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505
HIBHR	0	0	0	0	0	0
HISD1	0	0	0	0	0	0
HISTD	0.088373	0.088373	0.088373	0.088373	0.088373	0.088373
HISTP	0.088373	0.088373	0.088373	0.088373	0.088373	0.088373
HISTRS	0.088373	0.088373	0.088373	0.088373	0.088373	0.088373
HMBS	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505
HMGDx	0	0	0	0	0	0
HMGL	0	0	NA	NA	NA	NA
HMGSs	0	0	NA	NA	0	0
HOXPRx	0	0	NA	NA	NA	NA
HPPDO1	0	0	NA	NA	NA	NA
НРРК	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
HPYRRx	0	0	0	0	0	0
HPYRRy	0	0	0	0	0	0
	-	-	-	-		
HSDy	0.108051	0.108051	0.611937	0.611937	-1.60228	-1.60228
HSK	0	0	0.503885	0.503885	1.494229	1.494229
HSST	0.108051	0.108051	0.108051	0.108051	0.108051	0.108051
HSTPT	0.088373	0.088373	0.088373	0.088373	0.088373	0.088373
HTHBPD	0	0	0	0	0	0
HXAD	0	0	0	0	0	0
HXPRT	0	0	0	0	0	0
ICDHxi	0	9.795027	0	0	0	0
	-					
ICDHy	8.952831	0.842196	0.842196	0.842196	0.842196	0.842196
ICHORSi	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
ICL	1.494229	1.494229	0.990343	0.990343	0	0
IG3PS	0.088373	0.088373	0.088373	0.088373	0.088373	0.088373
IGPDH	0.088373	0.088373	0.088373	0.088373	0.088373	0.088373
IGPS			0.040007	0 040207	0 040207	0 040207
	0.049387	0.049387	0.049387	0.049387	0.049387	0.049387
	0.049387 -	0.049387	0.049387	0.049387	0.049387	0.049387
	-		-		-	
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ILETA	0.268394	5.914751	0.268394	5.914498	0.268394	5.942219
ILETRS	0.268394	0.268394	0.268394	0.268394	0.268394	0.268394
ILEt4	0	0	0	0	0	0
	-	-	-	-	-	-
IMPC	0.238914	0.238914	0.238914	0.238914	0.238914	0.238914
IMPD	0.072524	0.072524	0.072524	0.072524	0.072524	0.072524
INDOLEt2	NA	NA	NA	NA	0	0
INSK	0	0	0	0	0	0
IPDPS	0.003904	0.003904	0.003904	0.003904	0.003904	0.003904
IPMD	0.526852	0.526852	0.526852	0.526852	0.526852	0.526852
	-	-	-	-	-	-
IPPMIa	0.526852	0.526852	0.526852	0.526852	0.526852	0.526852
	-	-	-	-	-	-
IPPMIb	0.526852	0.526852	0.526852	0.526852	0.526852	0.526852
IPPS	0.526852	0.526852	0.526852	0.526852	0.526852	0.526852
IZPN	0	0	0	0	0	0
KARA2i	0.268394	0.268394	0.268394	0.268394	0.268394	0.268394
KAS15	0	0.661538	0	0.661538	0	0.661538
KAS16	0.047735	0.047735	0.047735	0.047735	0.047735	0.047735
KDOPP	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
KDOPS	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
Kt2i	0.21017	4.728404	0.21017	0.21017	0.21017	0.21017
Kt3	0	4.518233	0	0	0	0
LDH_Dir	0	0	0	0	0	0
	-		-		-	
LEUTA	0.433966	5.749179	0.433966	5.748927	0.433966	5.776647
LEUTRS	0.433966	0.433966	0.433966	0.433966	0.433966	0.433966
LEUt4	0	0	0	0	0	0
LIPID_SYNTHESIS	0.175	0.175	0.175	0.175	0.175	0.175
	-		-		-	
LLEUDr	6.183145	0	6.182892	0	6.210613	0
LPADSS	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
LPSSYN_core	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
LPS_SYNTHESIS	0.034	0.034	0.034	0.034	0.034	0.034
LYSTRS	0.218689	0.218689	0.218689	0.218689	0.218689	0.218689
LYSt3	NA	NA	0	0	NA	NA
MACPD	0	0	0	0	0	0
MALS	0	0	0	0	0	0
MAN1PT2	0	0	0	0	0	0
MCITD	0	0	NA	NA	0	0

MCITS	0	0	0	0	0	0
MCOATA	5.068387	5.068387	5.068387	5.068387	5.068387	5.068387
МОН	0	0	0	0	-	- 5 706/85
MDRPD	0 007633	0.007633	0 007633	0 007633	0.007633	0.007633
MERIE MF2	2 032317	2 032317	1 528431	1 528431	0.007033	0.007033
MFAMP1 GLU-ASP	0	0	1.520451	1.520451	0	0
MEAMP1 GLY-ASP	0	0	0	0	0	0
MEAMP1 GLY-GLU	0	0	0	0	0	0
MECDPDH	0.004471	0.004471	0.004471	0.004471	0.004471	0.004471
MECDPS	0.004471	0.004471	0.004471	0.004471	0.004471	0.004471
MEPCT	0.004471	0.004471	0.004471	0.004471	0.004471	0.004471
MET-LABC	0	0	0	0	0	0
METAT	0.009404	0.009404	0.009404	0.009404	0.009404	0.009404
METGL	0	0	NA	NA	0	0
METS	0.109566	0.109566	0.109566	0.109566	0.109566	0.109566
METTRS	0.107797	0.107797	0.107796	0.107796	0.107796	0.107796
MGCH	0	0	NA	NA	NA	NA
MGt3	0	0	0	0	0	0
	-	-	_	_	_	-
MGt5	0.009341	0.009341	0.009341	0.009341	0.009341	0.009341
MI1PP	0	0	0	0	0	0
MICITH	0	0	0	0	0	0
MICITL	0	0	0	0	0	0
MLACI	0	0	NA	NA	NA	NA
MLTS	0	0	NA	NA	NA	NA
MLTSp	0	0	0	0	0	0
MMSDHir	0	0	0	0	0	0
MNabc	0.000745	0.000745	0.000745	0.000745	0.000745	0.000745
MOAT3	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
MOBDabc	8.00E-06	8.00E-06	8.00E-06	8.00E-06	8.00E-06	8.00E-06
MOHMT	0.000615	0.000615	0.000615	0.000615	0.000615	0.000615
MTAN	0.007633	0.007633	0.007633	0.007633	0.007633	0.007633
	-	-	-	-	-	-
MTHFC	0.689787	0.689787	0.689787	0.689787	0.689787	0.689787
	-	-	-	-	-	-
MTHFD	0.689787	0.689787	0.689787	0.689787	0.689787	0.689787
MTHFR2	0.109818	0.109818	0.109818	0.109818	0.109818	0.109818
MTHPTGHM	0	0	NA	NA	NA	NA
MTRI	0.007633	0.007633	0.007633	0.007633	0.007633	0.007633
MTRK	0.007633	0.007633	0.007633	0.007633	0.007633	0.007633

NADH11	NA	NA	0	0.885911	0	5.008139
NADH12	0	0	0	0	0	0
						11.10800
NADH13	NA	NA	0	0.885911	6.099865	3
NADH14	0	0	0	0	0	0
NADH4	0	0	0	0	0	0
NADK	0.000506	0.000506	0.000506	0.000506	0.000506	0.000506
NADS1	0.002579	0.002579	0.002579	0.002579	0.002579	0.002579
NAabcO	0	0	NA	NA	NA	NA
NAt3	0	4.540349	0.022115	0.022115	0	0
NAt3_2	0	3.026899	0	0	0	0
	-	-	-	-	-	-
NAt9	0.005605	0.005605	0.005605	0.005605	0.005605	0.005605
		18.86626		13.85229		13.85229
NDPK1	0	1	0	4	0	4
NDPK2	0.233848	0.760477	0.233848	0.256592	0.233848	0.256592
NDPK3	0.06209	0.090686	0.06209	0.090686	0.06209	0.090686
NDPK4	0.022744	0.022744	0.022744	0.022744	0.022744	0.022744
	-					
NDPK5	0.503885	0.028596	0	0.028596	0	0.028596
	-		-		-	
NDPK6	0.526629	0	0.022744	0	0.022744	0
NDPK7	0	0.028596	0	0.028596	0	0.028596
	-					
NDPK8	0.503885	0.022744	0	0.022744	0	0.022744
	-	-	-	-	-	-
NII 1 4+	38.12459	38.12459	12.59320	12.59320	46.48356	46.48356
	3	3	ð 0	8	/	/
	0 002570	0 002570		0 002570	0 002570	0 002570
	0.002579	0.002579	0.002579	0.002579	0.002579	0.002579
	0.002579	0.002579	0.002579	0.002579	0.002579	0.002579
NODOX	0	0	0	0	0	0
	0 000252	0 000252	0 000252	0 000252	0 000252	0 000252
NPHS	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
NID1	0	0.503885	0 072524	0 072524	0	0
NID10	0.072524	0.072524	0.072524	0.072524	0.072524	0.072524
NIDII NIDII	0	0	0	0	0	0
NID12	0	0	NA	NA	NA	NA
NTD2	0	0	0	0	0	0
NTD3	0	0	0	0	0	0
NTD3_P	0	0	0	0	0	0

NTD4	0	0	0	0	0	0
NTD5	0	0	0	0	0	0
NTD5_P	0	0	0	0	0	0
NTD6	0	0.503885	0	0	0	0
NTD6_P	0	0	0	0	0	0
NTD7	0	0	0	0	0	0
NTD8	0	0.503885	0	0	0	0
NTD8_P	0	0	0	0	0	0
NTD9	0	0	0	0	0	0
NTPP10	0	0	NA	NA	0	0
NTPP11	0	0	NA	NA	0	0
NTPP9	0	0	NA	NA	0	0
NTR4	0	0	0	0	0	0
NTR5	0	0	0	0	0	0
O2t	0.820226	0.820226	1.010734	1.010734	2.5047	2.5047
OAADC	0	0	0	0	0	0
OBTFL	0.011345	0.011345	0.011345	0.011345	0.011345	0.011345
OCBT	0.221268	0.221268	0.221268	0.221268	0.221268	0.221268
ОНРВАТ	0.000252	0.000252	0	0	0	0
ОНРНМ	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
OIVD1i	0.092886	0.092886	0.092886	0.092886	0.092886	0.092886
OIVD2	0	0	0	0	0	0
OIVD3	0	0	0	0	0	0
OMBZLM	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
OMCDC	0.526852	0.526852	0.526852	0.526852	0.526852	0.526852
OMMBLHX	0.000252	0.000252	0	0.000252	0.000252	0.000252
OMMBLHXAN	0	0	0	0.000252	0	0
OMPDC	0.141483	0.141483	0.141482	0.141482	0.141482	0.141482
OMPHHX	0.000252	0.000252	0	0.000252	0.000252	0.000252
OMPHHXAN	0	0	0	0.000252	0	0
	-	-			-	-
	157.2119	157.2119	-	-	176.4624	176.4624
OMP_AC	01	01	52.06936	52.06936	18	18
	45.16035	45.16035	19.62897	19.62897	53.54705	53.54705
OMP_ACGAM	9	9	4	4	3	3
OMP_ADN	0	0	0	0	NA	NA
OMP_ALA-D	0	0	0	0	-0.02772	-0.02772
OMP_ALA-L	0	0	0	0	0	0
OMP_ASP-L	0	0	0	0	0	0
OMP_CA2	0.005605	0.005605	0.005605	0.005605	0.005605	0.005605
OMP_CBL1	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252

OMP_CHITOB	0	0	0	0	0	0
OMP_CHOL	0	0	0	0	0	0
OMP_CIT	0	0	0	0	0	0
OMP_CL	0.005605	0.005605	0.005605	0.005605	0.005605	0.005605
	-	-	-	-		
OMP_CO2	6.406695	6.406695	0.753705	0.753705	0	0
OMP_COBALT2	2.70E-05	2.70E-05	2.70E-05	2.70E-05	2.70E-05	2.70E-05
OMP_CU2	0.000763	0.000763	0.000763	0.000763	0.000763	0.000763
OMP_CYTD	0	0	0	0	NA	NA
OMP_DAD-2	0	0	0	0	NA	NA
OMP_DAMP	0	0	0	0	NA	NA
OMP_DCMP	0	0	0	0	NA	NA
OMP_DCYT	0	0	0	0	NA	NA
OMP_DGMP	0	0	0	0	NA	NA
OMP_DGSN	0	0	0	0	NA	NA
OMP_DMS	0	0	0	0	0	0
OMP_DMSO	0	0	0	0	0	0
OMP_DODCA	0	0	0	0	0	0
OMP_DTMP	0	0	0	0	NA	NA
OMP_DURI	0	0	0	0	NA	NA
OMP_FE2	0.007735	0.007735	0.007735	0.007735	0.007735	0.007735
			-	-		
			11.68699	11.68699	-	-
OMP_FOR	0	0	6	6	9.937768	9.937768
OMP_FUM	0	0	0	0	0	0
OMP_GLU-L	0	0	0	0	0	0
OMP_GLY	0	0	0	0	0	0
OMP_GLY-ASP-L	0	0	0	0	0	0
OMP_GLY-GLU-L	0	0	0	0	0	0
OMP_GLYB	0	0	0	0	0	0
OMP_GLYCLT	0	0	0	0	0	0
OMP_GTHRD	0	0	0	0	0	0
	-	-	-	-	-	-
	105.5119	105.5119	37.58775	37.58775	138.8303	138.8303
OMP_H	16	16	6	6	72	72
OMP_H2	0	0	0	0	0	0
	65.60584	65.60584	20.19606	20.19606	82.51363	82.51363
OMP_H2O	3	3	4	4	4	4
OMP_H2O2	0	0	0	0	0	0
OMP_H2S	0	0	0	0	0	0
OMP HDCA	0	0	0	0	0	0

OMP_ILE-L	0	0	0	0	0	0
OMP_INDOLE	0	0	0	0	0	0
OMP_INOSHP	0	0	0	0	0	0
OMP_INOSPP1	0	0	0	0	0	0
OMP_K	0.21017	0.21017	0.21017	0.21017	0.21017	0.21017
OMP_LAC-D	0	0	0	0	0	0
OMP_LAC-L	0	0	0	0	0	0
OMP_LEU-L	0	0	0	0	0	0
OMP_LYS-L	0	0	0	0	0	0
OMP_MAL-L	0	0	0	0	0	0
OMP_MET-L	0	0	0	0	0	0
OMP_MG2	0.009341	0.009341	0.009341	0.009341	0.009341	0.009341
OMP_MN2	0.000745	0.000745	0.000745	0.000745	0.000745	0.000745
OMP_MOBD	8.00E-06	8.00E-06	8.00E-06	8.00E-06	8.00E-06	8.00E-06
	-	-	-	-	-	-
	38.12459	38.12459	12.59320	12.59320	46.48356	46.48356
OMP_NH4	3	3	8	8	7	7
OMP_NMN	0	0	0	0	0	0
OMP_NO2	0	0	0	0	0	0
OMP_NO3	0	0	0	0	0	0
OMP_02	0.820226	0.820226	1.010734	1.010734	2.5047	2.5047
OMP_OCDCA	0	0	0	0	0	0
OMP_PI	0.421062	0.421062	0.421062	0.421062	0.421062	0.421062
OMP_PMCOA	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06	2.00E-06
OMP_PPA	0	0	0	0	0	0
OMP_PRO-L	0	0	0	0	0	0
OMP_PTRC	0	0	0	0	0	0
OMP_PYR	0	0	0	0	0	0
OMP_SER-L	0	0	0	0	0	0
OMP_SO3	0	0	0	0	0	0
OMP_SO4	0.155406	0.155406	0.155406	0.155406	0.155406	0.155406
					-	-
OMP_SUCC	0	0	0	0	6.244573	6.244573
OMP_THR-L	0	0	0	0	0	0
OMP_THYMD	0	0	0	0	NA	NA
OMP_TMA	0	0	0	0	0	0
OMP_TMAO	0	0	0	0	0	0
OMP_TRP-L	0	0	0	0	0	0
OMP_TSUL	0	0	0	0	0	0
OMP_TTDCA	0	0	0	0	0	0
OMP_TTTNT	0	0	0	0	0	0

OMP_TYR-L	0	0	0	0	0	0
OMP_URA	0	0	0	0	0	0
	-	-	-	_	-	-
OMP_UREA	0.045289	0.045289	0.045289	0.045289	0.045289	0.045289
OMP_URI	0	0	0	0	NA	NA
OMP_VAL-L	0	0	0	0	0	0
OMP_XAN	0	0	0	0	NA	NA
OMP_na1	0	0	0	0	0	0
OPHBDC	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
ОРННХ	0.000252	0.000252	0	0.000252	0.000252	0.000252
OPHHXAN	0	0	0	0.000252	0	0
ORNCD	0.155468	0.155468	0.155468	0.155468	0.155468	0.155468
	-	-	-	-	-	-
ORPT	0.141483	0.141483	0.141482	0.141482	0.141482	0.141482
OXGDC2	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
P5CD	0	0	0	0	0	0
P5CR	0	0	0	0	0	0
PANTS	0.000615	0.000615	0.000615	0.000615	0.000615	0.000615
PAP	0.101276	0.101276	0.101276	0.101276	0.101276	0.101276
PAPPT3	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
PAPSR	0.150736	0.150736	0.150736	0.150736	0.150736	0.150736
PASYN_WP2	0.175	0.175	0.175	0.175	0.175	0.175
PDH	0	5.314555	0	0	6.647166	6.647166
PDX5PO	0.000252	0.000252	0	0	0	0
PDX5PS	0.000252	0.000252	0	0	0	0
PEPTIDOXe	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
PEPTIDO_SYNTHES						
IS	0.025	0.025	0.025	0.025	0.025	0.025
PERD	0.000252	0.000252	0	0	0	0
			12.74524	12.74524	10.99601	10.99601
PFL	1.058245	1.058245	1	1	2	2
	-	-	-	-	-	-
PGAMT	0.079308	0.079308	0.079308	0.079308	0.079308	0.079308
PGCD	0	0	0	0	0	0
PGDH	0	5.314555	0.165955	0.165955	0	0
PGDHY	5.898494	11.21305	0	0	0	0
	-	-				
	11.71430	11.71430	-	-	-	-
PGI	7	7	0.667212	0.667212	0.501257	0.501257
	_	~	18.08912	18.08912	30.24969	30.24969
PGK	0	0	4	4	7	7

PGL	11.21305	11.21305	0.165955	0.165955	0	0
PGLYCP	0	0	0	0	0	0
			18.08912	18.08912	30.24969	30.24969
PGM	0	0	4	4	7	7
	-	-	-	-	-	-
PGMT	0.501257	0.501257	0.501257	0.501257	0.501257	0.501257
PGPPH	0.01653	0.01653	0.01653	0.01653	0.01653	0.01653
PGSA	0.01653	0.01653	0.01653	0.01653	0.01653	0.01653
PHE4MO	0	0	NA	NA	NA	NA
PHEAL	0	0	0	0	0	0
PHEMEabc	0	0	0	0	NA	NA
	-	-	-	-	-	-
PHETA1	0.166877	0.166877	0.166877	0.166877	0.166877	0.166877
PHETRS	0.166877	0.166877	0.166877	0.166877	0.166877	0.166877
Plabc	0	0	NA	NA	NA	NA
Plt6	0.421062	0.421062	0.421062	0.421062	0.421062	0.421062
PMANM	0	0	NA	NA	0	0
PMCOAt	-2.00E-06	-2.00E-06	-2.00E-06	-2.00E-06	-2.00E-06	-2.00E-06
PMDPHT	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505
PNTK	0.000615	0.000615	0.000615	0.000615	0.000615	0.000615
PPA	6.160486	6.160486	6.160486	6.160486	6.160486	6.160486
PPAtNa	0	0	0	0	0	0
PPBNGS	0.002019	0.002019	0.002019	0.002019	0.002019	0.002019
PPC	3.782013	3.782013	3.782013	3.782013	9.488498	9.488498
PPCDC	0.000615	0.000615	0.000615	0.000615	0.000615	0.000615
РРСК	0	0	0	0	0	0
	-	-	-	-	-	-
PPM	0.511521	0.511521	0.007635	0.007635	0.007635	0.007635
PPM2	0.503885	0.503885	0	0	0	0
PPNCL	0.000615	0.000615	0.000615	0.000615	0.000615	0.000615
PPND	0.126933	0.126933	0.126933	0.126933	0.126933	0.126933
PPNDH	0.166877	0.166877	0.166877	0.166877	0.166877	0.166877
PPPGFUM	0	0.000252	0	0.000252	0	0.000252
PPPGMEN	0	0.000252	0	0.000252	0	0.000252
PPPGNO3	0	0	0	0	0	0
PPPGO	0	0.000252	0	0	0	0
PPS	4.510081	4.510081	0	0	0	0
PPTGSe	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
PPTT	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505
PRAGS	0.150793	0.150793	0.150793	0.150793	0.150793	0.150793
PRAIS	0.150793	0.150793	0.150793	0.150793	0.150793	0.150793

PRAIi	0.049387	0.049387	0.049387	0.049387	0.049387	0.049387
PRAMPC	0.088373	0.088373	0.088373	0.088373	0.088373	0.088373
PRASCS	0.150541	0.150541	0.150541	0.150541	0.150541	0.150541
PRATPP	0.088373	0.088373	0.088373	0.088373	0.088373	0.088373
PRFGS	0.150793	0.150793	0.150793	0.150793	0.150793	0.150793
PRKIN	0	0	0	0	0	0
PRMICIi	0.088373	0.088373	0.088373	0.088373	0.088373	0.088373
PRO1q	0	0	0	0	0	0
PROTRS	0.155468	0.155468	0.155468	0.155468	0.155468	0.155468
PROT_SYNTHESIS	0.528	0.528	0.528	0.528	0.528	0.528
PROt4	0	0	0	0	0	0
PRPPS	0.432615	0.432615	0.432615	0.432615	0.432615	0.432615
PSCVT	0.344207	0.344207	0.344207	0.344207	0.344207	0.344207
PSD	0.057136	0.057136	0.057136	0.057136	0.057136	0.057136
PSERT	0	0	0	0	0	0
PSP_L	0	0	0	0	0	0
PSSA	0.057136	0.057136	0.057136	0.057136	0.057136	0.057136
PSUDS	0	0	0	0	0	0
	-	-			10.92745	10.92745
PTAr	8.142054	2.827499	4.048828	4.048828	1	1
PTPATi	0.000615	0.000615	0.000615	0.000615	0.000615	0.000615
	-	-	-	-	-	-
PUNP1	0.511521	0.007635	0.007635	0.007635	0.007635	0.007635
PUNP2	0	0.503885	0	0	0	0
	-	-	-	-	-	-
PUNP3	0.576409	0.072524	0.072524	0.072524	0.072524	0.072524
PUNP4	0	0.503885	0	0	0	0
PUNP5	0	0	0	0	0	0
PUNP6	0	0	0	0	0	0
PUNP7	0.072524	0.072524	0.072524	0.072524	0.072524	0.072524
ΡΥΑΜ5ΡΟ	0	0	0	0	0	0
PYDXL5PSYN	0	0	0.000252	0.000252	0.000252	0.000252
			13.57904	13.57904	20.03313	20.03313
РҮК	0	0	3	3	1	1
	-	0	0	0	0	0
	0.503885	0	0	0	0	0
	0	0	0	0	0	0
QULINS	0.002579	0.002579	0.002579	0.002579	0.002579	0.002579
KBFK	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
KBF29	0.00101	0.00101	0.00101	0.00101	0.00101	0.00101
RBFSb	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505

RBK	0	0	0	0	0	0
RHCCE	0	0	0	0	0	0
RIBabc	NA	NA	NA	NA	0	0
RNA_SYNTHESIS	0.09	0.09	0.09	0.09	0.09	0.09
RNDR1	0	0.526629	0	0.022744	0	0.022744
RNDR2	0	0.532482	0	0.028596	0	0.028596
RNDR3	0	0.028596	0	0.028596	0	0.028596
RNDR4	0	0.526629	0	0.022744	0	0.022744
RNTR1	0	0.526629	0	0.022744	0	0.022744
RNTR2	0	0.532482	0	0.028596	0	0.028596
RNTR3	0	0.028596	0	0.028596	0	0.028596
RNTR4	0	0.526629	0	0.022744	0	0.022744
	37.35238	42.66693			36.72451	36.72451
RPE	3	8	8.969698	8.969698	3	3
	37.36532	37.36532			36.73745	36.73745
RPI	7	7	8.816687	8.816687	7	7
S7PI	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
SADH	0	0	0	0	0	0
SADT2	0.150736	0.150736	0.150736	0.150736	0.150736	0.150736
SDPDS	0.246409	0.246409	0.246409	0.246409	0.246409	0.246409
	-	-	-	-	-	-
SDPTA	0.246409	0.246409	0.246409	0.246409	0.246409	0.246409
SELNPS	0	0	0	0	0	0
SERAI	0.150736	0.150/36	0.150/36	0.150/36	0.150736	0.150/36
SERD_L	0	0	0	0	0	0
SERGLYX	0	0	0	0	0	0
SERIRS	0.299352	0.299352	0.299352	0.299352	0.299352	0.299352
SERt4	0	0	0	0	0	0
SERt6	0	0	0	0	0	0
SFGTH	0	0	0	0	0	0
SGDS	0	0	0	0	0	0
SGSAD	0	0	0	0	0	0
SHCHCS2	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
SHCHD2	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
SHCHF	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
SHK3D	0.344207	0.344207	0.344207	0.344207	0.344207	0.344207
SHKK	0.344207	0.344207	0.344207	0.344207	0.344207	0.344207
SHSL1	0.108051	0.108051	0.108051	0.108051	0.108051	0.108051
SLCYSS	0	0	0	0	0	0
SO4t2	0.155406	0.155406	0.155406	0.155406	0.155406	0.155406
SOD	0	0	0	0	0	0

SOTA	0	0	0	0	0	0
SPA	0	0	0	0	0	0
SPMS	0.007633	0.007633	0.007633	0.007633	0.007633	0.007633
SPRS	NA	NA	NA	NA	0	0
SSALx	0	0	0	0	0	0
SUCBZL	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
SUCBZS	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
SUCCtex	0	0	0	0	6.244573	6.244573
SUCD7	1.494118	1.638937	0.990989	2.020962	0	5.008139
SUCOAS	0.354571	0.354571	0.354571	0.354571	0.354571	0.354571
SUCP	0	0	0	0	0	0
SUCRPTS	0	0	0	0	0	0
SULR	- 0.150736 -	- 0.150736 -	- 0.150736	- 0.150736	- 0.150736 -	- 0.150736 -
	38.32139	38.32139	-	-	37.18989	37.18989
TAL	6	6	9.269123	9.269123	3	3
TDP3AAAT	0	0	0	0	0	0
TDPDRE	0	0	0	0	0	0
TDPDRR	0	0	0	0	0	0
TDPGDH	0	0	0	0	0	0
TDSK	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
THD2	0	4.518233	11.92667 1	11.92667 1	15.76769 9	15.76769 9
THD5	0	9.79427	0	0	0	0
THDPS	0.246409	0.246409	0.246409	0.246409	0.246409	0.246409
THMDt2	0	0	0	0	0	0
THRA	- 0.503885	- 0.503885	0	0	0	0.990343
THRD	0	0	0	0	0	0.990343
THRD_L	0.279739	0.279739	0.279739	0.279739	0.279739	0.279739
THRHT	NA	NA	0	0	- 0.005605	- 0.005605
THRLAD	0	0	0	0	0	0
THRS	0	0	0.503885	0.503885	1.494229	1.494229
THRTRS	0.224147	0.224147	0.224147	0.224147	0.224147	0.224147
THRt3	0	4.518233	NA	NA	0	0
THRt4	0	4.518233	0	0	0.005605	0.005605
THZPSN	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252

	-	-				
	38.30946	38.30946			-	-
TKT1	3	3	-9.25719	-9.25719	37.17796	37.17796
	-	-				
T 1/ T 0	38.66585	38.66585	0.64.000	0.64000	07 50 44	07 50 44
	6	6	-9.61333	-9.61333	-37.5341	-37.5341
TMAOR3e	0	0	0	0	0	0
TMDK1	0	0	0	0	0	0
	0	0	0	0	0	0
TMDS	0.022744	0.022744	0.022744	0.022744	0.022744	0.022744
TMPKr	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
ТМРРР	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
	-	-			-	-
	43.81461	43.81461	0 4 0 4 4 4	0 1 0 1 1 1	21.95161	21.95161
	8	8	-0.19411	-0.19411	5	5
TRACE_ELEMENTS	0.021	0.021	0.021	0.021	0.021	0.021
	0.757301	0.757301	0.253416	0.253416	0.253416	0.253416
TRE6PP	0	0	0	0	0	0
TREH	0	0	0	0	0	0
TREHtex	0	0	0	0	0	0
TRPOR	0	0	0	0	0	0
TRPS2	0.049387	0.049387	0.049387	0.049387	0.049387	0.049387
TRPS3	0.049387	0.049387	0.049387	0.049387	0.049387	0.049387
TRPTRS	0.049387	0.049387	0.049387	0.049387	0.049387	0.049387
TRPt6	NA	NA	0	0	0	0
TSULST	0	0	NA	NA	0	0
	-	-	-	-	-	-
TYRTA	0.126933	0.126933	0.126933	0.126933	0.126933	0.126933
TYRTRS	0.126681	0.126681	0.126681	0.126681	0.126681	0.126681
TYRt6	NA	NA	0	0	0	0
U23GAAT	0.023868	0.023868	0.023868	0.023868	0.023868	0.023868
UAAGDS	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
UAGAAT	0.023868	0.023868	0.023868	0.023868	0.023868	0.023868
UAGCVT	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
UAGDP	0.079308	0.079308	0.079308	0.079308	0.079308	0.079308
UAGPT3	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
UAMAGS	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
UAMAS	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
UAPGR	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
UDCPDP	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
UDCPDPS	6.20E-05	6.20E-05	6.20E-05	6.20E-05	6.20E-05	6.20E-05

UDPG4E	0.035802	0.035802	0.035801	0.035801	0.035801	0.035801
UDPHEXURI	NA	NA	NA	NA	0	0
UGMDDS	0.02772	0.02772	0.02772	0.02772	0.02772	0.02772
UHGADA	0.023868	0.023868	0.023868	0.023868	0.023868	0.023868
UMPK	0.19307	0.696956	0.19307	0.19307	0.19307	0.19307
UNK3	0.007633	0.007633	0.007633	0.007633	0.007633	0.007633
UPP3MT	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
UPP3S	0.000505	0.000505	0.000505	0.000505	0.000505	0.000505
UPPDC1	0.000252	0.000252	0.000252	0.000252	0.000252	0.000252
UPPRT	0	0	0	0	0	0
UQOR	0	0	0	0	0	0
URAt6	0	0	0	0	0	0
URCN	0	0	0	0	0	0
URHYDROX	0	0	0	0	0	0
	-	-	-	-	-	-
URIDK2	0.526629	0.022744	0.022744	0.022744	0.022744	0.022744
URIH	0	0	0	0	0	0
URIK1	0	0.503885	0	0	0	0
URIK2	0	0.503885	0	0	0	0
URIK3	0	0.503885	0	0	0	0
URIt2	0	0	0	0	0	0
USHD	0.011934	0.011934	0.011934	0.011934	0.011934	0.011934
UreaExp	0.045289	0.045289	0.045289	0.045289	0.045289	0.045289
	-		-		-	
VALALAMOB	0.272345	5.9108	0.272345	5.910547	0.272345	5.938268
	-		-		-	
VALDHr	6.183145	0	6.182892	0	6.210613	0
	-		-		-	
VALTA	2.168105	5.9108	1.664219	5.910547	0.701596	5.938268
VALTRS	0.272345	0.272345	0.272345	0.272345	0.272345	0.272345
VALt4	0	0	0	0	0	0
WO4abc	0	0	0	0	0	0
XAND	0	0	0	0	0	0
XANt	0	0	0	0	0	0
	114.3277	119.6422	27.84021	27.84021	111.4365	111.4365
ХРК	02	57	8	8	74	74

Appendix V Data S3 for Manuscript II

Data S3 Index

Each page in the workbook represents a unique comparison between two transcriptomes. The name of the tab is in the format of {condition 1}_{condition 2}_{growth phase}

Table A: Comparison between early log phase samples from 15°C and 4°C cultures.

Table B: Comparison between late log phase samples from 15°C and 4°C cultures.

Table C: Comparison between stationary phase samples from 15°C and 4°C cultures.

Table D: Comparison between early log phase samples from 20°C and 15°C cultures.

Table E: Comparison between late log phase samples from 20°C and 15°C cultures.

Table F: Comparison between stationary phase samples from 20°C and 15°C cultures.

Table G: Comparison between early log phase samples from 20°C and 4°C cultures.

Table H: Comparison between late log phase samples from 20°C and 4°C cultures.

Table I: Comparison between stationary phase samples from 20°C and 4°C cultures.

Column

_				
Des	cri	pti	or	IS

Descriptions	
gene	Refseq locus tag
log2FoldChange	Log2 Fold change calculated by DESeq2. Negative log 2 fold changes indicate that the expression of the gene was higher in condition 1. Positive log2 fold changes indicate that expression was higher in condition 2.
padj	P-value of the log2 fold change adjusted for multiple testing calcualted by DESeq2
name	Gene name based on EggNOG functional annotation
cats	COG functional category based on EggNOG functional annotation

log2FoldCh ange (<0 higher in 4, >0 higher in 15) padj cats gene name Amino Acid sps_RS00 metabolism and 915 4.55E-08 oligopeptidase A transport 2.45713272 Amino Acid sps RS03 2.00988101 0.000229053 PLP-dependent cysteine metabolism and 160 9501 synthase family protein transport 6 Amino Acid sps RS06 3.26042724 ATP metabolism and 490 6.51E-13 phosphoribosyltransferase transport 8 Amino Acid sps RS06 3.11443840 metabolism and 495 1.64E-07 histidinol dehydrogenase transport Amino Acid sps_RS06 2.76354676 histidinol-phosphate metabolism and 500 6.04E-05 transaminase transport 5 bifunctional histidinolphosphatase/imidazoleglyc Amino Acid 2.27988736 0.000888896 erol-phosphate metabolism and sps RS06 505 4923 dehydratase HisB transport imidazole glycerol Amino Acid phosphate synthase subunit metabolism and sps RS06 2.69092154 510 2.09E-05 HisH transport 4 Amino Acid sps RS07 3.71488465 1-aminocyclopropane-1metabolism and 005 6.25E-10 carboxylate deaminase 3 transport aminotransferase class V-Amino Acid sps RS09 2.58272049 fold PLP-dependent metabolism and 130 3.05E-08 enzyme transport Amino Acid sps RS09 2.19597818 branched-chain amino acid metabolism and 555 6.87E-09 ABC transporter permease transport Amino Acid sps RS11 pyrroline-5-carboxylate metabolism and 2.08E-07 reductase 505 transport 2.33616171 Amino Acid metabolism and sps RS12 2.24545348 glutamate synthase large

Data S3 Table A: Comparison between early log phase samples from 15°C and 4°C cultures.

transport

5.03E-07 subunit

9

080

sps_RS12 085	2.12102450 5	1.12E-06	glutamate synthase small subunit	Amino Acid metabolism and transport
sps_RS12 610	- 3.12720512 6	8.68E-08	aspartate aminotransferase family protein	Amino Acid metabolism and transport
sps_RS13 315	- 3.84666756 5	1.78E-16	EamA/RhaT family transporter	Amino Acid metabolism and transport
sps_RS15 440	2.03900977 6	0.000567452 7167	ketol-acid reductoisomerase	Amino Acid metabolism and transport
sps_RS16 205	2.09481493 7	1.32E-05	3-isopropylmalate dehydratase small subunit	Amino Acid metabolism and transport
sps_RS16 210	2.41238893 3	3.26E-13	3-isopropylmalate dehydratase large subunit	Amino Acid metabolism and transport
sps_RS16 215	2.82406003 7	3.47E-24	3-isopropylmalate dehydrogenase	Amino Acid metabolism and transport
sps_RS16 220	2.11633424	1.17E-11	2-isopropylmalate synthase	Amino Acid metabolism and transport
sps_RS17 470	2.30478034	1.57E-09	cysteine synthase A	Amino Acid metabolism and transport
sps_RS21 065	- 2.57424858 9	7.60E-09	EamA/RhaT family transporter	Amino Acid metabolism and transport
sps_RS22 050	3.65518078 9	1.94E-23	5- methyltetrahydropteroyltri glutamatehomocysteine S-methyltransferase	Amino Acid metabolism and transport
sps_RS24 965	- 2.07965274 4	4.38E-05	type 1 glutamine amidotransferase	Amino Acid metabolism and transport
sps_RS19 520	- 2.57677572 2	4.51E-07	allantoinase PuuE	Carbohydrate metabolism and transport
sps_RS00 455	- 2.67943112 3	4.61E-13	hypothetical protein	Cell motility
sps_RS00 460	- 2.84527207 4	1.71E-09	flagellar motor stator protein MotA	Cell motility

sps RS00			flagellar hook-length	
475	-3.61274973	2.14E-14	control protein FliK	Cell motility
sps RS00		0.000723946	flagellar export chaperone	
485	-2.55181689	3908	FliS	Cell motility
sps_RS00				
490	-2 13382262	8 66F-09	flagellar book protein FliD	Cell motility
470	2.13302202	0.001 07	nagenar nook protein ThD	
and PS00	2 20120572		flagaller basel body rod	
520	2.29130373	1 24E 05	nrotoin ElaG	Coll motility
550	/	1.54E-05		
	-			
sps_KS00	2.1/0/6601	2 405 06		C 11 ('1')
610 D (11)	9	2.49E-06	OmpA family protein	Cell motility
sps_RS11	2.00965976		type IV pili twitching	G 11
495	6	2.38E-09	motility protein PilT	Cell motility
			EscN/YscN/HrcN family	
sps_RS27	2.42359494		type III secretion system	
410	4	5.36E-06	ATPase	Cell motility
				Cell
				wall/membrane/e
sps_RS09	2.11070827			nvelope
045	5	1.41E-08	energy transducer TonB	biogenesis
				Cell
				wall/membrane/e
sps RS10			outer membrane protein	nvelope
100	2.76022882	8.46E-14	OmpW	biogenesis
			1	Cell
				wall/membrane/e
sps RS11	2.45555992	0.000240443		nvelope
770	6	8064	OmpA family protein	biogenesis
110				Cell
				wall/membrane/e
sns RS12				nvelone
490	2 24682787	6 80E-06	hypothetical protein	hiogenesis
	2.2 1002707	0.001-00	ng pomonour protom	Cell
				wall/membrane/a
ong DS14	2 24018562			wall/inclinitatic/c
sps_K514	2.24010302	2 52E 05	transporter	hiogeneoig
443	0	2.32E-03	transporter	
DO16	0.50704461			wall/membrane/e
sps_KS15	2.52/24461			nvelope
300	4	/.0/E-20	OmpA family protein	biogenesis
				Cell
	-			wall/membrane/e
sps_RS18	3.20418097			nvelope
185	8	2.70E-13	glycosyl transferase	biogenesis

				Cell
DC10	-			wall/membrane/e
sps_KS18	2.06055189			nvelope
190	2	4.80E-06	nucleotidyl transferase	biogenesis
ana DC19	-	0 000227620	CDD alwaysel	wall/memorane/e
sps_K510	2.1/3013/0	0.00052/059	CDP-glycerol	hiogenegia
195	0	010	grycerophosphotransferase	Call
				Uell wall/mombrana/a
ene PS24	2 27540360			wall/inclinitatic/c
sps_1324 070	2.27340300	2 20F-08	energy transducer TonB	hiogenesis
070		2.271-00	energy transducer rollb	biogenesis
sps RS13	2 34448263		type 3 dihydrofolate	Coenzyme
240	2.34440203	3 36E-11	reductase	metabolism
sns RS20	2 04403407	5.501 11		Coenzyme
3p3_1(520 075	2.04403407	943E-09	glutamatecysteine ligase	metabolism
010	,	9.15E 09	heme anaerobic	
			degradation radical SAM	
sps RS24			methyltransferase	Coenzyme
100	-2.09186263	9.24E-06	ChuW/HutW	metabolism
		,		Energy
sps RS03	2.19838672			production and
735	1	2.30E-07	hypothetical protein	conversion
				Energy
sps RS04	2.41532099		cytochrome-c oxidase,	production and
545	1	1.05E-10	cbb3-type subunit III	conversion
				Energy
sps_RS04	2.63159381		cbb3-type cytochrome c	production and
550	8	6.20E-08	oxidase subunit 3	conversion
				Energy
sps_RS04	2.29906161		cytochrome-c oxidase,	production and
555	5	2.63E-07	cbb3-type subunit II	conversion
	-			Energy
sps_RS07	3.14339884			production and
560	6	2.99E-07	hydrogenase	conversion
				Energy
sps_RS09	2.39560605	0.000634247		production and
325	2	2103	cytochrome C	conversion
				Energy
sps_RS10	2.37112094			production and
985	5	4.95E-09	isocitrate dehydrogenase	conversion
	-			Energy
sps_RS15	2.41090199	0.000157089	NADH-dependent alcohol	production and
885	2	0195	dehydrogenase	conversion

				Energy
sps RS20	3.00012640		sodium ion-translocating	production and
125	5	4.95E-09	decarboxylase subunit beta	conversion
	-			Energy
sps_RS23	3.58696267			production and
415	1	9.10E-15	alkene reductase	conversion
			pyruvate dehydrogenase	
			complex	Energy
sps_RS26	2.15590780		dihydrolipoyllysine-	production and
460	3	6.40E-06	residue acetyltransferase	conversion
			NAD(P)H-dependent	Energy
sps_RS27	2.03905041	0.000122375	glycerol-3-phosphate	production and
670	1	6457	dehydrogenase	conversion
				Energy
sps_RS27	2.81596090		F0F1 ATP synthase	production and
845	9	2.81E-07	subunit epsilon	conversion
				Energy
sps_RS27	2.42880403		F0F1 ATP synthase	production and
850	1	4.76E-05	subunit beta	conversion
				Energy
sps_RS27		0.000227161	F0F1 ATP synthase	production and
855	2.22246063	9999	subunit gamma	conversion
DGOO	-			D
sps_RS00	2.32533924	2 01 5 05		Function
060	1	3.01E-05	LysE family translocator	Unknown
DCOO	-	0.00015(710		
sps_KS00	2.3/83430/	0.000156/18	11	Function
385	8	6126	collagenase	Unknown
ana DCOO	- 2 21609544	0.000200051	mathyltransforma damain	Eurotion
sps_K500	5.51096544	0.000399031	methyltransferase domain-	Function
075	4	909	containing protein	UIIKIIOWII
ene RCOO	2 32027810	0.000100240		Function
sps_1300 870	2.52027810	6.000109240	VIIT family protein	Unknown
sns RSA1	3 26811262	0723		Function
100	5.20011202	4 27F-08	hypothetical protein	Unknown
sps RS02		4.2712 00	ABC transporter ATP-	Function
165	-2 1134215	1 15E-08	hinding protein	Unknown
105		1.151 00		
sps RS02	2,10413225			Function
645	5	1.98E-05	hypothetical protein	Unknown
sps RS04		0.000601054		Function
630	-2.47485543	3627	hypothetical protein	Unknown
sps RS05	2.02126106		type VI secretion system	Function
145	1	7.06E-05	protein TssA	Unknown

sps_RS06	2.74166398		23S rRNA accumulation	Function
735	1	7.00E-13	protein YceD	Unknown
sps_RS07 010	- 2.32020319 4	5.31E-13	YccF domain-containing protein	Function Unknown
sps_RS07 015	- 2.90527438 7	2.34E-09	ABC transporter	Function Unknown
sps_RS07 580	- 2.90096398 5	7.82E-11	DUF1566 domain- containing protein	Function Unknown
sps_RS07 765	3.09994495	6.14E-10	curlin	Function Unknown
sps_RS08 435	2.14432426 7	1.95E-20	cytotoxic necrotizing factor	Function Unknown
sps_RS08 545	- 2.58144089 6	0.000253830 8085	N-acetyltransferase	Function Unknown
sps_RS08 925	- 2.62367077 4	7.64E-07	NADP-dependent oxidoreductase	Function Unknown
sps_RS09 140	- 2.00538267 7	3.18E-07	ATPase	Function Unknown
sps_RS09 320	2.50764786 2	0.000120654 1052	cytochrome C	Function Unknown
sps_RS09 560	2.45495819 4	5.18E-13	AzlD domain-containing protein	Function Unknown
sps_RS09 605	3.00005382 1	0.000410977 9478	N-acetyltransferase	Function Unknown
sps_RS09 770	- 2.55712167 5	5.75E-10	hypothetical protein	Function Unknown
sps_RS09 930	- 2.27667004 7	3.38E-08	tetratricopeptide repeat protein	Function Unknown
sps_RS10 070	2.36337947	2.81E-17	protease	Function Unknown
sps_RS10 625	3.28550120 4	1.57E-15	hypothetical protein	Function Unknown
sps_RS11 140	2.91031872	9.49E-07	peptidase	Function Unknown
sps_RS11 145	2.66366113	7.59E-07	hypothetical protein	Function Unknown

	-			
sps_RS11	3.11462917		DUF2884 domain-	Function
540	5	1.92E-15	containing protein	Unknown
	-			
sps RS12	2.13751781	0.000312574	cupin domain-containing	Function
620	6	8346	protein	Unknown
sps RS12			-	Function
860	4.04554213	1.62E-06	hypothetical protein	Unknown
	_			
sps RS13	3.79112846			Function
245	6	7.89E-24	hypothetical protein	Unknown
	_			
sps RS13	2.13956147			Function
250	8	7.89E-24	threonine/serine exporter	Unknown
	-		·····	
sps RS13	2.05135785	0.000702633		Function
985	7	1602	transposase	Unknown
sps RS14			F	Function
360	4.29282835	1.09E-19	hypothetical protein	Unknown
sps RS14	2.58983223			Function
370	5	6.77E-07	hypothetical protein	Unknown
sps RS14	2.15629700	0.000164773	curli production assembly	Function
450	8	0646	protein CsgF	Unknown
sps_RS15	2.16189700		p	Function
065	4	1.06E-07	adhesin	Unknown
sps RS15	2.22557809		type I secretion system	Function
070	4	4.57E-07	permease/ATPase	Unknown
sps RS15			<u>r</u>	Function
570	3.02008577	7.77E-06	hypothetical protein	Unknown
	-			
sps RS16	3.36705074			Function
965	5	4.34E-10	hypothetical protein	Unknown
	_		- 71	
sps RS16	4.56591891			Function
980	4	1.04E-06	hypothetical protein	Unknown
	-			
sps RS16	4.59123608		DUF1320 domain-	Function
990	3	3.91E-05	containing protein	Unknown
	-			
sps RS17	4.22412632			Function
000	6	7.95E-12	hypothetical protein	Unknown
	-		***	
sps RS17	5.27099435			Function
005	8	2.99E-08	hypothetical protein	Unknown

sps RS17	- 2.26629337			Function
010	6	4.21E-06	hypothetical protein	Unknown
sps_RS18	3.18944852			Function
960	5	1.42E-25	hypothetical protein	Unknown
sps_RS19 515	- 2.93348953 5	1.14E-08	OHCU decarboxylase	Function Unknown
sps_RS20 300	- 2.94367693 9	5.70E-17	hypothetical protein	Function Unknown
sps_RS20 305	- 2.27907748 2	1.03E-09	KR domain-containing protein	Function Unknown
sps_RS20 565	- 2.91839028 6	0.000186294 2119	PAP2 family protein	Function Unknown
sps_RS20 570	- 2.45521380 5	0.000310056 2264	putative porin	Function Unknown
sps_RS21 070	- 3.08307112 7	6.02E-06	hypothetical protein	Function Unknown
sps_RS21 845	3.06462664 4	1.34E-13	hypothetical protein	Function Unknown
sps_RS22 705	- 2.46861753 7	5.42E-05	NADPH-dependent oxidoreductase	Function Unknown
sps_RS22 710	2.16368413 3	4.30E-09	VOC family protein	Function Unknown
sps_RS23 235	- 2.03042131 8	1.06E-05	DUF3560 domain- containing protein	Function Unknown
sps_RS23 400	- 4.85083901 2	4.43E-16	SRPBCC family protein	Function Unknown
sps_RS23 405	- 3.73716543 5	4.43E-16	hypothetical protein	Function Unknown
sps_RS23 410	- 3.74735610 2	4.92E-25	patatin	Function Unknown
sps_RS24	2.15638404		ABC transporter ATP-	Function
525	7	4.61E-12	binding protein	Unknown

sps_RS25	2.03127525	0.000218419	how other tight watching	Function
345	Z	2448	nypotnetical protein	Unknown
sps_RS25 710	- 2.83457127 2	6.20E-06	hypothetical protein	Function Unknown
sps_RS27 290	2.68565870 5	1.25E-06	hypothetical protein	Function Unknown
sps_RS27 295	2.70222601 5	1.15E-08	hypothetical protein	Function Unknown
sps_RS27 350	3.86686893 7	2.80E-16	hypothetical protein	Function Unknown
sps_RS27 355	3.37408373	9.73E-14	hypothetical protein	Function Unknown
sps_RS27	3.58329184	9 10E 19	CesD/SycD/LcrH family type III secretion system	Function
sps_RS27	2.67931755 2	1.25E-11	hypothetical protein	Function
sps_RS27 395	2.86284689 9	1.35E-07	type III secretion chaperone SycN	Function Unknown
sps_RS27 405	3.28509245 8	2.26E-15	YopN family type III secretion system gatekeeper subunit	Function Unknown
sps_RS06 925	- 2.04669403 9	4.03E-07	MFS transporter	Inorganic ion transport and metabolism
sps_RS07 025	- 3.47268335 2	6.12E-14	cytochrome C biogenesis protein CcsA	Inorganic ion transport and metabolism
sps_RS09 050	2.44518709 2	3.82E-06	biopolymer transporter ExbD	Inorganic ion transport and metabolism
sps_RS09 125	- 2.89335232 7	2.04E-12	Anion transporter	Inorganic ion transport and metabolism
sps_RS13 780	2.13962444 9	4.85E-15	phosphoadenylyl-sulfate reductase	Inorganic ion transport and metabolism
sps_RS14 125	- 2.73847647 5	8.82E-05	hypothetical protein	Inorganic ion transport and metabolism
sps_RS17 560	3.04098523	7.93E-10	TonB-dependent receptor	Inorganic ion transport and metabolism

sps_RS24	- 2.46721855		iron ABC transporter	Inorganic ion transport and
090	2	6.99E-06	permease	metabolism
sps_RS24 125	- 2.10216932 1	3.53E-07	TonB-dependent siderophore receptor	Inorganic ion transport and metabolism
sps_RS24 165	- 2.12855548 3	6.35E-07	potassium transporter Kef	Inorganic ion transport and metabolism
sps_RS09 055	2.13759388	1.50E-06	MotA/TolQ/ExbB proton channel family protein	Intracellular trafficking and secretion
sps_RS14 610	- 2.19764693 6	4.79E-05	type II secretion system F family protein	Intracellular trafficking and secretion
sps_RS14 615	- 2.37625426 9	1.67E-10	type II secretion system protein F	Intracellular trafficking and secretion
sps_RS17 775	2.51470516 4	1.01E-05	protein translocase subunit SecF	Intracellular trafficking and secretion
sps_RS17 780	2.36681931 1	2.53E-07	protein translocase subunit SecD	Intracellular trafficking and secretion
sps_RS17 785	2.46402867 9	2.09E-06	preprotein translocase subunit YajC	Intracellular trafficking and secretion
sps_RS26 490	2.12102174	3.75E-33	prepilin-type N-terminal cleavage/methylation domain-containing protein	Intracellular trafficking and secretion
sps_RS27 675	2.64353463 3	6.38E-05	protein-export chaperone SecB	Intracellular trafficking and secretion
sps_RS01 105	2.23253779 4	7.89E-05	hypothetical protein	Lipid metabolism
sps_RS01 110	2.75892813	1.28E-06	hypothetical protein	Lipid metabolism
sps_RS01 115	3.98161412 8	1.48E-14	hypothetical protein	Lipid metabolism
sps_RS17 815	- 2.49506463 1	0.000915568 9982	acyltransferase	Lipid metabolism
sps_RS25 165	- 2.16992300 8	4.27E-08	enoyl-CoA hydratase	Lipid metabolism

				Nucleotide
sps RS04	2.27377100		adenylosuccinate	metabolism and
270	2	2.08E-07	synthetase	transport
				Post-translational
				modification.
				protein turnover.
sps_RS05	2.25691458	0.000276839	type VI secretion system	chaperone
160	2.220091100	344	ATPase TssH	functions
100	,	511		Post-translational
				modification
	_			protein turnover
sps RS06	2 96102230			chaperone
895_R500	2.90102230	2 71E-05	serine protease	functions
075	· · · · · · · · · · · · · · · · · · ·	2.7112.05	serine proteuse	Post-translational
				nodification
				nrotein turnovor
one DCOA	2 22524170			chaperona
sps_K500	2.22324170	504E11	hypothetical protain	functions
900	3	3.04E-11	nypotnetical protein	Tunctions
				Post-translational
				modification,
DC07	-	0 000110150		protein turnover,
sps_KSU/	2.43//4322	0.000118156	1 41 - 41 1	chaperone
385	2	8298	hypothetical protein	Tunctions
				Post-translational
				modification,
DCOT	0 10105445			protein turnover,
sps_RS07	2.10195445	0.000		chaperone
830	9	9.32E-07	protease HtpX	functions
				Post-translational
				modification,
D G 0.0				protein turnover,
sps_RS08	2.63080938			chaperone
175	5	7.37E-09	co-chaperone YbbN	functions
				Post-translational
				modification,
				protein turnover,
sps_RS08	2.82448454			chaperone
180	6	1.45E-07	molecular chaperone HtpG	functions
				Post-translational
				modification,
				protein turnover,
sps_RS09	2.20007367			chaperone
205	1	1.79E-06	peptidylprolyl isomerase	functions
				Post-translational
sps_RS09	2.36838386			modification,
215	7	8.94E-09	endopeptidase La	protein turnover,

				1
				chaperone
				functions
				Post-translational
				modification,
				protein turnover,
sps_RS11	2.11341406		nucleotide exchange factor	chaperone
045	3	3.39E-08	GrpE	functions
				Post-translational
				modification,
	-			protein turnover,
sps_RS18	2.18603063			chaperone
045	8	3.63E-05	peptidylprolyl isomerase	functions
				Post-translational
				modification,
				protein turnover,
sps_RS20	2.14735896		ATP-dependent zinc	chaperone
985	2	1.70E-07	metalloprotease FtsH	functions
				Post-translational
				modification,
				protein turnover,
sps_RS21	2.24368187			chaperone
055	4	6.80E-07	molecular chaperone DnaJ	functions
				Post-translational
				modification,
				protein turnover,
sps_RS21	2.48059371	0.000173408	molecular chaperone	chaperone
060	6	0891	DnaK	functions
				Post-translational
				modification,
				protein turnover,
sps_RS21	2.29568931		ATP-dependent chaperone	chaperone
670	4	1.87E-06	ClpB	functions
				Post-translational
				modification,
			glutathione-dependent	protein turnover,
sps_RS22			disulfide-bond	chaperone
460	2.96625476	1.49E-15	oxidoreductase	tunctions
				Post-translational
				modification,
				protein turnover,
sps_RS25	2.49919848		DegQ family serine	chaperone
550	2	3.08E-14	endoprotease	tunctions
				Post-translational
sps_RS25	2.19900770	0.000136018		modification,
925	6	5061	chaperonin GroEL	protein turnover,

				chaperone
				functions
				Post-translational
				protein turnover
sns RS25	2 41321638			chaperone
930	2.41521050	1.49E-05	co-chaperone GroES	functions
,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	<u> </u>			Post-translational
				modification,
				protein turnover,
sps_RS26	2.55546487		ATP-dependent protease	chaperone
410	5	2.86E-11	subunit HslV	functions
				Post-translational
				modification,
				protein turnover,
sps_RS26	2.81996626		ATP-dependent protease	chaperone
415	2	2.78E-10	ATPase subunit HsIU	functions
				Post-translational
				modification,
and DS26	2 40505073		Han22 family molecular	protein turnover,
sps_K320 850	2.40393973	1 28F-06	chaperone HslO	functions
0.50	0	1.201 00		Post-translational
				modification.
				protein turnover,
sps RS27	4.10955785			chaperone
340	3	4.76E-21	hypothetical protein	functions
	-			
sps_RS04	2.21263489			Replication and
595	9	9.56E-11	replication endonuclease	repair
	-			
sps_RS06	2.52831285			Replication and
160	3	1.11E-05	integrase	repair
DC12	-			
sps_KS13	5.911961//	1 115 07	IS256 formily them an a second	Replication and
310	8	1.11E-07	18256 family transposase	repair
and DS22	2 56502058			Poplication and
sps_K322 930	2.30392938	8 22F-17	hypothetical protein	repair
250	2	0.22L-1/	nypometical protein	repuir
sps RS22	2,11758149			Replication and
990	2	7.41E-07	IS30 family transposase	repair
	-		FF>•	4
sps RS23	2.24745991			Replication and
700	9	3.46E-08	IS21 family transposase	repair

sps RS15				Secondary
280	2.22318351	1.24E-07	tandem-95 repeat protein	Structure
	-		sigma-54-dependent Fis	
sps RS00	2.33719045		family transcriptional	Signal
605	9	6.51E-13	regulator	Transduction
sns RS11	2 09714429		PAS domain-containing	Signal
3p3_K511 800	2.07714427	2 25E 05	nrotoin	Transduction
800	1	5.2512-05	protein	Transduction
DCOO	-			C:1
sps_K522	2.93090313	4.005 11	1,	
/45	9	4.02E-11	response regulator	Iransduction
sps_RS00	2.75894184		RNA polymerase sigma	
465	7	2.36E-09	factor FliA	Transcription
sps_RS09	2.53551543		YafY family	
570	5	3.66E-30	transcriptional regulator	Transcription
sps_RS09	3.32013114		AraC family	
575	8	4.94E-10	transcriptional regulator	Transcription
	-		- <u> </u>	
sps RS09	3.19003774		GntR family	
965	3	2.36E-16	transcriptional regulator	Transcription
sns RS13	3 01456071			
205	0.01450071	1 13E-05	cold-shock protein	Transcription
275)	т. т . <u>т</u>	cold-shock protein	Transcription
and DS14	-		LycD family	
sps_K514	2.00022072	1.570.00	Lysk failing	Turneralistica
033 DC17	Z	1.3/E-09		Transcription
sps_RS1/	0.00000177	4.005 13	transcriptional regulator	
430	-2.36366177	4.00E-12	Betl	Transcription
	-			
sps_RS23	2.45019509			
225	4	4.28E-09	hypothetical protein	Transcription
sps_RS27	3.31410323			
370	8	4.02E-07	hypothetical protein	Transcription
	-			
sps_RS00	2.41396132		ribonuclease P protein	
180	2	7.27E-06	component	Translation
sps RS01	2.01076051			
780	8	9.40E-06	30S ribosomal protein S12	Translation
sps_RS01	2,42743155			
785	1	1.05E-05	30S ribosomal protein S7	Translation
sps RS01	2 46168614	1.051 05		I I MII DI MII OII
3ps_1301 700	2.40108014	2 10E 07	alongation factor G	Translation
/90	2 24611202	2.10E-U/		
sps_KS11	2.24611393	0.00012/326	ribosome-associated	T 1.4
822	6	6449	translation inhibitor KaiA	I ranslation

sps_RS11				
900	2.88007929	2.98E-06	50S ribosomal protein L19	Translation
sps_RS11	2.76213947		tRNA (guanosine(37)-N1)-	
905	7	9.14E-09	methyltransferase TrmD	Translation
sps_RS11	2.47503214		ribosome maturation factor	
910	6	2.75E-05	RimM	Translation
sps_RS11	2.21875695			
915	9	2.21E-05	30S ribosomal protein S16	Translation
sps_RS14	2.11229414		30S ribosomal protein S6	
235	5	1.29E-07	L-glutamate ligase	Translation
sps_RS17	2.22316729		tRNA guanosine(34)	
790	5	2.31E-05	transglycosylase Tgt	Translation
sps_RS19	2.30486709		ribosome-associated	
945	6	2.68E-05	translation inhibitor RaiA	Translation
			23S rRNA (uridine(2552)-	
sps_RS20	2.48793462		2'-O)-methyltransferase	
990	2	1.33E-08	RlmE	Translation

Data S3 Tab	le B: Comparison be	tween late log phas	se samples from 1	5°C and 4°C
cultures.	-		-	

	log2FoldChang e (<0 higher in			
gene	4, >0 higher in 15)	nadi	name	cats
800		PJ		Amino Acid
			serine	metabolism and
sps_RS05410	-2.251297573	1.17E-07	dehydratase	transport
			DSD1 family	Amino Acid
			PLP-dependent	metabolism and
sps_RS05415	-2.188101251	6.08E-10	enzyme	transport
			1-	
			aminocycloprop	A · A · 1
		0 00002222022	ane-1-	Amino Acid
sps PS07005	2 204573376	0.00085552955	deaminase	transport
sps_K307003	-2.20+373370	19	low-specificity	Amino Acid
			L-threonine	metabolism and
sps RS11430	-2.295816048	6.81E-08	aldolase	transport
- <u>r</u>			3-deoxy-7-	Amino Acid
			phosphoheptulo	metabolism and
sps_RS11890	-2.799793394	8.19E-07	nate synthase	transport
			methylenetetrah	Amino Acid
			ydrofolate	metabolism and
sps_RS14555	-2.78520259	3.89E-06	reductase	transport
			dihydrodipicoli	Amino Acid
DC1(775	2 (51(0)747	1 425 21	nate synthase	metabolism and
sps_RS16//5	-2.651691/4/	1.42E-21	family protein	transport
			nhaanhaltatalaa	Carbonydrate
sps RS11765	2 474339026	1 44F-13	e family protein	transport
505_10511705	2.171339020	1.112 13	e fulling protein	Carbohydrate
			allantoinase	metabolism and
sps RS19520	-2.450764521	2.89E-06	PuuE	transport
			sugar ABC	•
			transporter	Carbohydrate
			substrate-	metabolism and
sps_RS20810	2.227328424	5.89E-07	binding protein	transport
			hypothetical	~ 11
sps_RS17255	-3.349087296	3.79E-06	protein	Cell motility
			HrpE/YscL	
			lamily type III	
			annaratus	
sps RS27270	2.006547001	4.59E-05	protein	Cell motility
SPS_102/2/0	2.000347001	-r.57L-05	Protoni	

			EscN/YscN/Hrc	
			N family type	
			III secretion	
sps RS27410	4 017940358	1 62F-15	system ATPase	Cell motility
<u>sps_R527410</u>	4.017740330	1.02L-13	VscO/HrcO	
			family type III	
			socration	
			opporatus	
ong RS27425	2 063367258	183E 11	apparatus	Cell motility
sps_K327423	2.905507258	1.05E-11	protein	Coll
				Util wall/mombrana/
			hypothetical	wall/inclinoralic/
ang DS00225	2 020707642	4 44E 00	nypothetical	biogenesis
sps_K309333	2.929797042	4.44E-09	protein	Call
			4 1	wall/memorane/
DC10100	2 751020040	0.015 14	outer membrane	envelope
sps_RS10100	2./51039948	9.01E-14	protein Ompw	biogenesis
				wall/membrane/
DG10055	2 7 ((1 7 1 2 0 4	4 105 11	LrgB family	envelope
sps_RS12855	3.766171284	4.18E-11	protein	biogenesis
			oxygen-	
			independent	~
Danacco	2 1 2 2 4 5 5 0 0 0		coproporphyrin	Coenzyme
sps_RS00660	2.123457099	8.79E-06	ogen III oxidase	metabolism
				Energy
			hypothetical	production and
sps_RS01075	2.57099078	4.36E-06	protein	conversion
				Energy
				production and
sps_RS03745	-4.054348131	3.46E-26	isocitrate lyase	conversion
			bifunctional	
			acetaldehyde-	Energy
			CoA/alcohol	production and
sps_RS03765	2.118466909	3.11E-09	dehydrogenase	conversion
			cytochrome-c	Energy
			oxidase, cbb3-	production and
sps_RS04555	2.232442027	7.83E-07	type subunit II	conversion
			cytochrome-c	Energy
			oxidase, cbb3-	production and
sps_RS04560	2.069631451	5.32E-08	type subunit I	conversion
				Energy
				production and
sps RS08005	-2.306217513	9.53E-09	citrate synthase	conversion

				Energy
sps R S 08860	-3.028955554	1 09F-06	malate synthase	production and
sps_K508800	-3.020733334	1.072-00	malate synthase	Energy
				production and
sps_RS09325	3.726408731	2.44E-08	cytochrome C	conversion
				Energy
D C00220	2 ((0002020	2 01E 07	cystathionine	production and
sps_RS09330	3.660893039	2.91E-06	beta-synthase	conversion
			NADH:ubiquin	
			(Na(+)-	Energy
		0.00033190233	transporting)	production and
sps_RS11115	2.058018349	47	subunit D	conversion
			Na(+)-	
			translocating	
			NADH-quinone	Energy
ang PS11120	2 22/82602	4 05E 06	reductase	production and
sps_K311120	2.33462092	4.9512-00	NADH ubiquin	conversion
			one reductase	
			(Na(+)-	Energy
			transporting)	production and
sps_RS11125	3.096698864	2.49E-05	subunit B	conversion
			Na(+)-	
			translocating	Enorgy
			reductase	production and
sps RS11130	3.126630001	7.93E-12	subunit A	conversion
				Energy
			L-threonine	production and
sps_RS11370	2.156652566	3.22E-05	dehydrogenase	conversion
			SDR family	.
			NAD(P)-	Energy
sps_R\$15005	-3.030073652	1 47E-07	oxidoreductase	conversion
3p3_R015005	5.050075052	1.472.07	fumarate	conversion
			reductase	Energy
		0.00031700117	flavoprotein	production and
sps_RS15135	2.412280418	45	subunit	conversion
			formate C-	Energy
ana DO17575	2 45114(051	1 055 07	acetyltransferas	production and
sps_K51/3/3	2.451146051	1.85E-07	e	Energy
			malate synthase	production and
sps RS18985	-3.955351693	1.89E-19	A	conversion

			dicarboxylate/a	
			mino	Energy
			acid:cation	production and
sps_RS19370	-2.479899085	4.41E-08	symporter	conversion
			coproporphyrin	Energy
			ogen III oxidase	production and
sps RS27115	2.92511801	2.58E-08	family protein	conversion
			4Fe-4S dicluster	
			domain-	Energy
		0.00024651865	containing	production and
sps RS27125	2.030416571	74	protein	conversion
<u> </u>			1	Energy
			formate	production and
sps RS27130	3.058889745	1.63E-09	dehvdrogenase	conversion
1			NAD(P)H-	
			dependent	
			glycerol-3-	Energy
			phosphate	production and
sps RS27670	2.260576312	2.16E-05	dehvdrogenase	conversion
	2.2000 / 0012	2.102.00	cytochrome o	
			ubiquinol	Energy
			oxidase subunit	production and
sps_RS27795	2 467801715	6 70E-06	III	conversion
505_1027795	2.107001713	0.701 00	cytochrome o	
			ubiquinol	Energy
			oxidase subunit	production and
sps RS27800	2 68423386	3 20E-11	I	conversion
5p5_10527000	2.00123300	5.201 11	ubiquinol	Energy
			oxidase subunit	production and
sps_RS27805	2 088397482	1 09E-05	II	conversion
<u></u>	2.000377102	1.072 05	nutative sulfate	
			exporter family	Function
sps_RS00895	2 133987127	2 41E-19	transporter	Unknown
5P5_1000075	2.133907127	2.711.17	hypothetical	Function
sps_RS01100	5 2081 572 53	1 64F-14	nrotein	Unknown
<u>sps_Roo1100</u>	5.200157255	1.042 14	protein	Function
sps RS01375	3 719617102	6 03F-30	ATPase P	Unknown
sps_K501575	5./1901/102	0.951-50	DUE2057	UIIKIIUWII
			domain-	
			containing	Function
sps RS01285	3 281145605	3 20F 07	protein	Unknown
sps_1201202	5.201145095	3.20E-07	hypothetical	Function
ene RS02265	2 52552004	071000	nypoinctical	Linknown
sps_11302203	2.32332984	9./1E-08	protein phytophalatin	Eurotion
DC02275	2.000000000		pnytocnelatin	r unction
sps_KS02275	2.006963933	6.56E-07	synthase	Unknown

			hypothetical	Function
sps_RS04385	-2.500539512	3.88E-06	protein	Unknown
			N-	
			acetyltransferas	Function
sps_RS04390	-2.808524718	7.53E-12	e	Unknown
			type III	
			secretion	Function
sps_RS04880	-2.000214882	5.14E-05	apparatus	Unknown
			META domain-	
			containing	Function
sps_RS05225	-3.210814348	4.16E-09	protein	Unknown
			YtoQ family	Function
sps_RS05430	-2.041015208	4.77E-07	protein	Unknown
			hypothetical	Function
sps_RS06230	2.985365231	3.41E-05	protein	Unknown
			hypothetical	Function
sps_RS06235	3.54904298	4.98E-19	protein	Unknown
			anaerobic C4-	
		0.00058325153	dicarboxylate	Function
sps_RS07520	2.515603667	31	transporter	Unknown
				Function
sps_RS09320	4.116488482	3.07E-11	cytochrome C	Unknown
			AzlD domain-	
			containing	Function
sps_RS09560	2.184493683	1.23E-09	protein	Unknown
			GNAT family	
			N-	
			acetyltransferas	Function
sps_RS09825	-2.125806196	1.32E-09	e	Unknown
			hypothetical	Function
sps_RS10625	2.748262219	5.02E-11	protein	Unknown
			hypothetical	Function
sps_RS12860	4.768188285	8.68E-09	protein	Unknown
		0.00015614330	oxidative stress	Function
sps_RS13860	2.450838133	71	defense protein	Unknown
			hypothetical	Function
sps_RS14205	-2.34496438	4.95E-06	protein	Unknown
		0.00012696222		Function
sps_RS14420	2.472539876	73	collagenase	Unknown
				Function
sps_RS15065	2.172604671	1.24E-07	adhesin	Unknown
			type I secretion	
			system	
			permease/ATPa	Function
sps_RS15070	2.553243551	1.28E-08	se	Unknown

			type I secretion	
			system (A TD	
DC15205	0.114710550	0.715 10	permease/ATPa	Function
sps_RS15285	2.114/13559	2./IE-I2	se	Unknown
	2 25010/5		hypothetical	Function
sps_RS15570	3.3791067	5.09E-07	protein	Unknown
			hypothetical	Function
sps_RS17000	-2.598562794	5.12E-05	protein	Unknown
		0.00048904629	hypothetical	Function
sps_RS17005	-3.377431967	35	protein	Unknown
			methyl-	
			accepting	
			chemotaxis	Function
sps_RS18820	3.100621417	1.99E-22	protein	Unknown
			OHCU	Function
sps_RS19515	-2.752274116	1.98E-07	decarboxylase	Unknown
			MipA/OmpV	Function
sps_RS20500	2.23184764	2.38E-05	family protein	Unknown
			DUF3019	
			domain-	
			containing	Function
sps_RS20505	2.327663668	3.41E-05	protein	Unknown
			hypothetical	Function
sps_RS21080	3.03966257	1.68E-13	protein	Unknown
			SRPBCC	Function
sps_RS23400	-3.116756196	1.77E-07	family protein	Unknown
			hypothetical	Function
sps_RS27275	2.686319692	5.37E-10	protein	Unknown
			EscI/YscI/HrpB	
			family type III	
			secretion	
			system inner	Function
sps_RS27285	3.005269776	7.44E-10	rod protein	Unknown
			hypothetical	Function
sps_RS27290	3.556104216	4.78E-11	protein	Unknown
			hypothetical	Function
sps_RS27295	4.25002937	8.77E-22	protein	Unknown
			EscD/YscD/Hrp	
			Q family type	
			III secretion	
			system inner	
			membrane ring	Function
sps_RS27310	3.392255294	1.83E-21	protein	Unknown
			hypothetical	Function
sps RS27350	3.866446239	6.10E-17	protein	Unknown

			hypothetical	Function
sps_RS27355	4.058696582	2.02E-20	protein	Unknown
			CesD/SycD/Lcr	
			H family type	
			III secretion	
			system	Function
sps_RS27360	4.504790823	1.63E-31	chaperone	Unknown
			hypothetical	Function
sps_RS27365	3.760290094	1.33E-23	protein	Unknown
			hypothetical	Function
sps_RS27385	3.670547054	1.38E-11	protein	Unknown
			type III	
			secretion	Function
sps_RS27395	4.850126293	8.77E-22	chaperone SycN	Unknown
			TyeA family	
			type III	
			secretion	
			system	- ·
	4 50 50000 5 6		gatekeeper	Function
sps_RS27400	4.705800356	8.37E-07	subunit	Unknown
			YopN family	
			type III	
			secretion	
			system	
DC27405	2.04(57010(0.005.04	gatekeeper	Function
sps_R527405	3.9403/8180	9.28E-24		Unknown
ana DC27455	2 152070740	7 91E 20	hypothetical	Function
sps_K52/455	3.1530/0/49	7.81E-30	protein	Unknown
			DUF2061	
		0.00051294072	domain-	Encention
ang DS27760	2 026740921	0.00031284973	containing	Function
sps_152/100	5.950749821	08	protein	Inorgania ion
			$\Lambda \circ n \mathbf{D} / \Lambda \circ n \mathbf{D} / \Lambda \circ n$	transport and
ong DS01265	2 020740504	1 42E 05	ACTD/ACTD/ACT	matabalism
sps_K501505	2.029749304	4.4312-03	offlux PND	Inclabolisii
			transporter	Inorganic ion
			nerinlasmic	transport and
sps_RS01370	2 950226404	5 10F-19	adaptor subunit	metabolism
525_1001570	2.750220404	5.101-17	adaptor Suburit	Inorganic ion
				transport and
sps_RS01620	2 180320034	2 66F-08	catalase	metabolism
<u>5p5_1001020</u>	2.100520054	2.001-00	ARC	Inorganic ion
			transporter	transport and
sps_RS02090	2,411588947	1 01E-07	nermease	metabolism
sps_RS02090	2.411588947	1.01E-07	transporter permease	transport and metabolism
				Inorganic ion
---------------------	--------------	---------------	-------------------	-----------------
			sodium/proton	transport and
sps_RS06305	2.098316747	5.90E-07	antiporter NhaB	metabolism
	21070210711	0.002.07	rhodanese-like	
			domain-	Inorganic ion
			containing	transport and
sps RS08845	-2 269209062	1.03E_06	protein	metabolism
<u>sps_1000045</u>	-2.207207002	1.05L-00	protein	Incraonia ion
				transport and
enc PS1 /015	2 551774014	0 18F 07	catalaca	metabolism
sps_K314015	2.331774014	9.101-07	Catalase	metabolism
			C4-	
			dicarboxylate	
			ABC	т
		0.00010152514	transporter	Inorganic ion
DC15(40	0 411000 447	0.00010152514	substrate-	transport and
sps_RS15640	-2.411088447	18	binding protein	metabolism
			formate	Inorganic ion
			transporter	transport and
sps_RS17570	2.91015431	2.02E-09	FocA	metabolism
			DNA	
			starvation/statio	
			nary phase	Inorganic ion
			protection	transport and
sps_RS21625	2.564272938	2.98E-06	protein	metabolism
			EscJ/YscJ/HrcJ	
			family type III	
			secretion inner	Intracellular
			membrane ring	trafficking and
sps_RS27280	3.314108907	8.77E-22	protein	secretion
			EscF/YscF/Hrp	
			A family type	
			III secretion	Intracellular
			system needle	trafficking and
sps_RS27300	3.272136692	2.47E-07	major subunit	secretion
			EscC/YscC/Hrc	
			C family type	
			III secretion	
			system outer	Intracellular
			membrane ring	trafficking and
sps_RS27315	3.70202654	1.33E-43	protein	secretion
			EscV/YscV/Hrc	
			V family type	
			III secretion	
			system export	Intracellular
			apparatus	trafficking and
sps_RS27380	3.905493093	5.12E-37	protein	secretion

			YscX family	
			type III	Intracellular
			secretion	trafficking and
sps RS27390	3.878461197	1.95E-19	protein	secretion
			1	Intracellular
			hypothetical	trafficking and
sps_RS27415	3 575094311	4 46E-06	protein	secretion
	0.070071011		type III	
			secretion	
			system needle	Intracellular
			length	trafficking and
sps_RS27420	3 1 5 2 4 1 3 2 5 8	5 40E-15	determinant	secretion
<u>bps_1027120</u>	5.152 115250	2.102.12	EscR/YscR/Hrc	
			R family type	
			III secretion	
			system export	Intracellular
			apparatus	trafficking and
sps_RS27430	3 105151559	4 23E-07	protein	secretion
			EscS/YscS/Hrc	
			S family type	
			III secretion	
			system export	Intracellular
			apparatus	trafficking and
sps RS27435	3.464001301	1.18E-05	protein	secretion
			hypothetical	Lipid
sps RS01090	2.575788805	4.13E-06	protein	metabolism
<u> </u>			hypothetical	Lipid
sps RS01105	3.240604938	4.65E-09	protein	metabolism
			hypothetical	Lipid
sps RS01110	3.476868577	9.24E-10	protein	metabolism
			hypothetical	Lipid
sps RS01115	3.961007549	4.11E-14	protein	metabolism
			-	Lipid
sps RS08835	-2.387161901	1.62E-09	transporter	metabolism
		0.00055528298	hypothetical	Lipid
sps_RS20665	2.146523738	19	protein	metabolism
			alpha/beta	Lipid
sps_RS21950	-2.570844826	3.97E-08	hydrolase	metabolism
				Nucleotide
			adenylosuccinat	metabolism and
sps_RS04270	2.365655531	6.08E-08	e synthetase	transport
				Post-
				translational
			heme ABC	modification,
			transporter	protein
sps_RS01955	2.137531674	3.06E-05	permease	turnover,

				chaperone
				functions
				Post-
				translational
				modification,
			peptide-	protein
			methionine (S)-	turnover,
D.G.02050	0 0 1 0 0 1 1 0 7 0		S-oxide	chaperone
sps_RS03850	-2.3108119/3	6.44E-05	reductase	functions
				Post-
				translational
				modification,
				protein
			1122 family	urnover,
ang DS20670	2 655295552	1.05E.05	U32 family	functions
sps_K520070	2.033383333	1.03E-05	pepudase	Dest
				rusi-
				modification
				niounication,
				turnover
		0.0001/303501	1132 family	chaperone
sps RS20675	2 114799468	0.00014303351	nentidase	functions
5p5_10520075	2.111777100		peptiduse	Post-
				translational
				modification
			ATP-dependent	protein
			zinc	furnover.
			metalloprotease	chaperone
sps RS20985	2.062360328	7.47E-07	FtsH	functions
1		, 2 37		Post-
				translational
				modification.
			glutathione-	protein
			dependent	turnover,
			disulfide-bond	chaperone
sps_RS22460	2.155503673	2.33E-08	oxidoreductase	functions
				Post-
				translational
				modification,
			alkyl	protein
			hydroperoxide	turnover,
		0.00010867295	reductase	chaperone
sps_RS24220	2.111736663	67	subunit F	functions
				Post-
sps_RS24225	3.250360652	5.00E-05	peroxiredoxin	translational

				modification,
				protein
				turnover,
				chaperone
				functions
				Post-
				translational
				modification,
				protein
			Hsp33 family	turnover,
			molecular	chaperone
sps RS26850	2.055703911	6.91E-05	chaperone HslO	functions
				Post-
				translational
				modification,
				protein
				turnover,
			hypothetical	chaperone
sps RS27340	3.604478108	3.14E-17	protein	functions
			hypothetical	Secondary
sps RS01085	2.603124452	2.74E-06	protein	Structure
			hypothetical	Secondary
sps RS01095	3.301386047	8.68E-09	protein	Structure
			copper	
			resistance	
			system	
			multicopper	Secondary
sps RS06040	2.359080321	1.30E-10	oxidase	Structure
			tandem-95	Secondary
sps_RS15280	2.448583378	4.99E-09	repeat protein	Structure
			PrkA family	
		0.00031589519	serine protein	Signal
sps_RS03040	-2.292840491	79	kinase	Transduction
			methyl-	
			accepting	
			chemotaxis	Signal
sps_RS11275	2.221007313	9.67E-15	protein	Transduction
			DNA-binding	
			response	Signal
sps_RS20510	2.696642555	1.45E-05	regulator	Transduction
		0.00094929356	hypothetical	Signal
sps_RS27835	2.005497069	37	protein	Transduction
			YafY family	
			transcriptional	
sps_RS09570	2.258567275	1.33E-23	regulator	Transcription

			LysR family	
			transcriptional	
sps_RS22055	-2.413152654	2.11E-08	regulator	Transcription
			hypothetical	
sps_RS27370	3.423565507	1.22E-07	protein	Transcription
		0.00087719368	hypothetical	
sps_RS27375	2.55325427	5	protein	Transcription
			threonine	
sps_RS20540	3.127015948	4.56E-48	tRNA ligase	Translation

Data S3 Tab	le C: Comparison	between stati	ionary phase	samples from	15°C and 4	°C
cultures.						

	log2FoldChang e (<0 higher in			
gene	4, >0 higher in 15)	nadi	name	cats
8)	<u>l</u>		Amino Acid
			amino acid	metabolism and
sps RS03105	4.37910112	6.38E-15	transporter	transport
			anthranilate	Amino Acid
			synthase	metabolism and
sps_RS08280	2.087042264	2.98E-06	component 1	transport
			bifunctional	
			indole-3-	
			glycerol-	
			phosphate	
			synthase	
			TrpC/phosphori	
			bosylanthranilat	Amino Acid
			e isomerase	metabolism and
sps_RS08295	2.031765077	2.61E-05	TrpF	transport
			branched-chain	
			amino acid	
			ABC	Amino Acid
DC00555	2.2502(1((2	5 91E 00	transporter	metabolism and
sps_R809555	2.259261662	5.81E-09	permease	transport
			1 / . 1	Amino Acid
ang DC10240	2 067555755	2 70E 12	sodium/giulama	metabolism and
sps_K519540	2.00/333/33	2./0E-12	armithing	Amino Agid
		0.00021085554	ormunite	motobolism and
ene R\$26675	_2 288105052	0.00021085554	erase	transport
sps_R520075	-2.200175752	<u>∠</u>	clase	Amino Acid
			acetylolutamate	metabolism and
sps_RS26680	-3 111911488	1 79E-06	kinase	transport
<u>-p5_1020000</u>		1.772.00	N-acetyl-	
			gamma-	
			glutamyl-	Amino Acid
			phosphate	metabolism and
sps RS26685	-2.85621217	1.95E-10	reductase	transport
				Carbohydrate
		0.00069273190		metabolism and
sps_RS02380	2.257975208	27	gluconokinase	transport
			carbohydrate	Carbohydrate
			ABC	metabolism and
sps_RS06180	2.829391151	5.15E-05	transporter	transport

			substrate-	
			binding protein	
			glycogen/starch	Carbohydrate
			/alpha-glucan	metabolism and
sps_RS11340	2.004652578	7.34E-06	phosphorylase	transport
			rRNA (guanine-	
			N1)-	
			methyltransfera	
sps_RS11685	2.588920966	5.41E-22	se	Cell motility
			flagellar	
			biosynthesis	
sps_RS18555	2.17870521	1.24E-15	protein FlhA	Cell motility
			flagellar basal	
			body M-ring	
sps RS18630	2.232872733	1.11E-05	protein FliF	Cell motility
		0.00025822926		-
sps RS18675	2.088934191	25	flagellin	Cell motility
<u> </u>			flagellar hook-	-
			associated	
sps RS18690	2.054108501	4.02E-05	protein FlgK	Cell motility
			flagellar	
			biosynthesis	
sps RS18705	2.184230157	2.64E-07	protein FlgH	Cell motility
<u> </u>			chemotaxis	
sps RS26085	2.027632119	5.75E-07	protein CheD	Cell motility
<u> </u>			EscN/YscN/Hrc	
			N family type	
		0.00018314141	III secretion	
sps RS27410	2.092808444	08	system ATPase	Cell motility
<u> </u>			efflux RND	Cell
			transporter	wall/membrane/
			periplasmic	envelope
sps RS08020	2.319638101	4.34E-06	adaptor subunit	biogenesis
· -			•	Cell
				wall/membrane/
			hypothetical	envelope
sps RS09305	2.885430188	1.93E-05	protein	biogenesis
			· ±	Cell
				wall/membrane/
				envelope
sps RS11360	2.000094358	7.45E-05	porin	biogenesis
· -			-	Cell
				wall/membrane/
			porin family	envelope
sps_RS15945	4.099235757	1.72E-06	protein	biogenesis

			thiamine	
			biosynthesis	Coenzyme
sps_RS05830	-2.409758079	8.03E-06	protein ThiS	metabolism
				Energy
		0.00083422750	cytochrome-c	production and
sps_RS00020	2.019700949	41	oxidase	conversion
				Energy
			cystathionine	production and
sps_RS09300	3.083648602	6.06E-07	beta-synthase	conversion
				Energy
				production and
sps_RS09310	2.966842289	1.35E-07	cytochrome C	conversion
			cytochrome d	
			terminal	Energy
			oxidase subunit	production and
sps_RS13470	2.276821633	7.68E-13	1	conversion
			NADH-quinone	Energy
			oxidoreductase	production and
sps_RS17485	2.273372901	5.85E-10	subunit A	conversion
			NADH-quinone	Energy
		0.00029492465	oxidoreductase	production and
sps_RS17495	2.884528314	13	subunit NuoC/D	conversion
			NADH	_
			dehydrogenase	Energy
		0.00021227838	(quinone)	production and
sps_RS17510	2.39658358	29	subunit G	conversion
			NADH-quinone	Energy
D.G.1.5500	0.1.00.1100000	0.0008/1664/8	oxidoreductase	production and
sps_RS17520	3.168413939	41	subunit Nuol	conversion
			NADH:ub1qu1n	-
		0.0001 (10.1000	one	Energy
DG17505	2 25 ((0 (0 2 0	0.00016424008	oxidoreductase	production and
sps_K51/525	2.356696929	04	subunit J	conversion
				Energy
ang DC10005	2 254095242	1.500.00	marate synthase	production and
sps_R518985	-2.234085342	1.50E-06	A	conversion
DC00000	2 07000000	1.04E.05	1	Function
sps_K500990	2.078960086	1.04E-05	acylase	Unknown
ang DS01425	2 211060520	2 04E 07	nhaanhalinaaa	runction
sps_K501023	2.211909329	2.04E-07	hymothetics1	Ulikilown
ana DC01620	2 466512606	0.00027072052	nypoinetical	r unction
sps_K501630	2.400313096	35	protein	Unknown
	2.925((404	2 AOF 1 -	pilus assembly	runction
sps_KS03620	2.82566494	3.49E-15	protein	Unknown

			N-	
			acetyltransferas	Function
sps RS04390	-2.364565947	3.18E-08	e	Unknown
			hypothetical	Function
sps_RS04940	2.802345908	6.70E-05	protein	Unknown
			hypothetical	Function
sps_RS04950	2.125889945	6.04E-05	protein	Unknown
			secretion	Function
sps_RS04955	2.223263065	9.76E-05	protein	Unknown
			pathogenicity	
			island effector	Function
sps_RS04960	3.237935951	1.57E-09	protein	Unknown
			type III	
			secretion	
			system	
			translocon	Function
sps_RS04965	2.924395747	2.47E-06	protein	Unknown
			CesD/SycD/Lcr	
			H family type	
			III secretion	D
D G 6 40 50	0 515 (100 0 5		system	Function
sps_RS04970	2.717640935	6.23E-05	chaperone	Unknown
D.G.0.4075	0.000450005	0.000119/6910	secretion	Function
sps_RS049/5	2.329453385	4/	protein EspA	Unknown
DCOCOOO	2 210(02(01	2.055.07	hypothetical	Function
sps_RS06080	2.310693691	2.05E-07	protein	Unknown
			cytotoxic	т. (¹
ana DC00425	2.040642227	0 55 E 10	necrotizing	Function
sps_K508433	2.049043337	9.33E-18		Unknown
			AZID domain-	Exaction
ang DS00560	2 887520060	1 24E 15	rotain	Function
sps_K309300	2.887329009	1.24E-13	DUE/126	UIIKIIOWII
			domain	
		0 00015667094	containing	Function
sps R \$09805	2 048842281	39	protein	Unknown
sps_R507005	2.040042201	57	protein	Function
sps_RS10070	2 522915853	2 48E-18	protease	Unknown
5p5_10510070	2.322713033	2.101 10	penicillin	
			acylase family	Function
sps RS10785	2.786006729	1.92E-09	protein	Unknown
1			hypothetical	Function
sps RS10795	2.894915251	2.75E-16	protein	Unknown
1			cupin domain-	
		0.00062271205	containing	Function
sps_RS12620	-2.282292448	77	protein	Unknown

		0.00023644941	hypothetical	Function
sps_RS12860	3.381831849	3	protein	Unknown
			hypothetical	Function
sps_RS13850	2.0480048	4.44E-05	protein	Unknown
			UPF0016	
			domain-	
			containing	Function
sps_RS14010	2.211041965	5.53E-06	protein	Unknown
			type I secretion	
			system	
			permease/ATPa	Function
sps_RS15070	2.293237294	4.67E-07	se	Unknown
		1 505 10	1 1 1	Function
sps_RS15400	3.269553257	1.52E-10	hydrolase	Unknown
D.G.1.5570	0.500010000	0.00027453024	hypothetical	Function
sps_RS15570	2.582318308	57	protein	Unknown
			HlyD family	D (*
DG15(25	4.0.42070.002	1.5(1) 12	secretion	Function
sps_RS15625	4.9438/0692	1.56E-13	protein	Unknown
ana DC15905	2 2220 421 52	5 01E 00	phasin family	Function
sps_R515895	-2.332942153	5.21E-09	protein	Unknown
			DUF2219	
			domain-	Function
sps RS10160	2 208046055	1 91F-05	protein	Linknown
sps_K517100	2.270040733	0.00020761398	Min A/OmnV	Function
sps RS20500	2 013106444	0.00020701378	family protein	Unknown
3p3_R520500	2.013100444	0	DUF3019	
			domain-	
			containing	Function
sps RS20505	2.517833068	1.19E-05	protein	Unknown
		0.00040354931	hypothetical	Function
sps RS21020	2.413610054	81	protein	Unknown
1_			hypothetical	Function
sps RS21315	3.390832229	6.25E-15	protein	Unknown
			GTP	
			pyrophosphokin	Function
sps_RS21730	2.677035022	1.87E-05	ase	Unknown
			SRPBCC	Function
sps_RS23400	-2.455679562	6.40E-05	family protein	Unknown
			multidrug	Function
sps_RS24450	3.052074741	5.08E-08	transporter	Unknown
			ABC	
			transporter	Function
sps_RS24545	2.354940588	2.10E-09	permease	Unknown

			hypothetical	Function
sps_RS27295	2.397746348	9.01E-07	protein	Unknown
			hypothetical	Function
sps_RS27350	2.384724326	1.79E-06	protein	Unknown
D.C.27255	0 701000446		hypothetical	Function
sps_RS27355	2.701208446	6.84E-09	protein	Unknown
			type III	
DG27205	2 501579215	1.005.05	secretion	Function
sps_K52/393	2.301378213	1.09E-03	DUE2061	Unknown
			DUF2001	
			domain-	Function
sps BS27760	1 71684520	2 22E 05	protein	Unknown
sps_K327700	4./1004323	2.22E-03	protein	Inorganic ion
				transport and
sps_RS01620	3 550908801	4 10F-21	catalase	metabolism
5p5_10501020	5.550700001	1.102 21	TonB-	Inorganic ion
			dependent	transport and
sps RS09075	2.817201186	9.47E-13	receptor	metabolism
<u></u>				Inorganic ion
				transport and
sps RS14015	3.775448563	4.17E-14	catalase	metabolism
				Inorganic ion
		0.00079356671	sorbose	transport and
sps_RS14130	-2.07521329	22	reductase	metabolism
				Inorganic ion
				transport and
		2 27E 00	MFS transporter	metabolism
sps_RS15620	3.96478885	2.3/E-08		
sps_RS15620	3.96478885	2.3/E-08	TonB-	Inorganic ion
sps_RS15620	3.96478885	2.57E-08	TonB- dependent	Inorganic ion transport and
sps_RS15620 sps_RS17675	3.96478885 -2.332152706	1.25E-10	TonB- dependent receptor	Inorganic ion transport and metabolism
sps_RS15620 sps_RS17675	3.96478885 -2.332152706	1.25E-10	TonB- dependent receptor DNA	Inorganic ion transport and metabolism
sps_RS15620 sps_RS17675	3.96478885 -2.332152706	1.25E-10	TonB- dependent receptor DNA starvation/statio	Inorganic ion transport and metabolism
sps_RS15620 sps_RS17675	3.96478885	1.25E-10	TonB- dependent receptor DNA starvation/statio nary phase	Inorganic ion transport and metabolism
sps_RS15620 sps_RS17675	3.96478885 -2.332152706	1.25E-10	TonB- dependent receptor DNA starvation/statio nary phase protection	Inorganic ion transport and metabolism Inorganic ion transport and
sps_RS15620 sps_RS17675 sps_RS21625	3.96478885 -2.332152706 3.709462096	1.25E-10 1.87E-12	TonB- dependent receptor DNA starvation/statio nary phase protection protein	Inorganic ion transport and metabolism Inorganic ion transport and metabolism
sps_RS15620 sps_RS17675 sps_RS21625	3.96478885 -2.332152706 3.709462096	1.25E-10 1.87E-12	TonB- dependent receptor DNA starvation/statio nary phase protection protein	Inorganic ion transport and metabolism Inorganic ion transport and metabolism Inorganic ion transport and
sps_RS15620 sps_RS17675 sps_RS21625	3.96478885 -2.332152706 3.709462096 2.378253811	1.25E-10 1.87E-12 2.47E-07	TonB- dependent receptor DNA starvation/statio nary phase protection protein	Inorganic ion transport and metabolism Inorganic ion transport and metabolism Inorganic ion transport and metabolism
sps_RS15620 sps_RS17675 sps_RS21625 sps_RS22160	3.96478885 -2.332152706 3.709462096 2.378253811	2.37E-08 1.25E-10 1.87E-12 2.47E-07	TonB- dependent receptor DNA starvation/statio nary phase protection protein MFS transporter prepilin-type N-	Inorganic ion transport and metabolism Inorganic ion transport and metabolism Inorganic ion transport and metabolism
sps_RS15620 sps_RS17675 sps_RS21625 sps_RS22160	3.96478885 -2.332152706 3.709462096 2.378253811	1.25E-10 1.87E-12 2.47E-07	TonB- dependent receptor DNA starvation/statio nary phase protection protein MFS transporter prepilin-type N- terminal	Inorganic ion transport and metabolism Inorganic ion transport and metabolism Inorganic ion transport and metabolism
sps_RS15620 sps_RS17675 sps_RS21625 sps_RS22160	3.96478885 -2.332152706 3.709462096 2.378253811	2.37E-08 1.25E-10 1.87E-12 2.47E-07	TonB- dependent receptor DNA starvation/statio nary phase protection protein MFS transporter prepilin-type N- terminal cleavage/methvl	Inorganic ion transport and metabolism Inorganic ion transport and metabolism Inorganic ion transport and metabolism
sps_RS15620 sps_RS17675 sps_RS21625 sps_RS22160	3.96478885 -2.332152706 3.709462096 2.378253811	1.25E-10 1.87E-12 2.47E-07	TonB- dependent receptor DNA starvation/statio nary phase protection protein MFS transporter prepilin-type N- terminal cleavage/methyl ation domain-	Inorganic ion transport and metabolism Inorganic ion transport and metabolism Inorganic ion transport and metabolism
sps_RS15620 sps_RS17675 sps_RS21625 sps_RS22160	3.96478885 -2.332152706 3.709462096 2.378253811	1.25E-10 1.87E-12 2.47E-07	TonB- dependent receptor DNA starvation/statio nary phase protection protein MFS transporter prepilin-type N- terminal cleavage/methyl ation domain- containing	Inorganic ion transport and metabolism Inorganic ion transport and metabolism Inorganic ion transport and metabolism

			type IV pilus	Intracellular
			modification	trafficking and
sps RS11700	2.446822552	1.68E-06	protein PilV	secretion
			-	Intracellular
			signal peptidase	trafficking and
sps_RS15755	2.111968534	3.32E-05	Ι	secretion
			EscC/YscC/Hrc	
			C family type	
			III secretion	
			system outer	Intracellular
			membrane ring	trafficking and
sps_RS27315	2.029832054	1.94E-12	protein	secretion
				Lipid
sps_RS08835	-2.188103952	6.99E-08	transporter	metabolism
			anaerobic	
			ribonucleoside-	Nucleotide
			triphosphate	metabolism and
sps_RS08910	-2.494691249	1.27E-15	reductase	transport
				Nucleotide
				metabolism and
sps_RS10470	-2.129270999	1.43E-07	UMP kinase	transport
				Post-
				translational
			CesD/SycD/Lcr	modification,
			H family type	protein
			III secretion	turnover,
			system	chaperone
sps_RS04945	2.760738177	2.92E-07	chaperone	functions
				Post-
				translational
				modification,
				protein
				turnover,
		0.00043680577	hypothetical	chaperone
sps_RS09315	2.586989251	25	protein	functions
				Post-
				translational
				modification,
				protein
		0.000.000000000000000000000000000000000		turnover,
	0.000 1000 10	0.00069988819		chaperone
sps_RS17270	-2.830498216	85	thiol peroxidase	tunctions
			organic	Post-
			hydroperoxide	translational
D G (G (F G		• • • • • •	resistance	modification,
sps_RS19150	3.526383355	2.45E-14	protein	protein

				turnover,
				chaperone
				functions
				Post-
				translational
				modification,
			alkyl	protein
			hydroperoxide	turnover,
5 6 4 6 6 6			reductase	chaperone
sps_RS24220	4.311808106	1.15E-17	subunit F	functions
				Post-
				translational
				modification,
				protein
				turnover,
DC24225	5 1051070(7	7010 10		chaperone
sps_RS24225	5.19519/96/	/.21E-12	peroxiredoxin	Tunctions
	2 205425720	451007	hypothetical	Replication and
sps_RS06255	2.305425729	4.51E-07	protein	repair
			group II intron	
			reverse	D
ma DC1(750	2 050040421	1 165 05	transcriptase/ma	Replication and
sps_K510/30	2.030949431	1.10E-03	lurase	repair Secondamy
ong DS16225	2 527140585	2 02E 10	nypotnetical	Secondary
sps_K310233	-2.33/149363	2.02E-10	CHKI domain	Suucluie
			ORKL domain-	Signal
sps R \$02065	2 219170531	3 75E-06	protein	Transduction
sps_K302003	2.217170331	5.751-00	DNA_binding	Tansauction
			response	Signal
sps_RS02070	2 383263365	6 87E-09	regulator	Transduction
5p5_10502070	2.303203303	0.0711 05	DNA-binding	
			response	Signal
sps RS03915	2.380049497	3.79E-07	regulator	Transduction
		0.172 01	DUF3369	
			domain-	
			containing	Signal
sps RS04570	2.805093996	6.79E-08	protein	Transduction
1 _			fused response	
			regulator/phosp	Signal
sps RS18155	2.540207047	8.43E-05	hatase	Transduction
			DNA-binding	
			response	Signal
sps_RS20510	2.552528657	5.49E-05	regulator	Transduction
			methyl-	Signal
sps_RS21025	2.726417378	2.56E-06	accepting	Transduction

			chemotaxis protein	
			YafY family	
			transcriptional	
sps_RS09570	2.157886905	1.16E-20	regulator	Transcription
			N-	
			acetyltransferas	
sps_RS08515	-2.069896604	4.52E-12	e	Translation

Data S3 Table D: Comparison betw cultures.	veen early log pha	ase samples from	20°C and 15°C

	Data S3 Table D	: Comparison betv	ween early log pha	ase samples from	20°C and 15°C
gene20padynamecatssps20padynamecatssps1secretionsecretionsps4.4932464072.27E-25protein HcpUnknownsps4.4932464072.27E-25protein HcpUnknownspsrulesecretionsystem tubeFunctionspsrule-4.3403081762.07E-22protein HcpUnknownspsrule-4.2611394541.23E-18proteinUnknownspsrule-4.0496969941.23E-18proteinUnknownspsrule-4.0496969944.25E-15protein HcpUnknownspsrule-4.0496969944.25E-15protein HcpUnknownspsrule-4.0496969942.24E-06malate synthaseconversionspsrule-3.1970283862.24E-06malate synthaseconversionspsrule-3.0133621575.06E-07protein VgrGbiogenesisspsrulescretionsystem tipenvelopespsrule-3.0133621575.06E-07protein VgrGbiogenesisspsrule-3.0133621575.03E-05protein VgrGbiogenesisspsrule-2.9219986323.38E-06protein VgrGbiogenesisspsrule-2.6046859195.03E-05proteinUnknownspsrule-2.6046859195.03E-05proteinUnknown		log2FoldChang e (<0 higher in 15, >0 higher in	nodi		aata
$sps_RS10195 = -4.493246407 = 2.27E-25 protein Hcp = Unknown$ $sps_RS10195 = -4.340308176 = 2.07E-22 protein Hcp = Unknown$ $sps_RS14360 = -4.261139454 = 1.23E-18 protein = Unknown$ $sps_RS24400 = -4.04969696994 = 4.25E-15 protein Hcp = Unknown$ $sps_RS24400 = -4.04969696994 = 4.25E-15 protein Hcp = Unknown$ $sps_RS08860 = -3.197028386 = 2.24E-06 malate synthase conversion$ $sps_RS19090 = -3.013362157 = 5.06E-07 protein VgrG biogenesis$ $sps_RS10190 = -2.921998632 = 3.38E-06 protein VgrG biogenesis$ $sps_RS10180 = -2.604685919 = 5.03E-05 protein = Unknown$ $LysM domain-containing = Function = VyrN = V = VYPN = VY = VYPN = VYP$	gene	20)	pauj	name	cats
sps_RS10195 -4.493246407 2.27E-25 sover tube secretion system tube system tube secretion system tip secretion system t				type VI	
sps_RS10195 -4.493246407 2.27E-25 protein Hcp Unknown sps_RS19095 -4.340308176 2.07E-22 protein Hcp Unknown sps_RS14360 -4.261139454 1.23E-18 protein Hcp Unknown sps_RS14360 -4.261139454 1.23E-18 protein Unknown sps_RS24400 -4.049696994 4.25E-15 protein Hcp Unknown sps_RS24400 -4.049696994 4.25E-15 protein Hcp Unknown sps_RS08860 -3.197028386 2.24E-06 malate synthase conversion sps_RS19090 -3.013362157 5.06E-07 protein VgrG biogenesis sps_RS10190 -2.921998632 3.38E-06 protein VgrG biogenesis sps_RS10180 -2.604685919 5.03E-05 protein Unknown sps_RS10180 -2.604685919 5.03E-05 protein Unknown sps_RS10180 -2.604685919 5.03E-05 protein Unknown sps_RS10190 -2.921998632 5.03E-05 protein VgrG biogenesis sps_RS10180 -2.604685919 5.03E-05 protein Unknown sps_RS10180 -2.604685919 5.03E-05 protein Unknown Sp				secretion	
sps_RS10195-4.4932464072.2/E-25protein HcpUnknowntype VI secretion system tubeFunctionsps_RS19095-4.3403081762.07E-22protein HcpUnknownhypothetical sps_RS14360-4.2611394541.23E-18proteinUnknownsps_RS14360-4.2611394541.23E-18proteinUnknownsps_RS24400-4.0496969944.25E-15proteinUnknownsps_RS24400-4.0496969944.25E-15protein HcpUnknownsps_RS08860-3.1970283862.24E-06malate synthase secretionconversionsps_RS10900-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknownLysM peptidoglycan- bindingLysM peptidoglycan- bindingFunction	DC10105	4 402246407	0.075.06	system tube	Function
type V1 secretion system tubeFunctionsps_RS19095-4.3403081762.07E-22protein HcpUnknownsps_RS14360-4.2611394541.23E-18proteinUnknownsps_RS14360-4.2611394541.23E-18proteinUnknownsps_RS24400-4.0496969944.25E-15protein HcpUnknownsps_RS24400-4.0496969944.25E-15protein HcpUnknownsps_RS24400-4.0496969944.25E-15protein HcpUnknownsps_RS24400-4.0496969942.24E-06malate synthaseconversionsps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown	sps_RS10195	-4.493246407	2.27E-25	protein Hcp	Unknown
sps_RS19095 -4.340308176 2.07E-22 protein Hcp Unknown sps_RS14360 -4.261139454 1.23E-18 protein Hcp Unknown sps_RS14360 -4.261139454 1.23E-18 protein Unknown sps_RS24400 -4.049696994 4.25E-15 protein Hcp Unknown sps_RS24400 -4.049696994 4.25E-15 protein Hcp Unknown sps_RS08860 -3.197028386 2.24E-06 malate synthase conversion sps_RS08860 -3.197028386 2.24E-06 malate synthase conversion sps_RS19090 -3.013362157 5.06E-07 protein VgrG biogenesis sps_RS10190 -2.921998632 3.38E-06 protein VgrG biogenesis sps_RS10180 -2.604685919 5.03E-05 protein VgrG biogenesis				type VI	
sps_RS19095 -4.340308176 2.07E-22 protein Hcp Unknown hypothetical Function sps_RS14360 -4.261139454 1.23E-18 protein Unknown type VI secretion system tube Function system tube Function system tube Function system tube Function system tube Function system tube Cell secretion system tube Function unknown Energy production and 2.24E-06 malate synthase conversion type VI Cell secretion wall/membrane/ system tip envelope sps_RS19090 -3.013362157 5.06E-07 protein VgrG biogenesis type VI Cell secretion system tip envelope biogenesis type VI Cell secretion System tip System System tip System Syst				secretion	
sps_RS19095-4.3403081762.07E-22protein HcpUnknownsps_RS14360-4.2611394541.23E-18proteinUnknownsps_RS14360-4.2611394541.23E-18proteinUnknownsps_RS24400-4.0496969944.25E-15protein HcpUnknownsps_RS24400-4.0496969944.25E-15protein HcpUnknownsps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown				system tube	Function
sps_RS14360 -4.261139454 1.23E-18 protein Unknown sps_RS24400 -4.049696994 4.25E-15 protein Hcp Unknown sps_RS24400 -4.049696994 4.25E-15 protein Hcp Unknown sps_RS08860 -3.197028386 2.24E-06 malate synthase conversion sps_RS08860 -3.197028386 2.24E-06 malate synthase conversion sps_RS10909 -3.013362157 5.06E-07 protein VgrG biogenesis sps_RS10190 -2.921998632 3.38E-06 protein VgrG biogenesis sps_RS10180 -2.604685919 5.03E-05 protein Unknown sps_RS10180	sps_RS19095	-4.340308176	2.07E-22	protein Hcp	Unknown
sps_RS14360-4.2611394541.23E-18proteinUnknownsps_RS24400-4.04969699944.25E-15secretionsystem tubeFunctionsps_RS24400-4.04969699944.25E-15protein HcpUnknownsps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown				hypothetical	Function
kype VI secretionkype VI secretionsps_RS24400-4.0496969944.25E-15system tube protein HcpFunctionsps_RS24400-4.0496969944.25E-15protein HcpUnknownsps_RS08860-3.1970283862.24E-06malate synthase secretionconversionsps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS10909-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06type VI secretionCell secretionwall/membrane/ system tipsps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10190-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown	sps_RS14360	-4.261139454	1.23E-18	protein	Unknown
sps_RS24400-4.049696994-4.25E-15secretion system tube protein HcpFunctionsps_RS08860-3.1970283862.24E-06malate synthase scretionEnergy production and conversionsps_RS08860-3.1970283862.24E-06malate synthase scretionCell secretionsps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06LysM domain- containing proteinFunctionsps_RS10180-2.6046859195.03E-05proteinUnknown				type VI	
sps_RS24400-4.0496969944.25E-15system tube protein HcpFunctionsps_RS08860-3.1970283862.24E-06malate synthaseEnergy production andsps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS10900-3.0133621575.06E-07protein VgrGbiogenesissps_RS10900-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06type VICellsps_RS10180-2.6046859195.03E-05protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown				secretion	
sps_RS24400-4.0496969944.25E-15protein HcpUnknownsps_RS08860-3.1970283862.24E-06malate synthaseEnergy production andsps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS10900-3.0133621575.06E-07protein VgrGbiogenesissps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown				system tube	Function
sps_RS08860-3.1970283862.24E-06Handlet synthaseEnergy production and conversionsps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS19090-3.0133621575.06E-07type VI protein VgrGenvelopesps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown	sps_RS24400	-4.049696994	4.25E-15	protein Hcp	Unknown
sps_RS08860-3.1970283862.24E-06malate synthaseproduction and conversionsps_RS08860-3.1970283862.24E-06malate synthasecellsecretiontype VICellsecretionwall/membrane/sps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06type VICellsps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown					Energy
sps_RS08860-3.1970283862.24E-06malate synthaseconversionsps_RS19090-3.0133621575.06E-07type VI secretionenvelope biogenesissps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06type VI secretioncell secretionsps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown					production and
sps_RS19090-3.0133621575.06E-07type VI secretion protein VgrGCell wall/membrane/ system tip protein VgrGsps_RS10190-2.9219986323.38E-06type VI secretion protein VgrGCell secretion system tipsps_RS10180-2.6046859195.03E-05protein proteinLysM peptidoglycan- binding	sps RS08860	-3.197028386	2.24E-06	malate synthase	conversion
sps_RS19090-3.0133621575.06E-07wall/membrane/ system tipsps_RS19090-3.0133621575.06E-07protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown				type VI	Cell
sps_RS19090-3.0133621575.06E-07system tip protein VgrGenvelope biogenesissps_RS10190-2.9219986323.38E-06rype VI secretioncell wall/membrane/ system tipsps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknownsps_ns_rs_rs_rs_rs_rs_rs_rs_rs_rs_rs_rs_rs_rs				secretion	wall/membrane/
sps_RS19090-3.0133621575.06E-07protein VgrGbiogenesistype VICellsecretionwall/membrane/sps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownsps_RS10180-2.6046859195.03E-05proteinUnknown				system tip	envelope
sps_RS10190 -2.921998632 3.38E-06 rotein VgrG biogenesis sps_RS10180 -2.604685919 5.03E-05 protein Unknown sps_RS10180 -2.604685919 5.03E-05 protein Unknown sps_ns_rs_rs_rs_rs_rs_rs_rs_rs_rs_rs_rs_rs_rs	sps RS19090	-3.013362157	5.06E-07	protein VgrG	biogenesis
sps_RS10190-2.9219986323.38E-06wall/membrane/ system tipsps_RS10190-2.6046859193.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05proteinUnknownLysM peptidoglycan- bindingLysM peptidoglycan- binding				type VI	Cell
sps_RS10190 -2.921998632 3.38E-06 system tip envelope biogenesis LysM domain- containing Function sps_RS10180 -2.604685919 5.03E-05 protein Unknown LysM peptidoglycan- binding				secretion	wall/membrane/
sps_RS10190-2.9219986323.38E-06protein VgrGbiogenesissps_RS10180-2.6046859195.03E-05LysM domain- containing proteinFunctionsps_RS10180-2.6046859195.03E-05proteinUnknownLysM peptidoglycan- bindingLysM				system tip	envelope
sps_RS10180 -2.604685919 5.03E-05 LysM domain- containing Function LysM protein Unknown LysM peptidoglycan- binding	sps RS10190	-2.921998632	3.38E-06	protein VgrG	biogenesis
sps_RS10180 -2.604685919 5.03E-05 containing Function LysM peptidoglycan- binding				LvsM domain-	
sps_RS10180 -2.604685919 5.03E-05 protein Unknown LysM peptidoglycan- binding				containing	Function
LysM peptidoglycan- binding	sps RS10180	-2.604685919	5.03E-05	protein	Unknown
peptidoglycan- binding	<u>-r</u>			LvsM	
binding				peptidoglycan-	
Chitching				binding	
domain-				domain-	
containing Function				containing	Function
sps R\$19080 -2 561880809 1 59E-05 protein Unknown	sps_RS19080	-2 561880809	1 59E-05	protein	Unknown
5 <u><u><u></u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u></u>	<u>-po_1017000</u>	2.001000000	1.571 05	5-	
methyltetrahydr				nethyltetrahydr	
onterovitrigiuta				onterovitrigiuta	
mate Amino Aoid				mate	Amino Acid
homocysteine metabolism and				homocysteine	metabolism and
sps RS22050 -2 541738045 1 00F-10 S- transport	sps RS22050	-2 541738045	1.00F-10	S-	transport

			methyltransfera	
			se	
			DUF4123	
			domain-	
			containing	Function
sps_RS19085	-2.534230144	5.03E-05	protein	Unknown
			type VI	Cell
			secretion	wall/membrane/
			system tip	envelope
sps_RS24405	-2.397993379	1.90E-05	protein VgrG	biogenesis
			hypothetical	Function
sps_RS04175	-2.276038852	4.25E-15	protein	Unknown
			sulfate	
			adenylyltransfer	Inorganic ion
		0.00077795709	ase subunit	transport and
sps_RS18235	-2.001295119	47	CysD	metabolism
				Inorganic ion
		0.00066968516		transport and
sps_RS04420	2.244682356	4	bacterioferritin	metabolism
			DUF1611	
			domain-	
			containing	Function
sps_RS10355	2.706572509	1.55E-08	protein	Unknown
				Cell
				wall/membrane/
			dipeptide	envelope
sps_RS10360	2.717091443	7.43E-13	epimerase	biogenesis

Data S	S3 Table E:	Comparison betw	veen late log phas	e samples from 2	0°C and 15°C
cultur	es.				

	log2FoldChang e (<0 higher in			
	15, >0 higher			
gene	in 20)	padj	name	cats
			PLP-dependent	
			cysteine	Amino Acid
		0.00053890515	synthase family	metabolism and
sps_RS03160	2.002902784	66	protein	transport
			HAAAP family	Amino Acid
			serine/threonine	metabolism and
sps_RS13055	-2.356820823	6.17E-05	permease	transport
				Carbohydrate
				metabolism and
sps_RS05545	-2.302160549	6.72E-06	pyruvate kinase	transport
				Carbohydrate
			phosphoketolas	metabolism and
sps_RS11765	-3.03084186	1.16E-19	e family protein	transport
			PAS domain-	
		0.00029809669	containing	
sps_RS01230	2.763101264	25	protein	Cell motility
				Cell
				wall/membrane/
				envelope
sps_RS09080	-2.396033577	6.17E-05	porin	biogenesis
				Cell
				wall/membrane/
D C10100	0.405155077	1 (05 10	outer membrane	envelope
sps_RS10100	-2.435155977	1.60E-10	protein OmpW	biogenesis
				Cell
			1	wall/membrane/
DC102(0	2 215(2557		dipeptide	envelope
sps_RS10360	2.21563557	5.//E-08	epimerase	biogenesis
			efflux KND	
			ransporter	waii/membrane/
ang DC15250	2 545029021	1 11E 06	peripiasmic	biogonosia
sps_K515550	-2.343028021	1.11E-06	adaptor subunit	Call
				Util wall/mombrane/
			porin family	envelope
sps R\$150/0	-2 043748405	5 58F_07	portinianiny	hiogenesis
sps_13513940	-2.043740493	J.JOE-07	protein	Cell
				wall/membrane/
			norin family	envelone
sps_RS15945	-3.694176774	3 30F-05	protein	hiogenesis
	J.071 /07/ T	J.JUL-0J	Protein	orogeneois

			oxygen- independent	
			coproporphyrin	Coenzyme
sps_RS00660	-2.702930697	9.66E-09	ogen III oxidase	metabolism
			8-amino-7-	
			oxononanoate	Coenzyme
sps_RS07855	2.090386533	6.75E-14	synthase	metabolism
				Energy
D G 0 0 0 0		0.00087881334	cytochrome-c	production and
sps_RS00020	2.139152844	28	oxidase	conversion
				Energy
D G 0 1 (1 0	2 4000 (5 0 (1	0.00085045684	aldehyde	production and
sps_RS01610	-2.488865061	13	dehydrogenase	conversion
			bifunctional	-
			acetaldehyde-	Energy
D.0.27(5	2 4201 40070	1.205 11	CoA/alcohol	production and
sps_RS03/65	-2.429140979	1.36E-11	dehydrogenase	conversion
		0.00020070027	1	Energy
DC00200	2 272960792	0.000389/082/	cystathionine	production and
sps_KS09300	2.3/3809/82	51	Deta-synthase	conversion
			INa(+)-	
			NADU guinono	Enorm
			NADH-quinone	nroduction and
sps RS11130	-2 34283737	1 46F-06	subunit Δ	conversion
sps_K511150	-2.3+203737	1.401-00	NADH-quinone	Energy
		0 00091489579	oxidoreductase	production and
sps_RS17495	2.802754881	77	subunit NuoC/D	conversion
	21002701001		NADH	
			oxidoreductase	Energy
		0.00073947945	(quinone)	production and
sps RS17505	3.745847465	4	subunit F	conversion
· -			NADH	
			dehydrogenase	Energy
		0.00097372842	(quinone)	production and
sps_RS17510	2.269945306	62	subunit G	conversion
			formate C-	Energy
			acetyltransferas	production and
sps_RS17575	-2.995452748	1.39E-10	e	conversion
				Energy
				production and
sps_RS22755	3.230782563	1.74E-05	MFS transporter	conversion
				Energy
			formate	production and
sps_RS27130	-2.760980488	1.56E-07	dehydrogenase	conversion

			cytochrome o	Enonex
		0 00036282541	ubiquinoi oxidase subunit	production and
sps BS27700	3 648404321	0.00030282341	IV	conversion
sps_K327790	-3.040404321	03	1 v	CONVERSION
			ubiquinol	Energy
			avidase subunit	production and
sps R\$27705	-2 601057005	8 21E-06	III	conversion
sps_R527775	-2.001037003	0.21L-00	cytochrome o	
			ubiquinol	Energy
			oxidase subunit	production and
sps_RS27800	-2.758814428	2.96E-11	I	conversion
<u></u>	21,00011120	2,,02,11	cell division	Function
sps RS01305	2.439577113	2.33E-06	protein	Unknown
			1	Function
sps RS01375	-2.801855816	7.15E-17	ATPase P	Unknown
			DUF1302	
			domain-	
			containing	Function
sps RS02895	2.133959769	8.36E-05	protein	Unknown
			hypothetical	Function
sps_RS04175	-2.333335158	5.37E-17	protein	Unknown
			hypothetical	Function
sps_RS04695	-2.297335684	5.35E-10	protein	Unknown
		0.00059131228	hypothetical	Function
sps_RS06230	-2.659744863	2	protein	Unknown
		0.00067725321	AcrB/AcrD/Acr	Function
sps_RS08025	2.057553817	11	F family protein	Unknown
			type VI	
			secretion	
			system tube	Function
sps_RS10195	-4.359549727	1.51E-23	protein Hcp	Unknown
			DUF1611	
			domain-	
DG10255	0 40 (11 5 41 5		containing	Function
sps_RS10355	2.486115417	2.20E-07	protein	Unknown
DG10(05	0.007202042	4.175 10	hypothetical	Function
sps_KS10625	-2.66/382642	4.15E-10	protein	Unknown
DC15000	5 42 4200 (01		phasin family	Function
sps_K515000	-5.424390691	3.06E-09	protein	Unknown
ana DC15400	2 2 ((10 9 1 0	2 AOF AF	1	Function
sps_K515400	-2.30610819	2.08E-05	nyaroiase	Unknown
ang DC17010	2 122715065	1 20E 05	nypotnetical	Function
sps_K51/010	2.122/13965	4.30E-05	protein	Unknown

			regulatory	Function
sps_RS17130	2.170363817	5.65E-06	protein GemA	Unknown
			DUF3164	
			domain-	
			containing	Function
sps_RS17135	2.913125883	2.23E-07	protein	Unknown
			XRE family	
			transcriptional	Function
sps_RS17145	2.747405263	3.15E-06	regulator	Unknown
		0.00058262383	hypothetical	Function
sps_RS17220	2.675985673	01	protein	Unknown
			methyl-	
			accepting	
			chemotaxis	Function
sps_RS18820	-2.273770317	7.25E-12	protein	Unknown
			type VI	
			secretion	
			system tube	Function
sps_RS19095	-3.388696805	9.55E-14	protein Hcp	Unknown
			nitrate ABC	
			transporter	
		0.00059412345	substrate-	Function
sps_RS19180	2.167682679	71	binding protein	Unknown
		0.00079236668	hypothetical	Function
sps_RS19895	2.406790088	71	protein	Unknown
			hypothetical	Function
sps_RS21080	-2.050962492	4.13E-06	protein	Unknown
			GTP	
			pyrophosphokin	Function
sps_RS21730	-2.675888793	3.25E-05	ase	Unknown
			tripartite	
			tricarboxylate	
			transporter	
D.G.21.500	0.50(450)((5		substrate	Function
sps_RS21780	2.536479667	2.56E-05	binding protein	Unknown
			type VI	
			secretion	
DC24400	4.005666001		system tube	Function
sps_RS24400	-4.095666081	1.1/E-15	protein Hcp	Unknown
DG25225	0.170051104	1 005 05	nypothetical	Function
sps_K825235	-2.1/8851194	1.22E-05	protein	Unknown
D.027207	0.100200010		nypothetical	Function
sps_KS2/295	-2.180390919	8.94E-06	protein	Unknown
			ESCD/YSCD/Hrp	F (*
D.007010	0 446701001		Q family type	Function
sps_RS2/310	-2.446/01824	5.24E-11	III secretion	Unknown

			system inner	
			membrane ring	
			protein	
			CesD/SycD/Lcr	
			H family type	
			III secretion	D
D.G.272(0	0.425050406	1.005.00	system	Function
sps_RS27360	-2.435979426	1.98E-09	chaperone	Unknown
DC272(5	2 555229 (41	0.455 11	hypothetical	Function
sps_RS2/365	-2.555258641	9.45E-11	protein	Unknown
DC27455	2 004050629	4 99E 13	hypothetical	Function
sps_R52/455	-2.004950638	4.88E-12	protein	Unknown
			eniux KND	Inonconicion
				morganic ion
sps PS01370	3 3/35///121	3 00F 23	adaptor subunit	metabolism
sps_1001370	-5.545544121	5.771-25	TonB-	Inorganic ion
			denendent	transport and
sps RS09075	2 446132199	1 60F-09	recentor	metabolism
sps_R507075	2.110132177	1.002 07	formate	Inorganic ion
			transporter	transport and
sps_RS17570	-2.26191516	1.31E-05	FocA	metabolism
				Inorganic ion
				transport and
sps RS19860	2.355978361	9.49E-05	arylsulfatase	metabolism
			DNA	
			starvation/statio	
			nary phase	Inorganic ion
		0.00051419598	protection	transport and
sps_RS21625	-2.078827136	35	protein	metabolism
				Inorganic ion
				transport and
sps_RS21785	2.276824723	3.22E-05	porin	metabolism
			HlyD family	
		0.0000000000000000000000000000000000000	type I secretion	Intracellular
	0.450440011	0.00031974113	periplasmic	trafficking and
sps_RS15075	2.473440211	83	adaptor subunit	secretion
			EscJ/YscJ/HrcJ	
			family type III	T., 4
			secretion inner	intracenular trofficience and
sps BS27280	2 102622866	0 20 00	nrotein	secretion
sps_122/200	-2.102022800	7.30E-09	VscX family	
			type III	Intracellular
			secretion	trafficking and
sns RS27300	-2 333410461	1 20F-07	nrotein	secretion
pp_102/5/0	2.333710701	1.201-0/	Protein	secteduti

			class I poly(R)-	
			hydroxyalkanoi	Lipid
sps RS14995	-2.657754139	1.18E-11	c acid synthase	metabolism
			anaerobic	
			ribonucleoside-	Nucleotide
			triphosphate	metabolism and
sps RS08910	-2 410888623	2 44F-14	reductase	transport
<u>sps_R500710</u>	2.410000023	2.112 11	Teductuse	Nucleotide
			uriding	metabolism and
ong P S15525	2 31//80/5/	2 73E 10	nhosnhorvlase	transport
sps_K515525	-2.31+07+3+	2.751-10	phosphorylase	Nucleotide
		0.00002706127	purme-	nucleotide
ana DC20065	2 24076006	0.00092706137	nucleoside	metabolism and
sps_K520805	-2.248/0890	3	phosphorylase	
			.1 . 1.	Nucleotide
DGQQQEE	0.011054005		thymidine	metabolism and
sps_RS20875	-2.2118/483/	8.33E-10	phosphorylase	transport
				Post-
				translational
				modification,
				protein
			YjjW family	turnover,
			glycine radical	chaperone
sps_RS01600	2.854376416	9.67E-05	enzyme activase	functions
				Post-
				translational
				modification,
			pyruvate	protein
			formate lyase 1-	turnover,
			activating	chaperone
sps RS17580	-2.222543587	1.60E-09	protein	functions
				Post-
				translational
				modification.
			organic	protein
			hydroperoxide	turnover.
			resistance	chaperone
sps RS19150	-2.254056794	1.94E-05	protein	functions
			1	Post-
				translational
				modification
			alkyl	protein
			hydroperoxide	turnover
			reductase	chaperope
sns RS24220	-2 410502007	1 34F-05	subunit F	functions
5p5_1027220	2.110302007	1.5412 05	group II introp	Replication and
sps BS12060	2 255820454	1 1/E 05	Stoup II IIIIOII	reprivation and
sps_123200	2.255050454	1.14E-03	10,00120	теран

			transcriptase/ma	
			turase	
			group II intron	
			reverse	
			transcriptase/ma	Replication and
sps_RS16750	2.044192656	1.71E-05	turase	repair
			ATP-binding	Replication and
sps_RS17155	3.223893077	2.78E-13	protein	repair
			hypothetical	Replication and
sps_RS17160	2.436528703	8.40E-16	protein	repair
			DNA	Replication and
sps_RS21135	2.699576704	5.07E-08	polymerase IV	repair
			universal stress	Signal
sps_RS23425	-2.035180285	5.56E-06	protein	Transduction
		0.00061918880	hypothetical	Signal
sps_RS27835	-2.157084295	4	protein	Transduction
			transcriptional	
sps_RS17125	2.796093484	2.56E-07	regulator	Transcription
			threonine	
sps_RS20540	-2.36599461	6.96E-27	tRNA ligase	Translation

Data S3 Table F: Comparison between stationary phase samples from 20°C and 15°C cultures.

	log2FoldChang			
	15. >0 higher			
gene	in 20)	padj	name	cats
8	,	1 9		Amino Acid
			amino acid	metabolism and
sps_RS03105	-3.202635613	4.24E-08	transporter	transport
			branched-chain	
			amino acid	
			ABC	Amino Acid
			transporter	metabolism and
sps_RS06470	-3.51141094	6.30E-13	permease	transport
			serine O-	Amino Acid
			acetyltransferas	metabolism and
sps_RS15460	2.927916676	8.82E-11	e	transport
				Amino Acid
			cysteine	metabolism and
sps_RS17470	2.213409416	2.43E-08	synthase A	transport
				Carbohydrate
			methylisocitrate	metabolism and
sps_RS09960	-2.394133885	8.78E-06	lyase	transport
				Carbohydrate
			allantoinase	metabolism and
sps_RS19520	-2.222460122	7.05E-05	PuuE	transport
			type VI	Cell
			secretion	wall/membrane/
			system tip	envelope
sps_RS05125	-4.020323389	4.81E-19	protein VgrG	biogenesis
			type VI	Cell
			secretion	wall/membrane/
D C10100	0.05500.4577	1.005.07	system tip	envelope
sps_RS10190	-2.855824577	1.89E-06	protein VgrG	biogenesis
				Cell
			· c ·1	wall/membrane/
DC15045	2 722079464	2 455 05	porin family	envelope
sps_R\$15945	-3./230/8464	3.45E-05	protein	biogenesis
			type VI	
			secretion	wall/membrane/
ang DC10000	2 015450077	1 420 07	system tip	envelope
sps_K519090	-3.0154599//	1.43E-07	protein VgrG	Diogenesis
			type v1	
		0.00021467020	secretion	wan/memorane/
ang DS24405	2 061742000	0.0002140/920	system up	biogonosia
sps_K524405	-2.001/43998	24	protein v gro	biogenesis

			efflux RND	Cell
			transporter	wall/membrane/
			periplasmic	envelope
sps_RS25955	-2.372619478	7.94E-07	adaptor subunit	biogenesis
				Cell
				wall/membrane/
		0.00042594798	TolC family	envelope
sps_RS26230	-2.174644658	66	protein	biogenesis
				Cell
				wall/membrane/
			dipeptide	envelope
sps_RS10360	2.833433804	2.13E-14	epimerase	biogenesis
			4-	
			hydroxyphenylp	
			yruvate	Coenzyme
sps_RS07040	-2.435262652	1.80E-09	dioxygenase	metabolism
			uroporphyrinog	
			en-III C-	
			methyltransfera	Coenzyme
sps_RS13735	3.525070299	4.29E-19	se	metabolism
				Energy
			hypothetical	production and
sps_RS01075	2.390514104	5.67E-05	protein	conversion
				Energy
		0.00099083206	(Fe-S)-binding	production and
sps_RS08485	-2.332244017	01	protein	conversion
			iron-sulfur	Energy
			cluster-binding	production and
sps_RS08490	-2.243610425	3.16E-05	protein	conversion
				Energy
			2-methylcitrate	production and
sps_RS09955	-2.1819561	1.51E-07	synthase	conversion
			NADH-	
			dependent	Energy
			alcohol	production and
sps_RS15885	-3.353221008	2.44E-07	dehydrogenase	conversion
			putative sulfate	
			exporter family	Function
sps_RS00895	2.417088107	2.64E-23	transporter	Unknown
			hypothetical	Function
sps_RS01100	2.886649995	8.05E-06	protein	Unknown
				Function
sps_RS01625	-2.472383773	5.52E-09	phospholipase	Unknown
			pathogenicity	
			island effector	Function
sps_RS04960	-2.388386624	3.67E-05	protein	Unknown

			type III	
			secretion	
			system	
		0.00033232250	translocon	Function
sps RS04965	-2.398345673	98	protein	Unknown
			hypothetical	Function
sps RS05115	-2.020156919	2.79E-06	protein	Unknown
			DUF4123	
			domain-	
			containing	Function
sps_RS05120	-2.928372778	3.87E-08	protein	Unknown
- <u>F</u>			type VI	
			secretion	
			system tube	Function
sps_RS05130	-3.16543868	3.71E-05	protein Hcp	Unknown
1			serine	
			dehvdratase	
			subunit alpha	Function
sps_RS06460	-2.077520069	3.06E-05	family protein	Unknown
	2.077020003		NADP-	
			dependent	Function
sps_RS08925	-4.082910269	5.62E-15	oxidoreductase	Unknown
500,1000,20	1.002910209	0.021 10	type VI	
			secretion	
			system tube	Function
sps_RS10195	-3.907036734	3.91E-17	protein Hcp	Unknown
		0.912 17	hypothetical	Function
sps RS10795	-2.009449356	3.54E-08	protein	Unknown
- <u>F</u>			DUF1611	
			domain-	
			containing	Function
sps RS10355	3.216066082	6.30E-13	protein	Unknown
<u> </u>			hypothetical	Function
sps_RS13850	-2.07151457	7.04E-05	protein	Unknown
		,	UPF0016	
			domain-	
			containing	Function
sps RS14010	-3.219900954	9.29E-12	protein	Unknown
1				Function
sps RS15400	-3.649446034	6.03E-13	hydrolase	Unknown
			HlyD familv	
			secretion	Function
sps RS15625	-4.645200008	4.73E-12	protein	Unknown
1			LvsM	
		0.00011930990	peptidoglycan-	Function
sps RS19080	-2.24641819	63	binding	Unknown

			domain-	
			containing	
			protein	
			DUF4123	
			domain-	
		0 00017311104	containing	Function
cmc PS10085	2 253073626	0.00017511104	protein	Unknown
sps_K517005	-2.233073020	70	type VI	UIIKIIOWII
			socration	
			system tubo	Function
spc PS 10005	1 138315573	0 37E 73	protein Hen	Unknown
sps_K319095	-4.430313373	9.521-25		UIIKIIUWII
			DUF2219	
			domain-	Eurotian
ang DS10160	2 112556122	8 55E 06	rotain	Function
sps_K319100	-2.445550452	0.JJE-00		
DC10515	2.095129905	0.00036826877		Function
sps_RS19515	-2.085128805	63	decarboxylase	Unknown
		0.000.4500.000.4	GIP	
D.C.21720	0.045660750	0.00047989224	pyrophosphokin	Function
sps_RS21730	-2.345662758	73	ase	Unknown
			type VI	
			secretion	
			system tube	Function
sps_RS24400	-3.628176643	4.94E-12	protein Hcp	Unknown
			multidrug	Function
sps_RS24450	-2.699696138	3.15E-06	transporter	Unknown
			EscI/YscI/HrpB	
			family type III	
			secretion	
			system inner	Function
sps_RS27285	-2.180590953	8.98E-05	rod protein	Unknown
			hypothetical	Function
sps_RS27350	-3.501607706	2.94E-13	protein	Unknown
			hypothetical	Function
sps_RS27355	-3.430098658	5.30E-14	protein	Unknown
			CesD/SycD/Lcr	
			H family type	
			III secretion	
			system	Function
sps_RS27360	-2.031476666	1.10E-05	chaperone	Unknown
			DUF2061	
			domain-	
		0.00056555018	containing	Function
sps_RS27760	-4.109080184	56	protein	Unknown

			phosphoadenyly	Inorganic ion
			1-sulfate	transport and
sps_RS13780	2.323269975	8.67E-14	reductase	metabolism
			NADPH-	
			dependent	
			assimilatory	
			sulfite reductase	Inorganic ion
			hemoprotein	transport and
sps RS13785	2.967518488	3.24E-17	subunit	metabolism
			assimilatory	
			sulfite reductase	
			(NADPH)	Inorganic ion
			flavoprotein	transport and
sps RS13790	3.247360256	4.70E-14	subunit	metabolism
_1 _			sulfate	
			adenvlvltransfer	Inorganic ion
			ase subunit	transport and
sps RS18235	2.737406565	2.32E-07	CvsD	metabolism
			5	Inorganic ion
				transport and
sps RS01620	-3.046111367	7.12E-16	catalase	metabolism
<u></u>		,		Inorganic ion
				transport and
sps_RS14015	-4.27679358	5.18E-18	catalase	metabolism
				Inorganic ion
				transport and
sps RS15620	-3 663188551	4 99E-07	MFS transporter	metabolism
505_1012020	5.005100551		DNA	
			starvation/statio	
			nary phase	Inorganic ion
			protection	transport and
sps_RS21625	-4 947268525	7 50E-21	protein	metabolism
- <u></u>	1.9 17200323	,	Protom	Inorganic ion
				transport and
sps_RS22160	-2 24007972	2 22E-06	MFS transporter	metabolism
505_10522100	2.21007972	2.221 00		Intracellular
			signal pentidase	trafficking and
eng R\$15755	-2 25/1300710	1 73E-05	I signal peptidase	secretion
sps_R515755	-2.23+370717	1.75L-05	1 hypothetical	Lipid
sns RS01000	2 776272702	1 07F 06	nypoincical	metabolism
sps_1\301020	2.110212102	0.0002452094	hypothetical	Linid
ang DS01105	2 068271729	0.00093433084	nypoinctical	Lipia motobolicm
sps_KSU1103	2.0085/1/28	0.00022215702	hymothetical	Linid
ang DC01110	2 214560026	0.00023213/93	nypoinetical	Lipia matabalian
sps_KSUIIIU	2.314308820	57		
DC01117	2 (20072 (21		nypotnetical	
sps_KSUIIIS	2.6388/3631	3.14E-06	protein	metabolism

		0.00016287523	acyl-CoA	Lipid
sps_RS05895	-2.063500883	87	dehydrogenase	metabolism
			succinyl-CoA	
		0.00017806016	3-ketoacid-CoA	Lipid
sps_RS10265	-2.138572107	91	transferase	metabolism
				Post-
				translational
				modification,
				protein
				turnover,
		0.00011968764	heat-shock	chaperone
sps_RS06940	2.608649332	98	protein	functions
				Post-
				translational
				modification,
			glutathione-	protein
			dependent	turnover,
			disulfide-bond	chaperone
sps_RS22460	2.67185539	2.34E-12	oxidoreductase	functions
				Post-
				translational
				modification,
			organic	protein
			hydroperoxide	turnover,
			resistance	chaperone
sps_RS19150	-4.579618501	8.27E-23	protein	functions
				Post-
				translational
				modification,
			alkyl	protein
			hydroperoxide	turnover,
			reductase	chaperone
sps_RS24220	-4.81913761	4.25E-22	subunit F	functions
				Post-
				translational
				modification,
				protein
				turnover,
DC24225	5 (10077201			chaperone
sps_K524225	-5.640077394	/.02E-14	peroxiredoxin	Iunctions
				POST-
				modification
			hypothetical	nrotain
ang DC27240	2 104825210	1 650 05	nypoinetical	protein
sps_rs2/340	-2.104823219	1.03E-03	protein	turnover,

				chaperone
				functions
			ATP-binding	Replication and
sps_RS17155	2.179774499	4.75E-06	protein	repair
		0.00047934864	hypothetical	Secondary
sps_RS01085	2.118191426	2	protein	Structure
		0.00015262054	hypothetical	Secondary
sps_RS01095	2.387248928	48	protein	Structure
			DNA-binding	
			response	Signal
sps_RS02070	-2.450966683	3.14E-09	regulator	Transduction
			PrkA family	
			serine protein	Signal
sps_RS03040	-2.701132009	3.00E-05	kinase	Transduction
			DNA-binding	
			response	Signal
sps_RS03915	-3.371103351	1.37E-13	regulator	Transduction
			MarR family	
			transcriptional	
sps_RS08920	-2.348014489	9.49E-08	regulator	Transcription
			RidA family	
sps_RS06465	-2.654320948	4.06E-05	protein	Translation

Data S3 Table G: Comparison between early log phase samples from 20°C and 4°C cultures.

	log2FoldCh ange (<0 higher in 4,			
gene	>0 higher in 20)	padj	name	cats
sps_RS00 915	2 473297838	3 70E-08	oligonentidase A	Amino Acid metabolism and transport
sps_RS05 300	2.504603871	0.000475648 4313	alanine dehydrogenase	Amino Acid metabolism and transport
sps_RS06 490	2.371543739	4.19E-07	ATP phosphoribosyltransferas e	Amino Acid metabolism and transport
sps_RS06 495	2.131181472	0.000641235 7818	histidinol dehydrogenase	Amino Acid metabolism and transport
sps_RS06 510	2.471111565	0.000110719 9133	imidazole glycerol phosphate synthase subunit HisH	Amino Acid metabolism and transport
sps_RS07 005	3.533727838	4.73E-09	1-aminocyclopropane-1- carboxylate deaminase	Amino Acid metabolism and transport
sps_RS08 295	2.09839961	6.74E-06	bifunctional indole-3- glycerol-phosphate synthase TrpC/phosphoribosylant hranilate isomerase TrpF	Amino Acid metabolism and transport
sps_RS08 300	2.24429259	5.59E-09	tryptophan synthase subunit beta	Amino Acid metabolism and transport
sps_RS08 305	2.461791484	2.12E-07	tryptophan synthase subunit alpha	Amino Acid metabolism and transport
sps_RS09 555	2.668739053	6.87E-13	branched-chain amino acid ABC transporter permease	Amino Acid metabolism and transport
sps_RS11 505	2.521527885	1.58E-08	pyrroline-5-carboxylate reductase	Amino Acid metabolism and transport
sps_RS12 080	2.564517547	6.28E-09	glutamate synthase large subunit	Amino Acid metabolism and transport

sps RS12			glutamate synthase small	Amino Acid metabolism and
085	2.305569872	9.62E-08	subunit	transport
			aspartate	Amino Acid
sps_RS12	-		aminotransferase family	metabolism and
610	2.378197835	7.42E-05	protein	transport
				Amino Acid
sps_RS13	-		EamA/RhaT family	metabolism and
315	2.741720974	6.31E-09	transporter	transport
				Amino Acid
sps_RS21	-		EamA/RhaT family	metabolism and
065	2.489422486	2.57E-08	transporter	transport
DCOF			keto-deoxy-	Carbohydrate
sps_KS05	2 540510755	1 (55 00	phosphogluconate	metabolism and
520	2.340319733	1.03E-09	aldolase	transport Carbabydrata
and DS05			nhamhadluaanata	Carbonyurate
525	2 310023/1/	4 28E-07	dehydratase	transport
525	2.317023414	H.20L-07	ucifyuratase	Carbobydrate
sps RS18	_			metabolism and
005	2.285462679	7.36E-09	MFS transporter	transport
		,		Carbohvdrate
sps RS19				metabolism and
520	-3.65110482	2.04E-13	allantoinase PuuE	transport
sps RS00	-			
455	2.317242626	5.48E-10	hypothetical protein	Cell motility
sps_RS00	-		flagellar motor stator	
460	2.139791625	6.07E-06	protein MotA	Cell motility
sps_RS00	-		flagellar hook-length	
475	2.807469452	1.69E-09	control protein FliK	Cell motility
sps_RS00	-		flagellar hook protein	~ ~ ~ ~ ~
490 DG00	2.029521657	5.49E-08	FliD	Cell motility
sps_RS00	-	1 225 07		C 11 ('1')
610	2.480335439	1.23E-07	OmpA family protein	Cell motility
ana DO27			ESCN/YSCN/HrcN family	
sps_K527	2 212727624	5 21E 10	ATPage	Call matility
410	5.212/5/034	5.51E-10	AIrast	Cell
sps RS00				wall/membrane/en
045	2 500768282	942E-12	energy transducer TonR	velone biogenesis
	2.000700202	7. TZL 12	energy numbuleer rollD	Cell
sps RS10	_		type VI secretion system	wall/membrane/en
190	2.733619814	2.07E-06	tip protein VgrG	velope biogenesis

				Cell
sps RS10				wall/membrane/en
360	2.995531524	1.34E-16	dipeptide epimerase	velope biogenesis
				Cell
sps RS11				wall/membrane/en
770	3.249946574	4.50E-07	OmpA family protein	velope biogenesis
				Cell
sns RS12				wall/membrane/en
490	2 130852348	2 15E-05	hypothetical protein	velone biogenesis
190	2.130032310	2.101 00	nypometical protein	Cell
sns RS15				wall/membrane/en
300	2 261167563	641E-16	OmnA family protein	velone biogenesis
500	2.201107303	0.41L-10	efflux PND transporter	
ene DS15			periplasmic adaptor	Wall/membrane/en
sps_K313	2 052201075	6 16E 05	subunit	valore biogenesis
330	2.033291973	0.10E-03	subuiit	Call
ana DC10				
sps_K516	-	2 5 4 E 00		wan/memorane/en
185	2.023030349	2.34E-09	glycosyl transferase	velope biogenesis
D C10				
sps_KS18	-	5 50F 00	1 (11)	wall/membrane/en
190	2.436568113	5.58E-08	nucleotidyl transferase	velope biogenesis
D C10		0 0002 (7425	CDP-glycerol	
sps_RS18	-	0.000367435	glycerophosphotransfera	wall/membrane/en
195	2.169826984	6292	se	velope biogenesis
DOIO				Cell
sps_RS19	-		type VI secretion system	wall/membrane/en
090	2.645529721	2.27E-06	tip protein VgrG	velope biogenesis
DGA				
sps RS24				Cell
			type VI secretion system	Cell wall/membrane/en
405	-2.06836203	5.78E-05	type VI secretion system tip protein VgrG	Cell wall/membrane/en velope biogenesis
405	-2.06836203	5.78E-05	type VI secretion system tip protein VgrG methyltransferase	Cell wall/membrane/en velope biogenesis
405 sps_RS07	-2.06836203	5.78E-05	type VI secretion system tip protein VgrG methyltransferase domain-containing	Cell wall/membrane/en velope biogenesis
405 sps_RS07 850	-2.06836203 2.149056974	5.78E-05 1.11E-11	type VI secretion system tip protein VgrG methyltransferase domain-containing protein	Cell wall/membrane/en velope biogenesis Coenzyme metabolism
405 sps_RS07 850 sps_RS07	<u>-2.06836203</u> 2.149056974	5.78E-05 1.11E-11	type VI secretion system tip protein VgrG methyltransferase domain-containing protein	Cell wall/membrane/en velope biogenesis Coenzyme metabolism Coenzyme
405 sps_RS07 850 sps_RS07 860	-2.06836203 2.149056974 2.151726239	5.78E-05 1.11E-11 1.34E-16	type VI secretion system tip protein VgrG methyltransferase domain-containing protein biotin synthase BioB	Cell wall/membrane/en velope biogenesis Coenzyme metabolism Coenzyme metabolism
405 sps_RS07 850 sps_RS07 860	-2.06836203 2.149056974 2.151726239	5.78E-05 1.11E-11 1.34E-16	type VI secretion system tip protein VgrG methyltransferase domain-containing protein biotin synthase BioB adenosylmethionine8-	Cell wall/membrane/en velope biogenesis Coenzyme metabolism Coenzyme metabolism
405 sps_RS07 850 sps_RS07 860 sps_RS07	-2.06836203 2.149056974 2.151726239	5.78E-05 1.11E-11 1.34E-16	type VI secretion system tip protein VgrG methyltransferase domain-containing protein biotin synthase BioB adenosylmethionine8- amino-7-oxononanoate	Cell wall/membrane/en velope biogenesis Coenzyme metabolism Coenzyme metabolism
405 sps_RS07 850 sps_RS07 860 sps_RS07 865	-2.06836203 2.149056974 2.151726239 2.019542502	5.78E-05 1.11E-11 1.34E-16 8.92E-07	type VI secretion system tip protein VgrG methyltransferase domain-containing protein biotin synthase BioB adenosylmethionine8- amino-7-oxononanoate transaminase	Cell wall/membrane/en velope biogenesis Coenzyme metabolism Coenzyme metabolism
405 sps_RS07 850 sps_RS07 860 sps_RS07 865 sps_RS13	-2.06836203 2.149056974 2.151726239 2.019542502	5.78E-05 1.11E-11 1.34E-16 8.92E-07	type VI secretion system tip protein VgrG methyltransferase domain-containing protein biotin synthase BioB adenosylmethionine8- amino-7-oxononanoate transaminase type 3 dihydrofolate	Cell wall/membrane/en velope biogenesis Coenzyme metabolism Coenzyme metabolism Coenzyme metabolism Coenzyme
405 sps_RS07 850 sps_RS07 860 sps_RS07 865 sps_RS13 240	-2.06836203 2.149056974 2.151726239 2.019542502 - 2.382932423	5.78E-05 1.11E-11 1.34E-16 8.92E-07 3.16E-11	type VI secretion system tip protein VgrG methyltransferase domain-containing protein biotin synthase BioB adenosylmethionine8- amino-7-oxononanoate transaminase type 3 dihydrofolate reductase	Cell wall/membrane/en velope biogenesis Coenzyme metabolism Coenzyme metabolism Coenzyme metabolism Coenzyme metabolism
405 sps_RS07 850 sps_RS07 860 sps_RS07 865 sps_RS07 865 sps_RS13 240 sps_RS03	-2.06836203 2.149056974 2.151726239 2.019542502 - 2.382932423	5.78E-05 1.11E-11 1.34E-16 8.92E-07 3.16E-11	type VI secretion system tip protein VgrG methyltransferase domain-containing protein biotin synthase BioB adenosylmethionine8- amino-7-oxononanoate transaminase type 3 dihydrofolate reductase	Cell wall/membrane/en velope biogenesis Coenzyme metabolism Coenzyme metabolism Coenzyme metabolism Coenzyme metabolism Energy production
405 sps_RS07 850 sps_RS07 860 sps_RS07 865 sps_RS03 745	-2.06836203 2.149056974 2.151726239 2.019542502 2.382932423 -2.69362479	5.78E-05 1.11E-11 1.34E-16 8.92E-07 3.16E-11 1.19E-11	type VI secretion system tip protein VgrG methyltransferase domain-containing protein biotin synthase BioB adenosylmethionine8- amino-7-oxononanoate transaminase type 3 dihydrofolate reductase isocitrate lyase	Cell wall/membrane/en velope biogenesis Coenzyme metabolism Coenzyme metabolism Coenzyme metabolism Coenzyme metabolism Energy production and conversion
405 sps_RS07 850 sps_RS07 860 sps_RS07 865 sps_RS07 865 sps_RS13 240 sps_RS03 745 sps_RS04	-2.06836203 2.149056974 2.151726239 2.019542502 2.382932423 -2.69362479	5.78E-05 1.11E-11 1.34E-16 8.92E-07 3.16E-11 1.19E-11	type VI secretion system tip protein VgrG methyltransferase domain-containing protein biotin synthase BioB adenosylmethionine8- amino-7-oxononanoate transaminase type 3 dihydrofolate reductase isocitrate lyase cbb3-type cytochrome c	Cell wall/membrane/en velope biogenesis Coenzyme metabolism Coenzyme metabolism Coenzyme metabolism Coenzyme metabolism Energy production and conversion

sps_RS04			cytochrome-c oxidase,	Energy production
555	2.254032868	4.63E-07	cbb3-type subunit II	and conversion
sps_RS07	-			Energy production
560	2.789205715	5.90E-06	hydrogenase	and conversion
sps_RS08	-	0.000481910		Energy production
860	2.247658685	5477	malate synthase	and conversion
sps_RS10				Energy production
985	2.206294141	6.15E-08	isocitrate dehydrogenase	and conversion
sps_RS15			NADH-dependent	Energy production
885	-2.9442779	2.45E-06	alcohol dehydrogenase	and conversion
			sodium ion-translocating	
sps_RS20			decarboxylase subunit	Energy production
125	3.32189275	6.36E-11	beta	and conversion
sps_RS23	-			Energy production
415	3.720547178	8.57E-16	alkene reductase	and conversion
			pyruvate dehydrogenase	
			complex	
sps_RS26			dihydrolipoyllysine-	Energy production
460	2.881707815	5.31E-10	residue acetyltransferase	and conversion
			pyruvate dehydrogenase	
sps_RS26			(acetyl-transferring),	Energy production
465	2.340016067	6.57E-06	homodimeric type	and conversion
			NAD(P)H-dependent	
sps_RS27			glycerol-3-phosphate	Energy production
670	2.814399213	3.47E-08	dehydrogenase	and conversion
sps_RS27			F0F1 ATP synthase	Energy production
845	2.939690752	7.27E-08	subunit epsilon	and conversion
sps_RS27			F0F1 ATP synthase	Energy production
850	2.568897463	1.41E-05	subunit beta	and conversion
sps_RS27			F0F1 ATP synthase	Energy production
855	2.452899459	3.62E-05	subunit gamma	and conversion
sps_RS00	-	0.000100169		Function
385	2.438451695	1601	collagenase	Unknown
sps_RS00	-			Function
480	3.357865272	2.93E-06	hypothetical protein	Unknown
			methyltransferase	
sps_RS00	-	0.000270051	domain-containing	Function
675	3.410372752	2618	protein	Unknown
sps_RS00		0.000562729	·	Function
870	-2.09140705	3187	VUT family protein	Unknown
sps_RS01	-			Function
010	2.068994411	9.02E-09	multidrug efflux protein	Unknown
sps_RS01				Function
100	3.452451363	5.98E-09	hypothetical protein	Unknown

sps_RS01	-	0.000281830		Function
525	2.364678586	8048	hypothetical protein	Unknown
sps_RS02			tol-pal system-associated	Function
490	2.054339731	6.53E-07	acyl-CoA thioesterase	Unknown
sps_RS02	-			Function
645	2.382569799	1.20E-06	hypothetical protein	Unknown
sps_RS04	-			Function
175	2.739588519	3.48E-23	hypothetical protein	Unknown
sps_RS05			type VI secretion system	Function
145	2.021617602	6.90E-05	protein TssA	Unknown
sps_RS05		0.000836798	type VI secretion system	Function
175	2.04013844	4236	lipoprotein TssJ	Unknown
sps_RS06			23S rRNA accumulation	Function
735	2.72571405	1.13E-12	protein YceD	Unknown
sps_RS07	-		YccF domain-containing	Function
010	2.248587365	3.89E-12	protein	Unknown
sps_RS07	-			Function
015	3.016140716	5.36E-10	ABC transporter	Unknown
sps_RS07				Function
765	2.613046822	2.82E-07	curlin	Unknown
sps_RS08				Function
245	2.125520543	9.54E-08	lipase	Unknown
sps_RS08	-	0.000271697		Function
545	2.604867121	6324	N-acetyltransferase	Unknown
sps_RS08	-			Function
915	2.177334425	1.03E-05	hypothetical protein	Unknown
sps_RS08	-		NADP-dependent	Function
925	3.099947187	3.64E-09	oxidoreductase	Unknown
sps_RS09		0.000284560		Function
040	2.22689469	7299	hypothetical protein	Unknown
sps_RS09			AzlD domain-containing	Function
560	2.99160466	3.75E-19	protein	Unknown
sps_RS09		0.000346842		Function
565	2.675003278	2222	NIPSNAP family protein	Unknown
sps_RS09	-			Function
770	2.207295056	8.63E-08	hypothetical protein	Unknown
sps_RS09				Function
985	2.542558234	1.47E-09	ABC-F family ATPase	Unknown
sps_RS10				Function
070	2.49292302	2.99E-19	protease	Unknown
sps_RS10	-		LysM domain-	Function
180	2.362245241	4.66E-05	containing protein	Unknown
sps RS10	_		type VI secretion system	Function
			51 5	

sps_RS10			DUF1611 domain-	Function
355	2.948049625	4.21E-11	containing protein	Unknown
sps_RS11				Function
140	3.386515655	6.90E-09	peptidase	Unknown
sps_RS11				Function
145	2.581952277	1.85E-06	hypothetical protein	Unknown
sps_RS11		0.000112307		Function
485	2.073199428	7603	hypothetical protein	Unknown
sps_RS11	-		DUF2884 domain-	Function
540	2.679444292	1.68E-11	containing protein	Unknown
sps_RS13	-			Function
245	3.274027702	4.44E-19	hypothetical protein	Unknown
sps_RS13	-			Function
420	2.035543108	2.74E-07	NINE protein	Unknown
sps_RS13		0.000131888		Function
985	-2.35758331	119	transposase	Unknown
sps_RS15				Function
065	2.31914063	8.94E-09	adhesin	Unknown
sps_RS15			type I secretion system	Function
070	2.236929601	4.08E-07	permease/ATPase	Unknown
sps RS15				Function
570	2.787310859	4.34E-05	hypothetical protein	Unknown
sps_RS16	-			Function
965	2.189085415	2.51E-05	hypothetical protein	Unknown
sps_RS16		0.000311931		Function
980	-3.26305389	7043	hypothetical protein	Unknown
sps_RS17	-			Function
000	3.829160263	5.31E-10	hypothetical protein	Unknown
sps_RS17	-			Function
005	3.833000674	8.19E-06	hypothetical protein	Unknown
sps_RS17	-			Function
010	2.182859691	1.05E-05	hypothetical protein	Unknown
sps_RS17			DUF2919 domain-	Function
325	2.219727118	3.42E-05	containing protein	Unknown
sps_RS18				Function
960	2.373636069	2.22E-14	hypothetical protein	Unknown
			LysM peptidoglycan-	
sps_RS19	-		binding domain-	Function
080	2.319984805	1.81E-05	containing protein	Unknown
sps_RS19	-		DUF4123 domain-	Function
085	2.833388455	2.46E-07	containing protein	Unknown
sps_RS19	-		type VI secretion system	Function
095	3.346506632	9.82E-14	tube protein Hcp	Unknown
sps_RS19				Function
145	2.023061679	2.05E-07	DoxX family protein	Unknown
sps_RS19	-			Function
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515	3.855546301	3.01E-14	OHCU decarboxylase	Unknown
sps RS19		0.000872634	DUF3604 domain-	Function
870	2.107869645	0514	containing protein	Unknown
sps RS20				Function
300	-2.32652502	5.38E-11	hypothetical protein	Unknown
sps RS21	-	0.000461692		Function
070	2.457959302	9371	hypothetical protein	Unknown
sps RS21			· · ·	Function
845	2.073556007	1.49E-06	hypothetical protein	Unknown
sps_RS23	-		DUF3560 domain-	Function
235	2.391021966	1.36E-07	containing protein	Unknown
sps_RS23	-			Function
400	4.548249722	1.93E-14	SRPBCC family protein	Unknown
sps_RS23	-			Function
405	3.751341329	4.14E-16	hypothetical protein	Unknown
sps_RS23	-			Function
410	3.769934146	3.42E-25	patatin	Unknown
sps_RS24	-		type VI secretion system	Function
400	3.085092994	2.58E-09	tube protein Hcp	Unknown
sps_RS24			ABC transporter ATP-	Function
525	2.135759473	9.42E-12	binding protein	Unknown
sps_RS25	-	0.000868627		Function
410	3.142198139	7586	hypothetical protein	Unknown
sps_RS27				Function
290	2.862005667	2.04E-07	hypothetical protein	Unknown
sps_RS27				Function
295	3.619354663	3.29E-15	hypothetical protein	Unknown
			EscD/YscD/HrpQ family	
			type III secretion system	
sps_RS27			inner membrane ring	Function
310	2.105398212	3.57E-08	protein	Unknown
sps_RS27				Function
350	5.094906906	3.28E-28	hypothetical protein	Unknown
sps_RS27				Function
355	5.07287112	8.24E-31	hypothetical protein	Unknown
			CesD/SycD/LcrH family	
sps_RS27			type III secretion system	Function
360	4.388459415	5.86E-27	chaperone	Unknown
sps_RS27				Function
365	3.40333133	1.42E-18	hypothetical protein	Unknown
sps_RS27		0.000162541		Function
385	2.063279245	0229	hypothetical protein	Unknown
sps_RS27			type III secretion	Function
395	3.457498409	8.19E-11	chaperone SycN	Unknown

			YopN family type III	
sps RS27			secretion system	Function
405	3.724153559	1.23E-19	gatekeeper subunit	Unknown
sps RS27			NAD(P)/FAD-dependent	Function
665	2.163219059	1.50E-07	oxidoreductase	Unknown
				Inorganic ion
sps_RS07	_		cytochrome C biogenesis	transport and
025	3.452734497	1.09E-13	protein CcsA	metabolism
020	51152751157	1.072 12		Inorganic ion
sns RS09			biopolymer transporter	transport and
050	2 401619441	5 75E-06	ExbD	metabolism
	2.101019111	0.,01 00		Inorganic ion
sns RS09	_			transport and
125	2 539404115	1 13E-09	Anion transporter	metabolism
123	2.339 10 1113	1.152 07		Inorganic ion
sps RS10			TonB-dependent	transport and
800	2 2/18756185	7 73E-00	receptor	metabolism
800	2.240730103	7.73L-07	receptor	Incraonic ion
ong DS11			TonP domandant	transport and
sps_K311	2 208520062	1 21E 05	rooptor	matabalism
030	2.308330902	1.211-03	receptor	
and DS12				transment and
sps_K512	-	2 825 06	allealing the substance	transport and
843	2.1/3403138	3.82E-00	arkanne prospratase	
ana DC17			TanD day and ant	Inorganic ion
sps_KS1/	2 75(179229	2 225 00	TonB-dependent	transport and
560	2./364/8238	3.32E-08	receptor	
DCOA				Inorganic ion
sps_RS24	-	7 275 05	. , ,	transport and
/05	2.058354598	/.3/E-05	10n transporter	
DGAT			phosphate ABC	Inorganic ion
sps_RS27	-	4 505 00	transporter substrate-	transport and
765	2.246593006	4.59E-09	binding protein	metabolism
DCOC			MotA/TolQ/ExbB	Intracellular
sps_RS09			proton channel family	trafficking and
055	2.537202941	6.31E-09	protein	secretion
				Intracellular
sps_RS17		0.000254887	protein translocase	trafficking and
775	2.133086832	5961	subunit SecF	secretion
				Intracellular
sps_RS17			protein translocase	trafficking and
780	2.455758424	7.86E-08	subunit SecD	secretion
				Intracellular
sps_RS17			preprotein translocase	trafficking and
785	2.300615414	1.12E-05	subunit YajC	secretion

			EscJ/YscJ/HrcJ family	Intracellular
sps RS27			type III secretion inner	trafficking and
280	2.186301508	1.69E-09	membrane ring protein	secretion
			EscF/YscF/HrpA family	Intracellular
sps RS27			type III secretion system	trafficking and
300	2.749933851	2.76E-05	needle major subunit	secretion
			EscC/YscC/HrcC family	
			type III secretion system	Intracellular
sps RS27			outer membrane ring	trafficking and
315	2.273483267	2.76E-16	protein	secretion
			-	Intracellular
sps RS27			YscX family type III	trafficking and
390	2.597053944	1.28E-08	secretion protein	secretion
			I	Intracellular
sps RS27			protein-export chaperone	trafficking and
675	2.645334886	6.07E-05	SecB	secretion
sps RS01		0.000201240		
105	2.119231787	2357	hypothetical protein	Lipid metabolism
sns RS01	2.11)201707	2007		
110	3 0303685	7 94E-08	hypothetical protein	Lipid metabolism
sns RS01	5.0505000	7.5 12 00	nypetiletieu protein	Lipid metaoonism
115	3 94073512	301F-14	hypothetical protein	Linid metabolism
sps RS26	5.94075512	0.000796974	hypothetical protein	
895_K520	-2 36426423	1748	PAP2 family protein	Linid metabolism
075	$= 2 \cdot 3 0 + 2 0 + 2 3$	1/70	1 Al 2 laining protein	Lipid metabolism
				Nucleotide
sps RS04			adenvlosuccinate	Nucleotide metabolism and
sps_RS04	2 757608805	1 51E-10	adenylosuccinate	Nucleotide metabolism and transport
sps_RS04 270	2.757608805	1.51E-10	adenylosuccinate synthetase	Nucleotide metabolism and transport
sps_RS04 270	2.757608805	1.51E-10	adenylosuccinate synthetase	Nucleotide metabolism and transport Post-translational modification
sps_RS04 270	2.757608805	1.51E-10	adenylosuccinate synthetase	Nucleotide metabolism and transport Post-translational modification, protein turnover
sps_RS04 270	2.757608805	1.51E-10	adenylosuccinate synthetase	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone
sps_RS04 270 sps_RS05	2.757608805	1.51E-10 0.000464036 5808	adenylosuccinate synthetase type VI secretion system	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions
sps_RS04 270 sps_RS05 160	2.757608805 2.183503379	1.51E-10 0.000464036 5808	adenylosuccinate synthetase type VI secretion system ATPase TssH	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational
sps_RS04 270 sps_RS05 160	2.757608805 2.183503379	1.51E-10 0.000464036 5808	adenylosuccinate synthetase type VI secretion system ATPase TssH	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification
sps_RS04 270 sps_RS05 160	2.757608805 2.183503379	1.51E-10 0.000464036 5808	adenylosuccinate synthetase type VI secretion system ATPase TssH	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover
sps_RS04 270 sps_RS05 160	2.757608805 2.183503379	1.51E-10 0.000464036 5808	adenylosuccinate synthetase type VI secretion system ATPase TssH	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone
sps_RS04 270 sps_RS05 160 sps_RS07 585	2.757608805 2.183503379	1.51E-10 0.000464036 5808	adenylosuccinate synthetase type VI secretion system ATPase TssH	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions
sps_RS04 270 sps_RS05 160 sps_RS07 585	2.757608805 2.183503379 2.900592623	1.51E-10 0.000464036 5808 5.54E-06	adenylosuccinate synthetase type VI secretion system ATPase TssH hypothetical protein	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational
sps_RS04 270 sps_RS05 160 sps_RS07 585	2.757608805 2.183503379 2.900592623	1.51E-10 0.000464036 5808 5.54E-06	adenylosuccinate synthetase type VI secretion system ATPase TssH hypothetical protein	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational modification
sps_RS04 270 sps_RS05 160 sps_RS07 585	2.757608805 2.183503379 2.900592623	1.51E-10 0.000464036 5808 5.54E-06	adenylosuccinate synthetase type VI secretion system ATPase TssH hypothetical protein	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein furnover
sps_RS04 270 sps_RS05 160 sps_RS07 585	2.757608805 2.183503379 2.900592623	1.51E-10 0.000464036 5808 5.54E-06	adenylosuccinate synthetase type VI secretion system ATPase TssH hypothetical protein	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone
sps_RS04 270 sps_RS05 160 sps_RS07 585 sps_RS07 830	2.757608805 2.183503379 2.900592623	1.51E-10 0.000464036 5808 5.54E-06	adenylosuccinate synthetase type VI secretion system ATPase TssH hypothetical protein	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions
sps_RS04 270 sps_RS05 160 sps_RS07 585 sps_RS07 830	2.757608805 2.183503379 2.900592623 2.096191537	1.51E-10 0.000464036 5808 5.54E-06 1.01E-06	adenylosuccinate synthetase type VI secretion system ATPase TssH hypothetical protein protease HtpX	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions
sps_RS04 270 sps_RS05 160 sps_RS07 585 sps_RS07 830 sps_RS07	2.757608805 2.183503379 2.900592623 2.096191537	1.51E-10 0.000464036 5808 5.54E-06 1.01E-06	adenylosuccinate synthetase type VI secretion system ATPase TssH hypothetical protein protease HtpX	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational modification protein turnover, chaperone functions
sps_RS04 270 sps_RS05 160 sps_RS07 585 sps_RS07 830 sps_RS08 180	2.757608805 2.183503379 2.900592623 2.096191537	1.51E-10 0.000464036 5808 5.54E-06 1.01E-06	adenylosuccinate synthetase type VI secretion system ATPase TssH hypothetical protein protease HtpX molecular chaperone	Nucleotide metabolism and transport Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions Post-translational modification, protein turnover, chaperone functions

				chaperone
				Tunctions
				Post-translational
				modification,
one RS00				chaperone
sps_K309	2 567339524	1 /0F_08	nentidulnrolul isomerase	functions
205	2.307337324	1.472-00	peptidyipioryi isoinerase	Post-translational
				modification
				protein turnover.
sps RS09				chaperone
215	2.381433794	6.90E-09	endopeptidase La	functions
				Post-translational
				modification,
				protein turnover,
sps_RS10		0.000358126		chaperone
150	2.223985425	277	peroxiredoxin	functions
				Post-translational
				modification,
				protein turnover,
sps_RS11			nucleotide exchange	chaperone
045	2.106795419	3.79E-08	factor GrpE	functions
				Post-translational
				modification,
DC17		0.000(2(515		protein turnover,
sps_KS1/	-	0.000626515	41.:	chaperone
270	2.779791093	5215	thiol peroxidase	Tunctions
				rost-translational
				notein turnover
sps RS18	_			chaperone
045	2 098696208	8 47E-05	nentidylprolyl isomerase	functions
	2.090090200	0.171 03	repring protyr isomorase	Post-translational
				modification.
				protein turnover.
sps RS19			organic hydroperoxide	chaperone
150	-2.88489726	3.40E-09	resistance protein	functions
				Post-translational
				modification,
				protein turnover,
sps_RS20			ATP-dependent zinc	chaperone
985	2.359155945	6.53E-09	metalloprotease FtsH	functions
				Post-translational
sps_RS21			molecular chaperone	modification,
055	2 552907327	1 00F-08	Dnal	protein turnover

				chaperone
				functions
				Post-translational
				modification,
			glutathione-dependent	protein turnover,
sps_RS22			disulfide-bond	chaperone
460	2.697848607	6.26E-13	oxidoreductase	functions
				Post-translational
				modification,
				protein turnover,
sps_RS25			DegQ family serine	chaperone
550	2.364603931	8.99E-13	endoprotease	functions
				Post-translational
				modification,
				protein turnover,
sps_RS25				chaperone
925	2.327738644	4.53E-05	chaperonin GroEL	functions
				Post-translational
				modification,
				protein turnover,
sps_RS25				chaperone
930	2.377174616	1.96E-05	co-chaperone GroES	functions
				Post-translational
				modification,
				protein turnover,
sps_RS26			ATP-dependent protease	chaperone
410	2.895426261	2.45E-14	subunit HslV	functions
				Post-translational
				modification,
				protein turnover,
sps_RS26			ATP-dependent protease	chaperone
415	2.721968851	1.31E-09	ATPase subunit HslU	functions
				Post-translational
				modification,
DGAC				protein turnover,
sps_RS26	0.00(105050		Hsp33 family molecular	chaperone
850	2.326135273	3.09E-06	chaperone HslO	functions
				Post-translational
				modification,
ana DCOZ				protein turnover,
sps_KS2/	5 01529(757	0 COT 01	hymothetical metric	cnaperone
34U	5.015286757	2.02E-31	nypotnetical protein	Tunctions
sps_KS06	-		• • • • • • • • • • • •	Keplication and
100	2.365/01168	4.55E-05	integrase	repair
sps_RS07	-		1 1 1 1	Keplication and
065	2.048/44908	3.59E-05	hypothetical protein	repair

sps_RS07	-	0.000603383		Replication and
090	3.306453599	6821	hypothetical protein	repair
sps RS13	-	0.000251528		Replication and
310	4.057716061	6607	IS256 family transposase	repair
sps RS14	-			Replication and
690	2.202480566	5.78E-05	endonuclease I	repair
sps RS22			DNA polymerase III	Replication and
645	2.07799625	6.73E-07	subunit chi	repair
sps RS22	-			Replication and
930	2.537815092	2.25E-16	hypothetical protein	repair
sps_RS22	-			Replication and
990	2.553880839	1.69E-09	IS30 family transposase	repair
sps RS25	-	0.000585810	phage N-6-adenine-	Replication and
405	2.239026615	9063	methyltransferase	repair
sps_RS01		0.000407240		Secondary
095	2.110059204	3602	hypothetical protein	Structure
sps_RS08				Secondary
660	2.304565309	2.27E-06	reductase	Structure
sps_RS08				Secondary
665	2.668936075	3.42E-07	thioesterase	Structure
sps RS15				Secondary
280	2.074222371	9.55E-07	tandem-95 repeat protein	Structure
			sigma-54-dependent Fis	
sps_RS00	-		family transcriptional	Signal
605	2.423661829	2.99E-13	regulator	Transduction
sps_RS03			DNA-binding response	Signal
915	-2.08519072	9.05E-06	regulator	Transduction
			type VI secretion	
sps_RS05		0.000201256	system-associated FHA	Signal
180	2.253665936	0198	domain protein TagH	Transduction
sps_RS11			methyl-accepting	Signal
275	2.118380441	2.04E-13	chemotaxis protein	Transduction
sps_RS11	-		PAS domain-containing	Signal
800	2.498305045	1.03E-06	protein	Transduction
sps_RS22	-			Signal
745	2.076660325	3.52E-06	response regulator	Transduction
sps_RS00	-		RNA polymerase sigma	
465	2.723170359	5.29E-09	factor FliA	Transcription
			DNA-directed RNA	
sps_RS01			polymerase subunit	
930	2.058575598	3.32E-05	alpha	Transcription
sps_RS09			AraC family	
550	2.215989432	1.94E-06	transcriptional regulator	Transcription
sps_RS09			YafY family	
570	3.044029388	5.92E-44	transcriptional regulator	Transcription

sps_RS09			AraC family	
575	2.789269135	2.65E-07	transcriptional regulator	Transcription
sps RS09	-		GntR family	
965	3.292570998	3.47E-17	transcriptional regulator	Transcription
sps RS12			RNA polymerase sigma	
545	2.326682345	4.72E-06	factor RpoD	Transcription
sps RS14	-		LysR family	
655	2.173970549	7.04E-07	transcriptional regulator	Transcription
sps RS17	-		transcriptional regulator	
430	3.588847108	4.27E-25	BetI	Transcription
sps RS23	-			
225	2.595386474	5.31E-10	hypothetical protein	Transcription
sps RS27			AraC family	
330	2.14769305	1.26E-09	transcriptional regulator	Transcription
sps RS27				
370	3.135921594	1.93E-06	hypothetical protein	Transcription
sps RS01			50S ribosomal protein	
750	2.064605896	5.34E-05	L11	Translation
sps RS01		0.000876705	50S ribosomal protein	
755	2.118288641	5618	L1	Translation
sps RS01			30S ribosomal protein	
780	2.012603546	8.86E-06	S12	Translation
sps RS01				
790	2.569529472	5.49E-08	elongation factor G	Translation
sps RS01			30S ribosomal protein	
915	2.190065274	8.98E-05	S13	Translation
sps RS06			phenylalaninetRNA	
555	2.448467325	6.46E-10	ligase subunit beta	Translation
sps RS06			phenylalaninetRNA	
560	3.10283222	5.49E-08	ligase subunit alpha	Translation
sps RS09				
255	2.130282884	4.57E-11	cysteinetRNA ligase	Translation
			tRNA (guanosine(37)-	
sps_RS11			N1)-methyltransferase	
905	2.400582141	8.38E-07	TrmD	Translation
sps_RS11			ribosome maturation	
910	2.424002401	4.11E-05	factor RimM	Translation
sps_RS11			30S ribosomal protein	
915	2.211626603	2.28E-05	S16	Translation
sps_RS12				
360	2.156367875	9.78E-07	tyrosinetRNA ligase	Translation
sps_RS12		0.000589851	30S ribosomal protein	
530	2.10071334	2769	S21	Translation
sps_RS14			30S ribosomal protein	
235	2.453785596	5.31E-10	S6L-glutamate ligase	Translation

			ribosome-associated	
sps_RS19		0.000136915	translation inhibitor	
945	2.115698622	3752	RaiA	Translation
sps_RS20			translation initiation	
940	2.307679905	1.55E-06	factor IF-2	Translation
			23S rRNA	
sps_RS20			(uridine(2552)-2'-O)-	
990	2.589762127	2.98E-09	methyltransferase RlmE	Translation
sps_RS24				
155	2.162200772	5.73E-08	lysinetRNA ligase	Translation
sps_RS26				
400	2.476358676	5.44E-13	argininetRNA ligase	Translation

	log2FoldCha nge (<0 higher in 4,			
gene	>0 higher in 20)	padj	name	cats
sps_RS02 585	2.432967432	3.68E-16	FAD-binding oxidoreductase	Amino Acid metabolism and transport
sps_RS02 815	-2.62325148	6.55E-09	cystathionine beta- lyase	Amino Acid metabolism and transport
sps_RS03 160	2.082832257	7.00E-05	PLP-dependent cysteine synthase family protein	Amino Acid metabolism and transport
sps_RS03 450	-2.146479288	4.12E-17	sarcosine oxidase subunit gamma family protein	Amino Acid metabolism and transport
sps_RS04 490	-2.889406809	1.16E-07	aspartate/tyrosine/aro matic aminotransferase	Amino Acid metabolism and transport
sps_RS06 510	2.237174457	0.0004314874 391	imidazole glycerol phosphate synthase subunit HisH	Amino Acid metabolism and transport
sps_RS07 005	-2.308603	0.0002489754 345	1- aminocyclopropane- 1-carboxylate deaminase	Amino Acid metabolism and transport
sps_RS08 380	2.152438385	0.0002934225 871	GMC family oxidoreductase	Amino Acid metabolism and transport
sps_RS09 555	3.530787099	2.74E-22	branched-chain amino acid ABC transporter permease	Amino Acid metabolism and transport
sps_RS10 075	-2.10549464	1.66E-05	homoserine O- succinyltransferase	Amino Acid metabolism and transport
sps_RS11 430	-2.942693883	9.00E-13	low-specificity L- threonine aldolase	Amino Acid metabolism and transport
sps_RS11 825	-2.929936891	1.45E-09	bifunctional aspartate kinase/homoserine dehydrogenase I	Amino Acid metabolism and transport

Data S3 Table H: Comparison between late log phase samples from 20°C and 4°C cultures.

			3-deoxy-7-	Amino Acid
sps RS11			phosphoheptulonate	metabolism and
890	-2.495200904	9.94E-06	synthase	transport
			5	Amino Acid
sps RS14			methylenetetrahydrof	metabolism and
5p5_10511	-3 141433946	7 97E-08	olate reductase	transport
555	-3.141433740	7.77L-00		Amino Aoid
and DC14				Amino Aciu
sps_K514	2 752005122	2 095 07	succinymomoserine	metabolism and
303	-2.755095155	3.08E-07	(thiof)-fyase	
DC14				Amino Acid
sps_RS14			HAD-IB family	metabolism and
755	-2.426600049	7.04E-05	hydrolase	transport
			branched-chain	Amino Acid
sps_RS15			amino acid	metabolism and
425	-2.377008819	4.75E-10	transaminase	transport
				Amino Acid
sps RS15			acetolactate synthase	metabolism and
430	-3.153787209	3.68E-14	2 small subunit	transport
				Amino Acid
sps_RS15		0 0001858064	acetolactate synthase	metabolism and
435	-2 122386236	363	2 catalytic subunit	transport
433	-2.122300230	505	2 catalytic subulit	Amino Aoid
and DS15			Iratal and	Ammo Actu
sps_K515	2 00151(74(0 425 00		metabolism and
440	-2.991310/40	9.42E-08	reductoisomerase	
Date				Amino Acid
sps_RS16			2-isopropylmalate	metabolism and
220	-2.172148186	2.42E-12	synthase	transport
			dihydrodipicolinate	Amino Acid
sps_RS16			synthase family	metabolism and
775	-3.277195875	2.41E-31	protein	transport
			serine	Amino Acid
sps RS20			hydroxymethyltransf	metabolism and
350	-2.288885307	1.20E-07	erase	transport
				Amino Acid
sps RS22			LysE family	metabolism and
605	-3.937882589	3.82E-06	translocator	transport
				Amino Acid
sns RS26			argininosuccinate	metabolism and
665	-2 821317124	6 38F_00	lvase	transnort
005	2.021317124	0.301-09	19000	Amino Acid
and DCOC			anginingguaginata	matahalian and
sps_K520	2 1 (07522 (0		argininosuccinate	metabolism and
0/0	-2.100/53368	8.98E-06	syntnase	transport
Dene			1 1 1 1 1	Carbohydrate
sps_RS03			glucan 1,4-alpha-	metabolism and
280	2.427088679	5.25E-05	glucosidase	transport

				Carbohydrate
sps_RS19				metabolism and
520	-2.66578705	1.75E-07	allantoinase PuuE	transport
				Carbohydrate
sps_RS20				metabolism and
400	-2.335405937	1.54E-07	chitinase	transport
sps_RS26				Cell cycle control
405	2.219417589	9.36E-11	sporulation protein	and mitosis
sps_RS01			PAS domain-	
230	3.049676229	1.20E-05	containing protein	Cell motility
sps_RS03		0.0001935587		
520	2.155648326	614	flagellin	Cell motility
sps_RS17				
255	-5.320852604	1.63E-14	hypothetical protein	Cell motility
sps_RS21				
855	2.06242213	2.54E-05	hypothetical protein	Cell motility
			EscN/YscN/HrcN	
			family type III	
sps_RS27			secretion system	
410	3.29631472	1.38E-10	ATPase	Cell motility
			YscQ/HrcQ family	
sps_RS27			type III secretion	
425	2.362221446	1.40E-07	apparatus protein	Cell motility
				Cell
sps_RS01			LTA synthase family	wall/membrane/env
180	2.322175038	3.00E-24	protein	elope biogenesis
			efflux RND	
			transporter	Cell
sps_RS05			periplasmic adaptor	wall/membrane/env
215	2.21295443	9.58E-10	subunit	elope biogenesis
				Cell
sps_RS05		0.0003800328		wall/membrane/env
385	-2.097023326	242	hypothetical protein	elope biogenesis
				Cell
sps_RS06			D-alanineD-alanine	wall/membrane/env
170	-2.290620345	2.27E-08	ligase	elope biogenesis
				Cell
sps_RS07			mechanosensitive ion	wall/membrane/env
000	2.184837644	6.05E-15	channel protein MscS	elope biogenesis
				Cell
sps_RS09				wall/membrane/env
080	-2.505318639	7.29E-06	porin	elope biogenesis
				Cell
sps_RS09				wall/membrane/env
305	2.70757643	4.37E-05	hypothetical protein	elope biogenesis

sps_RS12				Cell wall/membrane/env
855	2.851965957	9.41E-07	LrgB family protein	elope biogenesis
				Cell
sps_RS15	2 507014050	1 105 16	1,	wall/membrane/env
080	3.507014058	1.10E-15	agglutination protein	elope biogenesis
ong PS15				Cell wall/membrane/env
295	2.112759757	4.43E-06	channel protein TolC	elope biogenesis
				Cell
sps_RS20				wall/membrane/env
885	-2.838836009	4.43E-06	hypothetical protein	elope biogenesis
sps_RS05			thiamine biosynthesis	Coenzyme
830	-3.098180536	1.02E-07	protein ThiS	metabolism
ong DS07			4- hydroxyphonylnymyy	Coonzumo
5ps_K307 040	-2 168044418	1 42E-07	ate dioxygenase	metabolism
	2.100011110	1.121.07	methyltransferase	
sps RS07			domain-containing	Coenzyme
850	2.01750249	3.89E-10	protein	metabolism
			8-amino-7-	
sps_RS07	0 (7000 (404	2 005 22	oxononanoate	Coenzyme
855 ama DS07	2.670996484	2.09E-23	synthase	metabolism
sps_KS07 860	2 24594267	9 39F-18	hiotin synthase BioB	metabolism
sps_RS01	2.2-139-1207).5)E 10	olotini syntilase DioD	Energy production
075	2.883998093	1.04E-07	hypothetical protein	and conversion
sps_RS01			aldehyde	Energy production
610	-4.303511554	3.61E-11	dehydrogenase	and conversion
sps_RS03				Energy production
745	-3.62477364	4.27E-21	isocitrate lyase	and conversion
sps_KS04	2 101286572	1 56E 10	alcohol	Energy production
705	-3.494200372	1.301-10	electron transport	
sps_RS05			complex subunit	Energy production
675	2.420291361	2.46E-12	RsxB	and conversion
			electron transport	
sps_RS05			complex subunit	Energy production
680	2.054928972	2.98E-08	RsxC	and conversion
ana DOOS			electron transport	Farmers and 14
sps_KSU3 685	2 437428107	7 09F_10	Reserved Subunit	and conversion
sps RS08	2.437420107	7.071-10		Energy production
005	-2.707442742	4.83E-12	citrate synthase	and conversion

sps RS08				Energy production
860	-3.31396699	4.71E-08	malate synthase	and conversion
sps RS09			cystathionine beta-	Energy production
300	3.427884457	1.08E-08	synthase	and conversion
sps RS09				Energy production
310	2.277455159	4.83E-05	cytochrome C	and conversion
			SDR family	
sps_RS15			NAD(P)-dependent	Energy production
005	-4.50922875	6.16E-16	oxidoreductase	and conversion
			NADH-quinone	
sps_RS17		0.0001779416	oxidoreductase	Energy production
495	2.887194427	287	subunit NuoC/D	and conversion
			NADH	
sps_RS17		0.0001168160	oxidoreductase	Energy production
505	3.883386137	13	(quinone) subunit F	and conversion
			NADH	
sps_RS17		0.0006500355	dehydrogenase	Energy production
510	2.1576288	765	(quinone) subunit G	and conversion
			NADH-quinone	
sps_RS17			oxidoreductase	Energy production
520	3.834237896	2.94E-05	subunit NuoI	and conversion
sps_RS18				Energy production
985	-2.606652119	6.55E-09	malate synthase A	and conversion
sps_RS19				Energy production
850	2.891238878	6.15E-07	hypothetical protein	and conversion
			NAD(P)H-dependent	
sps_RS27			glycerol-3-phosphate	Energy production
670	2.592397258	4.16E-07	dehydrogenase	and conversion
sps_RS27			F0F1 ATP synthase	Energy production
870	2.101067784	6.14E-07	subunit B	and conversion
			SDR family	
sps_RS00		0.0009825280	NAD(P)-dependent	
050	-2.577267	082	oxidoreductase	Function Unknown
			putative sulfate	
sps_RS00			exporter family	
895	2.826129795	8.34E-34	transporter	Function Unknown
sps_RS01				
100	4.389501481	2.23E-10	hypothetical protein	Function Unknown
sps_RS01			SURF1 family	
275	2.22923224	7.32E-06	protein	Function Unknown
sps_RS02			DUF4336 domain-	
200	-2.079402124	1.53E-10	containing protein	Function Unknown
sps_RS02			DUF1302 domain-	
895	3.426785493	2.42E-12	containing protein	Function Unknown

sps_RS03			SpoVR family	
030	-3.221569136	4.89E-09	protein	Function Unknown
sps_RS03				
035	-3.317282472	1.84E-07	hypothetical protein	Function Unknown
sps_RS03			AcrB/AcrD/AcrF	
135	2.077704014	2.11E-06	family protein	Function Unknown
sps_RS03				
275	2.052588717	1.14E-10	hypothetical protein	Function Unknown
sps_RS04				
300	2.017569937	2.78E-12	hypothetical protein	Function Unknown
sps_RS04				
385	-3.34560232	1.24E-10	hypothetical protein	Function Unknown
sps_RS04				
390	-2.436963057	2.87E-09	N-acetyltransferase	Function Unknown
sps_RS04			KR domain-	
635	-2.088956496	3.30E-05	containing protein	Function Unknown
sps_RS04			type III secretion	
880	-2.465666497	4.94E-07	apparatus	Function Unknown
			type VI secretion	
sps_RS05		0.0004842217	system PAAR	D 1 1 1
080	2.246990291	867	protein	Function Unknown
DGOG		0.0001207006	type VI secretion	
sps_RS05	2 745400400	0.000138/996	system tube protein	
130 DC05	-2./45409498	399	Hcp	Function Unknown
sps_RS05	0 70055004	5 525 07	META domain-	F
223 DS05	-2.73255384	5.52E-07	containing protein	Function Unknown
sps_KS05	2 220155774	2.945.09	VtoO family motoin	Enn etien Hulmenn
430 DS0(-2.220133774	2.84E-08	Y loQ family protein	Function Unknown
sps_K506	2 662820008	0.15E.05	DUF29/5 domain-	Function Unknown
150 ang PS07	-2.003820908	9.13E-03	containing protein	Function Unknown
sps_K307	2 153068555	1 88E 05	ABC transporter	Function Unknown
$\frac{013}{\text{sps}}$ PS07	-2.133908333	1.88E-05	ADC transporter	
205	-2 022633894	4 40F-05	hypothetical protein	Function Unknown
sps RS07	2.022033074	0.0005612003	nypotnetieur protein	
690	-2 379338868	0.0003012003	hypothetical protein	Function Unknown
sps RS07	2.379330000	000	nypoineirear protein	
765	2 437462568	1 98 F- 06	curlin	Function Unknown
sps RS08		1.502.00	MBL fold metallo-	
035	2.285969608	1.00E-06	hydrolase	Function Unknown
sps RS08		1.002.00		
150	2.070443021	9.16E-08	hypothetical protein	Function Unknown
sps RS08			J1 Protein	
245	2.170047659	4.44E-08	lipase	Function Unknown

sps_RS08 455	-2.220241886	2.31E-06	hypothetical protein	Function Unknown
sps_RS08 545	-3.12456507	5.36E-05	N-acetyltransferase	Function Unknown
sps_RS09 320	2.793261752	1.14E-05	cvtochrome C	Function Unknown
sps_RS09	3 337708202	6 90F-23	AzlD domain-	Function Unknown
sps RS09	5.557700202	0.0009266646	NIPSNAP family	
565	2.478001394	586	protein	Function Unknown
sps RS09		0.0001693507	amphi-Trp domain-	
620	-2.560594684	442	containing protein	Function Unknown
sps RS09			GNAT family N-	
825	-2.025967941	4.92E-09	acetyltransferase	Function Unknown
sps_RS10 070	2.229095898	1.19E-15	protease	Function Unknown
sps_RS10 195	-5.611808363	2.89E-40	type VI secretion system tube protein Hcp	Function Unknown
sps RS10			1	
335	2.021844539	1.88E-05	acyltransferase	Function Unknown
sps_RS10			DUF1611 domain-	
355	2.488481358	4.64E-08	containing protein	Function Unknown
sps_RS11 140	3.48294448	1.83E-09	peptidase	Function Unknown
sps_RS11 145	3.0291171	8.07E-09	hypothetical protein	Function Unknown
sps_RS11 150	2.135676497	4.06E-05	PKD domain- containing protein	Function Unknown
sps_RS11				
395	2.498869509	3.15E-09	hypothetical protein	Function Unknown
sps_RS11			DUF469 domain-	
550	-3.418547846	3.16E-05	containing protein	Function Unknown
sps_RS11 785	2.140951315	6.37E-05	DUF3545 domain- containing protein	Function Unknown
sps_RS12				
740	2.12418513	2.76E-08	flotillin	Function Unknown
sps_RS12 840	-2 016008953	1 27E-05	hypoxanthine phosphoribosyltransf erase	Function Unknown
sns RS12	2.0100000000	0.0002859681		
860	3.113128985	946	hypothetical protein	Function Unknown
sps RS13		210		
330	-2.018703658	3.91E-20	hypothetical protein	Function Unknown

sps_RS14		0.0003287139	DUF5062 domain-	
215	-2.068149672	46	containing protein	Function Unknown
sps_RS15				
000	-7.381744578	1.16E-17	phasin family protein	Function Unknown
sps_RS15				
065	3.92002712	3.00E-24	adhesin	Function Unknown
			type I secretion	
sps_RS15	4.01000.045.0	1.0.00	system	T 1 T 1
070	4.219326456	1.96E-23	permease/ATPase	Function Unknown
DC15			type I secretion	
sps_RS15	2 701 402017	1 205 21	system	
285 DC15	2./9140281/	1.39E-21	permease/ATPase	Function Unknown
sps_KS15	2 472254016	4 72E 10	nhagin family protain	Function Unlynown
093	-2.4/3334910	4.75E-10	phasm ranning protein	Function Unknown
sps_K317	2 286215213	0.0002344019	hypothetical protain	Function Unknown
$\frac{000}{\text{sps}}$ RS17	-2.200213213	231	DUE1851 domain	
3ps_K317 110	-2 862382028	8 66E-07	containing protein	Function Unknown
sns RS17	2.002302020	0.001 07	DUF3164 domain-	
135	2 807805055	1 91E-07	containing protein	Function Unknown
sps_RS17	2.007002022	0.0005891068	MBL fold metallo-	
295	-2.612633074	503	hydrolase	Function Unknown
sps RS18				
960	2.014079869	1.53E-10	hypothetical protein	Function Unknown
			type VI secretion	
sps_RS19			system tube protein	
095	-4.420059061	4.93E-24	Нср	Function Unknown
sps_RS19			OHCU	
515	-3.072554762	3.44E-09	decarboxylase	Function Unknown
sps_RS19				
855	2.295386358	2.14E-06	hypothetical protein	Function Unknown
sps_RS19				
865 DC10	2.270814515	7.08E-07	hypothetical protein	Function Unknown
sps_RS19	2 200700244	2 705 00	DUF3604 domain-	
870 DC10	3.309/89244	2.70E-08	containing protein	Function Unknown
sps_KS19	2 500552626	1.62E-16	peptidyl-prolyl cis-	Enn stinn Hulmorry
8/3	2.309333030	1.03E-10	trans isomerase	Function Unknown
sps_K519	1 256068721	A 52E 11	hypothetical protain	Function Unknown
sns RS20	7.230908734	4 .55Ľ-11	$\frac{1}{1} \frac{1}{1} \frac{1}$	
500	2 15708208	3 05F-05	nrotein	Function Unknown
sns RS20	2.13700200	0.0001145200	DUF3019 domain_	
505	2,140126738	855	containing protein	Function Unknown
sps_RS21	2.110120790		eentuning protoni	
315	2 146389124	1.81E-06	hypothetical protein	Function Unknown

			tripartite	
sps RS21		0.0008861930	tricarboxylate	
770	2.033422272	531	transporter TctA	Function Unknown
			tripartite	
			tricarboxylate	
sps_RS21			transporter substrate	
780	2.509567189	6.14E-06	binding protein	Function Unknown
sps RS21				
845	2.132905791	6.51E-07	hypothetical protein	Function Unknown
sps RS21			GNAT family N-	
990	-2.385598881	1.57E-05	acetyltransferase	Function Unknown
sps RS22		0.0001352607		
115	2.41744448	219	hypothetical protein	Function Unknown
sps RS22		0.0006730640	DUF4255 domain-	
275	-3.089386699	067	containing protein	Function Unknown
sps_RS22			8F	
465	2.046785643	9.42E-08	hypothetical protein	Function Unknown
sps_RS22		<i></i>	HlvD family	
815	2.458659705	1.58E-06	secretion protein	Function Unknown
sns RS23	2.100003700	1.002.00	SRPBCC family	
3p3_1(323 400	-4 066881676	3 61F-11	protein	Function Unknown
sns RS23	1.000001070	5.01L 11	protein	
3p3_1(525 405	-2 204859237	4 00F-06	hypothetical protein	Function Unknown
sns RS23	2.204037237	4.001 00	nypotnetieur protein	
3p3_K525 410	-2 791142135	1 21F-13	natatin	Function Unknown
sns RS23	2.791112133	0.0002012957	pututin	
810	-2 332394833	584	hypothetical protein	Function Unknown
010	2.332374033	504	type VI secretion	
sns RS24			system tube protein	
3p3_1(524 400	-4 365802519	2 43F-18	Hcn	Function Unknown
$rac{100}{r$	4.303002317	2.4512 10	DUE2170 domain-	
sps_K524 685	-3 551423386	6 93E-07	containing protein	Function Unknown
enc RS2/	3.331423300	0.751-07	containing protoin	
sps_K324 605	-2 358368825	$1.32F_{-}10$	hypothetical protein	Function Unknown
075	-2.550500025	1.52E-10	TAT leader	
ene RS24			containing	
sps_K324	2 140214504	4 87E 05	containing	Function Unknown
090	-2.149514594	4.0/E-03	DUE602 domain	
sps_K520	2 272201061	1 45 0 06	DUF092 domain-	Eunstian Unknown
JIJ	5.575261601	1.43E-00	DI 152292 damain	
sps_K520	4 121122102	1 605 05	DUF2282 domain-	Function L'ulmour
70U	4.121123102	1.08E-05	containing protein	runction Unknown
sps_KS2/	2 522642702		have athentical matrix	Eurotion L'ul-
290	2.532643793	4.64E-06	nypotnetical protein	runction Unknown
sps_RS27	0.0000000	1 205 05	1 .1 1	T. (* TT 1
295	2.069638451	1.30E-05	hypothetical protein	Function Unknown

sps_RS27	0.005000104	2 445 06	1 ,1 , 1 , .	
330 ama DS27	2.285903194	2.44E-06	nypothetical protein	Function Unknown
355 sps_K527	2.433883181	1.14E-07	hypothetical protein	Function Unknown
			CesD/SycD/LcrH	
one RS27			iamily type III	
360	2.068811397	5.89E-07	chaperone	Function Unknown
sps RS27	2.000011337	5.072 07		
385	2.761816979	8.17E-07	hypothetical protein	Function Unknown
sps_RS27			type III secretion	
395	2.863663393	8.73E-08	chaperone SycN	Function Unknown
			YopN family type III	
sps_RS27	2.051025412	0.005.07	secretion system	
405	2.051835412	8.80E-07	gatekeeper subunit	Function Unknown
sns RS07			biogenesis protein	Inorganic ion
025	-2.008958713	4.23E-05	CcsA	metabolism
			rhodanese-like	Inorganic ion
sps_RS08			domain-containing	transport and
845	-2.708764964	2.87E-09	protein	metabolism
				Inorganic ion
sps_RS09	2 00051 4120		TonB-dependent	transport and
075	3.800/14138	2.09E-23	receptor	metabolism
and DS10			TonP domandant	Inorganic ion
sps_K310 800	2 203399361	1 62E-08	receptor	metabolism
	2.203377301	1.021 00		Inorganic ion
sps RS10			phosphate-binding	transport and
900	-2.419258938	5.87E-10	protein	metabolism
				Inorganic ion
sps_RS19	2 172001407		1 10	transport and
860	3.1/299149/	8.56E-09	arylsulfatase	
ene RS27			transporter substrate-	Inorganic ion
3p3_1(327 765	-2.301580733	1.83E-09	binding protein	metabolism
100		1.002.03	emeng protein	Intracellular
sps_RS11		0.0004489343	pilus assembly	trafficking and
690	2.696052531	168	protein PilX	secretion
			type IV pilus	Intracellular
sps_RS11	0.000040452	2 225 00	modification protein	trafficking and
/00	2.988940453	3.33E-08	P1IV	secretion
sns RS15			niyD lamily type I	Intracentular
075	4.492391622	2.29E-13	adaptor subunit	secretion

				Intracellular
sps RS26			type II/IV secretion	trafficking and
330	2.15873685	1.46E-09	system protein	secretion
			× 1	Intracellular
sps RS26				trafficking and
340	2.241358532	1.04E-06	AAA family ATPase	secretion
		110.12.00	type IV-A pilus	Intracellular
sps RS26			assembly ATPase	trafficking and
3p3_10520 495	2 90865955	3 32F-15	PilR	secretion
475	2.90003933	5.52E 15	EscE/VscE/HrnA	secretion
			family type III	Introcellular
and DS27		0 0002030003	family type m	trafficking and
sps_K327	2 10812268	0.0002030993	noodlo major subunit	correction
300	2.40043200	033	Free C/Vree C/Ure C	secretion
			EscU/Y scU/HrcU	
			family type III	T . 11 1
DGOT			secretion system	Intracellular
sps_RS27	• • • • • • • • •		outer membrane ring	trafficking and
315	2.09414861	8.37E-14	protein	secretion
			EscV/YscV/HrcV	
			family type III	
			secretion system	Intracellular
sps_RS27			export apparatus	trafficking and
380	2.74244719	4.54E-18	protein	secretion
				Intracellular
sps_RS27		0.0001654802		Intracellular trafficking and
sps_RS27 415	2.981590005	0.0001654802 532	hypothetical protein	Intracellular trafficking and secretion
sps_RS27 415	2.981590005	0.0001654802 532	hypothetical protein EscS/YscS/HrcS	Intracellular trafficking and secretion
sps_RS27 415	2.981590005	0.0001654802 532	hypothetical protein EscS/YscS/HrcS family type III	Intracellular trafficking and secretion
sps_RS27 415	2.981590005	0.0001654802 532	hypothetical protein EscS/YscS/HrcS family type III secretion system	Intracellular trafficking and secretion Intracellular
sps_RS27 415 sps_RS27	2.981590005	0.0001654802 532	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus	Intracellular trafficking and secretion Intracellular trafficking and
sps_RS27 415 sps_RS27 435	2.981590005 3.439431307	0.0001654802 532 8.71E-06	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein	Intracellular trafficking and secretion Intracellular trafficking and secretion
sps_RS27 415 sps_RS27 435 sps_RS01	2.981590005 3.439431307	0.0001654802 532 8.71E-06	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein	Intracellular trafficking and secretion Intracellular trafficking and secretion
sps_RS27 415 sps_RS27 435 sps_RS01 090	2.981590005 3.439431307 2.708564244	0.0001654802 532 8.71E-06 6.74E-07	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01	2.981590005 3.439431307 2.708564244	0.0001654802 532 8.71E-06 6.74E-07	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105	2.981590005 3.439431307 2.708564244 3.443090214	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105 sps_RS01	2.981590005 3.439431307 2.708564244 3.443090214	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105 sps_RS01 110	2.981590005 3.439431307 2.708564244 3.443090214 3.589755078	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10 1 53E-10	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105 sps_RS01 110 sps_RS01	2.981590005 3.439431307 2.708564244 3.443090214 3.589755078	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10 1.53E-10	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 110 sps_RS01 110 sps_RS01 115	2.981590005 3.439431307 2.708564244 3.443090214 3.589755078 3.726402891	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10 1.53E-10 1.26E-12	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein hypothetical protein	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105 sps_RS01 110 sps_RS01 115 sps_PS02	2.981590005 3.439431307 2.708564244 3.443090214 3.589755078 3.726402891	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10 1.53E-10 1.26E-12	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein hypothetical protein	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105 sps_RS01 110 sps_RS01 115 sps_RS08 825	2.981590005 3.439431307 2.708564244 3.443090214 3.589755078 3.726402891	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10 1.53E-10 1.26E-12	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein hypothetical protein	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105 sps_RS01 110 sps_RS01 115 sps_RS08 835	2.981590005 3.439431307 2.708564244 3.443090214 3.589755078 3.726402891 -3.283606596	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10 1.53E-10 1.26E-12 5.99E-18	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein hypothetical protein hypothetical protein	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism Lipid metabolism Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105 sps_RS01 115 sps_RS01 115 sps_RS08 835	2.981590005 3.439431307 2.708564244 3.443090214 3.589755078 3.726402891 -3.283606596	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10 1.53E-10 1.26E-12 5.99E-18	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein hypothetical protein hypothetical protein transporter class I poly(R)-	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism Lipid metabolism Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105 sps_RS01 110 sps_RS01 115 sps_RS08 835 sps_RS14 005	2.981590005 3.439431307 2.708564244 3.443090214 3.589755078 3.726402891 -3.283606596	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10 1.53E-10 1.26E-12 5.99E-18	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein hypothetical protein hypothetical protein transporter class I poly(R)- hydroxyalkanoic acid	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105 sps_RS01 110 sps_RS01 115 sps_RS08 835 sps_RS14 995	2.981590005 3.439431307 2.708564244 3.443090214 3.589755078 3.726402891 -3.283606596 -3.442924677	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10 1.53E-10 1.26E-12 5.99E-18 2.31E-20	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein hypothetical protein hypothetical protein transporter class I poly(R)- hydroxyalkanoic acid synthase	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism Lipid metabolism Lipid metabolism
sps_RS27 415 sps_RS27 435 sps_RS01 090 sps_RS01 105 sps_RS01 115 sps_RS08 835 sps_RS14 995 sps_RS21	2.981590005 3.439431307 2.708564244 3.443090214 3.589755078 3.726402891 -3.283606596 -3.442924677	0.0001654802 532 8.71E-06 6.74E-07 2.70E-10 1.53E-10 1.26E-12 5.99E-18 2.31E-20	hypothetical protein EscS/YscS/HrcS family type III secretion system export apparatus protein hypothetical protein hypothetical protein hypothetical protein hypothetical protein transporter class I poly(R)- hydroxyalkanoic acid synthase	Intracellular trafficking and secretion Intracellular trafficking and secretion Lipid metabolism Lipid metabolism Lipid metabolism Lipid metabolism

			anaerobic	
			ribonucleoside-	Nucleotide
sps_RS08			triphosphate	metabolism and
910	-2.435155858	3.14E-15	reductase	transport
				Post-translational
D G O 1			YJJW family glycine	modification,
sps_RS01	2 2107(054	0.455.07	radical enzyme	protein turnover,
600	3.319766854	8.45E-07	activase	chaperone functions
				Post-translational
DGOO			11 1 1 1 1 1	modification,
sps_RS02	0.405170105	1.245.00	alkyl hydroperoxide	protein turnover,
470	-2.485172135	1.34E-08	reductase	chaperone functions
				Post-translational
DGOO				modification,
sps_RS03	2 710025025	0.005.07	peptide-methionine	protein turnover,
850	-2.710025025	9.99E-07	(S)-S-oxide reductase	chaperone functions
				Post-translational
Daac				modification,
sps_RS06	2 2222 2 (0 40			protein turnover,
075	3.222826849	4.64E-08	DsbA family protein	chaperone functions
				Post-translational
DCOT		0.00000000		modification,
sps_RS07	2 591504225	0.0006686637	1 1 1 1 1 1	protein turnover,
320	-3.381304333	482	hypothetical protein	chaperone functions
				Post-translational
DC00				modification,
sps_KS09	2 017125064	2 795 05	hypethetical matein	protein turnover,
313	2.91/123904	2.78E-03	nypotnetical protein	Dest translational
				Post-translational
and DS17				modification,
sps_K317	2 021602202	4 28E 07	thial paravidasa	protein turnover,
270	-3.921002293	4.201-07	unor peroxidase	Doct translational
				rost-translational
sps PS27				nrotain turnover
340	2 0022/38/5	3 27E-06	hypothetical protein	chaperone functions
sps PS00	2.072243043	5.2712-00	DNA protecting	Replication and
375	3 235764735	3 55E-09	nrotein DnrA	repair
sps RS06	5.255707755	5.5512-07	evodeovyribonucleas	Replication and
065	2 327830814	3 79F_07	e V subunit heta	renair
sps RS06	2.527050014	5.772.07	evodeoxyribonucleas	Replication and
070	2 513452333	2 20F-07	e V suhunit alnha	renair
sns RS07	2.515152555	2.201-07	PKD domain-	Replication and
515 1 5	2 113235101	2 69E-05	containing protein	renair
sns RS08	2.113233101	2.071 03	transcription-repair	Replication and
100	2 014379309	2 13E-07	counling factor	renair
100	2.01.379509	2.1307	apring racion	· · · · · · · · · · · · · · · · · · ·

sps_RS08			DNA topoisomerase	Replication and
570	2.296125413	4.00E-08	III	repair
			recombination-	
sps_RS10			associated protein	Replication and
920	-2.688446282	6.67E-06	RdgC	repair
sps_RS13		0.0006362498	IS256 family	Replication and
310	-3.998922105	297	transposase	repair
			group II intron	
			reverse	
sps_RS13			transcriptase/maturas	Replication and
960	2.487163749	2.13E-07	e	repair
sps_RS13		0.0007613934		Replication and
980	2.508998287	646	hypothetical protein	repair
			group II intron	
			reverse	
sps_RS16			transcriptase/maturas	Replication and
750	3.612384475	6.28E-17	e	repair
sps_RS17				Replication and
155	2.503316519	2.68E-09	ATP-binding protein	repair
sps_RS19		0.0001144997		Replication and
405	2.451203332	91	hypothetical protein	repair
sps_RS23			IS66 family	Replication and
060	3.113012122	7.04E-06	transposase	repair
sps_RS01				
085	2.80898152	1.97E-07	hypothetical protein	Secondary Structure
sps_RS01				
095	3.353664761	3.44E-09	hypothetical protein	Secondary Structure
sps_RS08				
660	2.625786757	5.81E-08	reductase	Secondary Structure
sps_RS08		0.0001393987		
665	2.031948858	896	thioesterase	Secondary Structure
sps_RS15			tandem-95 repeat	
280	2.710056353	4.62E-11	protein	Secondary Structure
sps_RS03			PrkA family serine	
040	-3.650389943	5.43E-10	protein kinase	Signal Transduction
sps_RS05			GGDEF domain-	
495	-2.371953436	1.23E-06	containing protein	Signal Transduction
sps_RS07		_	ANTAR domain-	
805	-2.119680762	7.86E-05	containing protein	Signal Transduction
sps_RS11			methyl-accepting	
275	2.472278492	2.37E-18	chemotaxis protein	Signal Transduction
sps_RS20			DNA-binding	
510	2.659090494	1.27E-05	response regulator	Signal Transduction

			two-component	
sps_RS20			sensor histidine	
515	2.532492669	7.37E-07	kinase	Signal Transduction
sps_RS20			HDOD domain-	
610	2.374815581	1.62E-05	containing protein	Signal Transduction
			helix-turn-helix	
sps_RS07		0.0002751965	transcriptional	
760	2.376809105	031	regulator	Transcription
			AraC family	
sps_RS09			transcriptional	
550	3.207724158	1.03E-12	regulator	Transcription
			YafY family	
sps RS09			transcriptional	
570	3.795111604	5.06E-68	regulator	Transcription
			AraC family	
sps RS09			transcriptional	
575	2.577525217	2.21E-06	regulator	Transcription
sps_RS14			DNA-binding	
035	2.530147865	2.16E-08	response regulator	Transcription
			TetR family	
sps RS15			transcriptional	
345	-2.045666298	3.99E-05	regulator	Transcription
sps RS17			transcriptional	
125	2.954632007	8.07E-09	regulator	Transcription
			LysR family	
sps_RS22			transcriptional	
055	-2.586561867	1.04E-09	regulator	Transcription
sps RS24			phage shock protein	
690	-2.158612464	3.79E-20	A	Transcription
sps_RS26		0.0004253600	RNA polymerase	
965	2.975601593	056	sigma factor	Transcription
sps_RS27				
370	2.858287534	1.09E-05	hypothetical protein	Transcription
sps_RS08				
515	-2.384737104	2.09E-15	N-acetyltransferase	Translation
sps_RS10				
475	-2.252301132	4.95E-07	elongation factor Ts	Translation

	log2FoldCh ange (<0 higher in 4,			
gene	>0 higher in	nadi	name	cate
gene	20)	pauj	hifunctional asportato	Amino Aoid
ene PS11			kinase/homoserine	metabolism and
825	- 2.086325517	5 10E-05	debydrogenase I	transport
023	2.000323317	J.10L-0J		Amino Acid
ene PS13			PKD domain containing	metabolism and
sps_K313	- 2 285055658	$2.01E_{-}17$	nrotein	transport
170	2.203733030	2.011-17	protein	Amino Acid
and DS08			anthranilata synthese	motobolism and
sps_K508	2 536604478	2 00E 00	antifiannate Synthase	transport
200	2.330004478	2.901-09		Amino Asid
and DS09			tuna 1 alutamina	motobolism and
sps_K500	2 100072052	2 95E 05	type i glutamme	transport
203	2.100972033	5.63E-05	annuouransierase	Amino Asid
and DS09			antinamate phosphorihogyltrongforg	motobolism and
sps_K508	2 051722695	9 05E 05	phosphoribosyltransferas	metabolism and
290	2.031/32083	8.93E-03		transport
			bifunctional indole-3-	
			glycerol-phosphate	Amina Aaid
and DC09			Tran C/mhoon horihogy long	Ammo Acia motobolism and
sps_K508	2 775000405	1 12E 00	herenilate isomerses Tre	metabolism and
293	2.773880403	1.12E-09	Infamiliate isomerase Trpr	
and DCO9				Amino Acid
sps_K508	2 672805400	1 09E 12	suburit hete	metabolism and
300	2.0/2893499	1.96E-12	subunit beta	
and DCO9				Amino Acid
sps_KS08	2 425770529	5 225 07	tryptopnan synthase	metabolism and
303	2.423779328	3.33E-07	subunit alpha	
ana DCOO				Amino Acid
sps_RS09	2 050004942	1 21E 07		metabolism and
343	2.039004842	1.31E-07		
ana DOOO			oranched-chain amino	Amino Acid
sps_RS09	2 0 4 2 2 0 2 4 4 2	2 00E 16	acid ABC transporter	metabolism and
333	5.045292443	2.00E-10	permease	
D017				Amino Acid
sps_KS15	2 (51(00(01	2.065.00	serine U-	metabolism and
400	2.031090001	2.90E-09	acetyitransierase	
DOIC				Amino Acid
sps_RS15	0 40700 407	2 (05 12		metabolism and
655	-2.43738487	3.68E-13	S9 family peptidase	transport

Data S3 Table I: Comparison between stationary phase samples from 20°C and 4°C cultures.

sps_RS18			flagellar biosynthesis	
555	2.715688136	5.30E-25	protein FlhA	Cell motility
				Amino Acid
sps_RS16	-		dihydrodipicolinate	metabolism and
775	2.251720936	1.09E-14	synthase family protein	transport
				Amino Acid
sps_RS24	-			metabolism and
885	2.365114513	4.36E-13	FAD-binding protein	transport
				Amino Acid
sps_RS26	-			metabolism and
680	2.651808388	3.95E-05	acetylglutamate kinase	transport
			N-acetyl-gamma-	Amino Acid
sps_RS26	-		glutamyl-phosphate	metabolism and
685	2.768358045	3.58E-10	reductase	transport
				Carbohydrate
sps_RS02	-			metabolism and
600	2.242443129	1.15E-07	glycoside hydrolase	transport
				Carbohydrate
sps_RS19	-			metabolism and
520	3.558352271	7.96E-13	allantoinase PuuE	transport
				Cell
sps_RS05	-		type VI secretion system	wall/membrane/en
125	3.001026181	6.12E-11	tip protein VgrG	velope biogenesis
				Cell
sps_RS10	-	0.000740723	type VI secretion system	wall/membrane/en
190	2.053258727	2578	tip protein VgrG	velope biogenesis
				Cell
sps_RS14	-			wall/membrane/en
350	2.766353924	3.79E-13	porin	velope biogenesis
			efflux RND transporter	Cell
sps_RS15	-		periplasmic adaptor	wall/membrane/en
350	2.741884285	4.19E-08	subunit	velope biogenesis
sps_RS00	-		glycine C-	Coenzyme
715	2.602991744	2.44E-12	acetyltransferase	metabolism
sps_RS05			thiamine biosynthesis	Coenzyme
830	-2.30005303	6.48E-06	protein ThiS	metabolism
sps_RS01	-			Energy production
395	2.310842263	1.76E-05	cytochrome C	and conversion
sps_RS01	-			Energy production
610	2.829686908	4.79E-05	aldehyde dehydrogenase	and conversion
			flagellar type III	
sps_RS18		0.000580118	secretion system protein	
575	2.118374688	4741	FliQ	Cell motility
sps_RS03	-	0.000773479	NADPH-dependent 2,4-	Energy production
945	2.124259834	6049	dienoyl-CoA reductase	and conversion

sps_RS18			flagellar biosynthetic	
580	2.258650385	5.66E-14	protein FliP	Cell motility
sps RS08	-			Energy production
005	2.113956873	2.09E-07	citrate synthase	and conversion
			ammonia-forming	
sps_RS12	-		cytochrome c nitrite	Energy production
775	2.275217671	3.95E-05	reductase	and conversion
sps RS18			flagellar export protein	
610	2.012594933	1.07E-06	FliJ	Cell motility
sps_RS14	-		nitrate reductase	Energy production
135	2.864031186	1.78E-06	catalytic subunit NapA	and conversion
sps_RS14	-	0.000359661		Energy production
140	2.469483652	4777	nitrate reductase	and conversion
sps_RS15	-	0.000126983	NADH-dependent	Energy production
885	2.520782686	4222	alcohol dehydrogenase	and conversion
sps_RS18			flagellar protein export	
615	2.064429679	3.13E-06	ATPase FliI	Cell motility
sps_RS18	-			Energy production
985	2.293926767	6.29E-07	malate synthase A	and conversion
sps_RS18			flagellar assembly	
620	2.043344521	7.31E-11	protein FliH	Cell motility
sps_RS18			flagellar basal body M-	
630	2.564368176	1.92E-07	ring protein FliF	Cell motility
			flagellar assembly	
sps_RS18			peptidoglycan hydrolase	
695	2.571054518	3.99E-15	FlgJ	Cell motility
sps_RS18			flagellar biosynthesis	
705	2.259513619	5.16E-08	protein FlgH	Cell motility
			efflux RND transporter	Cell
sps_RS08			periplasmic adaptor	wall/membrane/en
020	3.028216055	2.62E-10	subunit	velope biogenesis
				Cell
sps_RS10				wall/membrane/en
360	3.035660556	3.93E-17	dipeptide epimerase	velope biogenesis
sps_RS07				Coenzyme
860	2.052389225	1.07E-14	biotin synthase BioB	metabolism
sps_RS13			uroporphyrinogen-III C-	Coenzyme
735	3.09273994	3.21E-15	methyltransferase	metabolism
sps_RS23	-			Energy production
415	2.339187067	1.84E-06	alkene reductase	and conversion
sps_RS02	-		DUF4336 domain-	Function
200	2.337950535	3.84E-13	containing protein	Unknown
sps_RS03				Function
030	-3.66950723	9.54E-12	SpoVR family protein	Unknown

sps_RS03	-			Function
035	3.634735125	7.13E-09	hypothetical protein	Unknown
sps RS04	-			Function
390	2.219934553	1.31E-07	N-acetyltransferase	Unknown
sps_RS01				Energy production
075	2.75998547	5.63E-07	hypothetical protein	and conversion
sps_RS09		0.000321129	cystathionine beta-	Energy production
300	2.286414353	6218	synthase	and conversion
sps_RS09		0.000277059		Energy production
310	2.116248143	7889	cytochrome C	and conversion
sps_RS13			cytochrome d terminal	Energy production
470	3.449003903	1.17E-30	oxidase subunit 1	and conversion
sps_RS13			cytochrome d ubiquinol	Energy production
475	2.350299934	9.41E-09	oxidase subunit II	and conversion
sps_RS00			putative sulfate exporter	Function
895	3.386665164	8.63E-47	family transporter	Unknown
sps_RS01				Function
100	4.518717602	9.69E-13	hypothetical protein	Unknown
sps_RS05				Function
725	2.450446706	4.49E-13	hypothetical protein	Unknown
sps_RS06				Function
080	2.641648686	4.53E-10	hypothetical protein	Unknown
sps_RS08	-		NADP-dependent	Function
925	2.511887893	4.87E-06	oxidoreductase	Unknown
sps_RS10	-	0.000108069	LysM domain-	Function
180	2.339326925	4783	containing protein	Unknown
sps_RS10	-		type VI secretion system	Function
195	4.724486792	1.44E-25	tube protein Hcp	Unknown
sps_RS08			AcrB/AcrD/AcrF family	Function
025	2.542095536	3.25E-06	protein	Unknown
sps_RS09				Function
540	2.303232347	2.41E-13	hypothetical protein	Unknown
sps_RS10				Function
625	-2.13771009	7.36E-07	hypothetical protein	Unknown
sps_RS12	-		CBS domain-containing	Function
850	2.131682055	4.38E-08	protein	Unknown
sps_RS09			AzlD domain-containing	Function
560	3.65703157	5.50E-26	protein	Unknown
sps_RS09				Function
565	2.997703539	6.66E-05	NIPSNAP family protein	Unknown
sps_RS13	-			Function
420	2.158078468	3.00E-08	NINE protein	Unknown
sps_RS15	-			Function
000	3.941554963	2.80E-06	phasin family protein	Unknown

sps_RS15		0.000734457		Function
695	-2.1291936	2115	hypothetical protein	Unknown
sps_RS15	-			Function
895	3.653886357	7.92E-22	phasin family protein	Unknown
sps_RS15		0.000279554	nitrous oxide-stimulated	Function
990	-2.50548815	0374	promoter family protein	Unknown
sps_RS10			DUF1611 domain-	Function
355	3.259831866	1.33E-13	containing protein	Unknown
sps_RS13		0.000613075		Function
465	2.230827052	8117	DoxX family protein	Unknown
sps_RS14				Function
330	2.517665813	1.11E-09	hypothetical protein	Unknown
sps_RS15			type I secretion system	Function
070	2.098789981	3.63E-06	permease/ATPase	Unknown
sps_RS18			flagellar biosynthesis	Function
780	2.328864675	1.27E-09	protein FlgT	Unknown
sps_RS20		0.000338313	DUF3019 domain-	Function
505	2.096420537	2647	containing protein	Unknown
			tripartite tricarboxylate	
sps_RS21		0.000400983	transporter substrate	Function
780	2.033904608	4389	binding protein	Unknown
sps_RS19	-		type VI secretion system	Function
095	4.431498858	3.77E-23	tube protein Hcp	Unknown
sps_RS19	-			Function
515	3.650844014	5.71E-13	OHCU decarboxylase	Unknown
sps_RS21		1 2 2 5 1 1	DUF2804 domain-	Function
295	-2.19513035	1.33E-11	containing protein	Unknown
sps_RS26				Function
885	2.289110257	1.07E-10	hypothetical protein	Unknown
sps_RS23	-			Function
400	3.020956044	3.83E-07	SRPBCC family protein	Unknown
sps_RS23	-			Function
405	2.559922242	8.68E-08	hypothetical protein	Unknown
DOM				Inorganic ion
sps_RS01	0.040100005			transport and
540	2.949123937	4.76E-07	MFS transporter	metabolism
sps_RS23	-			Function
410	2.490494981	2.26E-11	patatin	Unknown
sps_RS23	-	0.000314116	DUF3144 domain-	Function
905	2.309484558	1291	containing protein	Unknown
Data			1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Inorganic ion
sps_RS13	0 (01 (0000)	0.015.10	phosphoadenylyl-sulfate	transport and
/80	2.681608289	8.21E-19	reductase	metabolism
sps_RS24	-		type VI secretion system	Function
400	3.752421059	4.31E-13	tube protein Hcp	Unknown

sps_RS24	-	0.000118538	TAT leader-containing	Function
890	2.100698947	4367	periplasmic protein	Unknown
sps_RS27	-			Function
585	2.011851802	1.90E-05	acyl-CoA thioesterase	Unknown
sps_RS27	-			Function
595	2.117141526	7.88E-16	acyl-CoA thioesterase	Unknown
				Inorganic ion
sps_RS06		0.000174921		transport and
210	-2.85664545	1018	reductase	metabolism
				Inorganic ion
sps_RS14	-			transport and
130	3.634810536	1.24E-09	sorbose reductase	metabolism
sps_RS04	-			
040	2.954407519	7.02E-08	acyl-CoA dehydrogenase	Lipid metabolism
sps_RS05	-			
895	3.777084186	3.24E-15	acyl-CoA dehydrogenase	Lipid metabolism
			NADPH-dependent	.
DG10			assimilatory sulfite	Inorganic ion
sps_RS13	0.005006005	1.055 1.0	reductase hemoprotein	transport and
785	2.885336025	1.2/E-16	subunit	metabolism
DC10			assimilatory sulfite	Inorganic ion
sps_KS13	2.01/250700	0 415 10	reductase (NADPH)	transport and
/90	2.916258709	8.41E-12	flavoprotein subunit	metabolism
			prepilin-type N-terminal	Turtus e e 11-1 e u
and DC11			demain containing	trofficking and
sps_K511	2 220477484	0 18F 08	nrotein	secretion
095	2.220477404	9.18L-08	type IV pilus	Intracellular
one RS11			modification protein	trafficking and
700	2 620763421	1 25E-07	PilV	secretion
sps RS01	2.020703121	1.232 07		secretion
090	3 1 5 2 9 2 2 6 9 8	4 39E-09	hypothetical protein	Lipid metabolism
sps RS01	5.1102922090			
105	2.852160291	3.53E-07	hypothetical protein	Lipid metabolism
sps RS01				
110	3.323991059	3.71E-09	hypothetical protein	Lipid metabolism
sps RS01				1
115	3.984054049	2.91E-14	hypothetical protein	Lipid metabolism
			*1 I	Post-translational
				modification,
			glutathione-dependent	protein turnover,
sps RS22			disulfide-bond	chaperone
460	2.651852912	1.72E-12	oxidoreductase	functions
sps_RS01				Secondary
085	2.222729616	8.12E-05	hypothetical protein	Structure

sps_RS07	-			
490	3.319249274	2.06E-14	acyl-CoA dehydrogenase	Lipid metabolism
sps_RS08			acetyl-CoA C-	
785	-3.16374189	4.58E-13	acyltransferase FadI	Lipid metabolism
sps_RS08	-			
835	3.759680308	3.77E-23	transporter	Lipid metabolism
sps_RS19	-			
255	3.212734622	4.68E-08	acyl-CoA dehydrogenase	Lipid metabolism
sps RS21	-			
950	2.143255876	9.71E-06	alpha/beta hydrolase	Lipid metabolism
				Nucleotide
sps RS04	-		adenylosuccinate	metabolism and
270	2.095991154	2.80E-06	synthetase	transport
sps RS01				Secondary
095	3.455227412	1.02E-09	hypothetical protein	Structure
			histidine triad	Nucleotide
sps RS07	-		nucleotide-binding	metabolism and
710	2.037883931	2.97E-11	protein	transport
sps RS05			IclR family	
405	2.159857347	4.87E-12	transcriptional regulator	Transcription
				Nucleotide
sps RS18	-			metabolism and
865	2.318961237	2.71E-09	IMP dehydrogenase	transport
sps RS09			AraC family	
550	2.987652795	5.16E-11	transcriptional regulator	Transcription
				Post-translational
				modification,
				protein turnover,
sps_RS02	-		alkyl hydroperoxide	chaperone
470	2.050190978	6.40E-06	reductase	functions
				Post-translational
				modification,
				protein turnover,
sps_RS08	-		disulfide bond formation	chaperone
535	2.564478514	1.51E-12	protein B	functions
				Post-translational
				modification,
				protein turnover,
sps_RS09	-			chaperone
025	2.056768145	1.02E-06	peptidylprolyl isomerase	functions
				Post-translational
				modification,
				protein turnover,
sps_RS17	-	0.000113597		chaperone
270	3.124593296	6081	thiol peroxidase	functions

sps_RS03			replication initiation	Replication and
840	-2.23686316	2.76E-17	negative regulator SeqA	repair
sps_RS11	-	0.000154562	exodeoxyribonuclease	Replication and
030	2.066018398	1337	VII small subunit	repair
sps_RS16	-			Secondary
235	2.867743323	1.84E-13	hypothetical protein	Structure
sps_RS03	-		PrkA family serine	Signal
040	3.601063732	1.06E-09	protein kinase	Transduction
sps_RS25	-	0.000236252		Signal
995	2.844543104	4103	PhoH family protein	Transduction
sps_RS00	-		RNA polymerase sigma	
465	2.077200509	1.69E-05	factor FliA	Transcription
sps_RS05	-		TetR/AcrR family	
555	2.049872122	8.48E-19	transcriptional regulator	Transcription
sps_RS09			YafY family	
570	2.838227561	5.02E-37	transcriptional regulator	Transcription
sps_RS15	-		TetR family	
345	2.331821137	3.36E-06	transcriptional regulator	Transcription
sps_RS01	-	0.000186270	30S ribosomal protein	
785	2.129566304	355	S7	Translation

Appendix VI Supplemental Tables for Manuscript III

Metabolite Name	KEGG Id	MetaCyc ID
ATP	C00002	ATP
ADP	C00008	ADP
NAD+	C00003	NAD
NADH	C00004	NADH
NADP+	C00006	NADP
NADPH	C00005	NADPH
FAD	C00016	FAD
FADH2	C01352	FADH2
H+	C00080	PROTON
Water	C00001	WATER
Orthophosphate	C00009	Pi
Carbon Dioxide	C00011	CARBON_DIOXIDE
Diphosphate	C00013	PPI
Ammonia	C00014	AMMONIUM

Supplemental Table S1: List of compounds that are removed in the AP-filtered network representation.

Supplemental Table S2: Highest degree nodes from KEGG networks for the FPP, AP, and AP-Filtered network representations with all elements. The percentage of networks where each node was in the top 5% of highest degree nodes is shown along with the average degree of the node across all of the networks.

AP				
	Percent Networks with metabolite	Average		
	in top 5%	Degree of		
Metabolite	of nodes	Metabolite		
H2O	99.98%	228.04		
H+	99.75%	121.64		
Phosphate	99.75%	104.21		
ATP	99.61%	115.36		
ADP	99.29%	99.31		
NAD+	98.76%	84.62		
Diphosphate	98.67%	70.31		
NADH	97.24%	83.83		
NADP+	95.73%	52.04		
Carbon Dioxide (CO2)	95.56%	58.45		
NADPH	95.35%	51.09		
Ammonia	94.61%	51.94		
L-Glutamate	94.03%	50.00		
AMP	92.80%	34.56		
2-Oxoglutarate	91.47%	31.69		
Coenzyme A (CoA)	90.15%	36.65		
Pyruvate	89.69%	36.94		
L-Glutamine	87.87%	22.91		
5-Phospho-alpha-D-ribose 1-diphosphate (PRPP)	85.33%	19.31		
Tetrahydrofolate	82.45%	19.25		
GTP	79.28%	17.72		
L-Aspartate	78.80%	19.04		
Glyceraldehyde 3-				
phosphate	78.30%	17.72		
Acetyl-CoA	75.86%	31.18		
AP-Filtered				

	Percent Networks with metabolite in top 5%	Average
Metabolite	of nodes	Metabolite
L-Glutamate	96.35%	40.14
AMP	95.02%	28.18
Pyruvate	95.00%	29.35
Glyceraldehyde 3-		
phosphate	94.32%	12.88
2-Oxoglutarate	92.76%	25.85
СоА	92.35%	28.23
5-Phospho-alpha-D-ribose 1-diphosphate (PRPP)	90.17%	14.60
L-Glutamine	88.86%	15.84
GTP	87.08%	13.27
Acetyl-CoA	85.23%	25.22
L-Aspartate	83.14%	12.99
СМР	78.99%	13.15
UMP	78.51%	14.03
Tetrahydrofolate	78.18%	11.55
	P Domoont	
	Networks	
	with	
	metabolite	Average
	in top 5%	Degree of
Metabolite	of nodes	Metabolite
H2O	99.90%	144.80
Phosphate	99.71%	66.60
ATP	99.65%	82.44
H+	99.56%	79.04
NADH	98.78%	56.93
Ammonia	97.68%	44.73
Diphosphate	97.22%	31.87
NADPH	96.18%	33.95
L-Glutamate	96.14%	43.28
Carbon Dioxide (CO2)	94.92%	44.41
2-Oxoglutarate	93.34%	28.09

5-Phospho-alpha-D-ribose		
1-diphosphate (PRPP)	91.04%	15.61
Pyruvate	89.59%	26.07
GTP	86.19%	14.81
L-Glutamine	85.48%	15.20
Phosphoenolpyruvate	84.11%	12.30
L-Aspartate	84.03%	15.61
Acetyl-CoA	80.67%	26.01
Glycine	78.74%	15.70
СТР	78.66%	11.89
UTP	78.57%	11.37
UMP	78.26%	16.04
AMP	76.04%	16.05

		FPP	
	25th Percentile	Median	75th Percentile
Number of Nodes	531.00	713.00	921.00
Number of Edges	1080.50	1489.00	1931.00
Average Degree	3.98	4.12	4.26
Density	0.00	0.01	0.01
Transitivity	0.04	0.05	0.05
Degree Assortativity	-0.15	-0.15	-0.13
Average Betweenness			
Centrality	728.75	988.14	1246.07
Average Closeness			
Centrality	0.27	0.28	0.28
Diameter	8.00	9.00	9.00
Average Shortest Path			
Length	3.68	3.73	3.80

Supplemental Table S3: Median network statistics values across all KEGG networks for the all-elements networks.

		AP	
	25th Percentile	Median	75th Percentile
Number of Nodes	531.00	714.00	922.00
Number of Edges	1539.00	2102.00	2735.00
Average Degree	5.67	5.85	5.99
Density	0.01	0.01	0.01
Transitivity	0.04	0.05	0.06
Degree Assortativity	-0.23	-0.22	-0.21
Average Betweenness			
Centrality	541.90	737.68	947.54
Average Closeness			
Centrality	0.33	0.33	0.34
Diameter	7.00	7.00	8.00
Average Shortest Path			
Length	3.03	3.06	3.09

	A	AP-Filtered		
	25th Percentile	Median	75th Percentile	
Number of Nodes	450.50	608.00	772.50	
Number of Edges	743.00	1024.00	1318.00	
Average Degree	3.24	3.33	3.43	
Density	0.00	0.01	0.01	
Transitivity	0.04	0.05	0.06	

Degree Assortativity	-0.08	-0.05	-0.02
Average Betweenness			
Centrality	998.50	1324.23	1635.72
Average Closeness			
Centrality	0.19	0.19	0.20
Diameter	14.00	15.00	17.00
Average Shortest Path			
Length	5.16	5.32	5.50
	FPP		
------------------------------	-----------------	---------	-----------------
	25th Percentile	Median	75th Percentile
Number of Nodes	436.00	569.00	721.00
Number of Edges	605.00	820.00	1042.00
Average Degree	2.75	2.83	2.90
Density	0.00	0.00	0.01
Transitivity	0.05	0.06	0.07
Degree Assortativity	-0.05	-0.04	-0.02
Average Betweenness			
Centrality	1137.07	1431.66	1779.08
Average Closeness Centrality	0.16	0.17	0.18
Diameter	16.00	16.00	18.00
Average Shortest Path			
Length	5.88	6.04	6.28

Supplemental Table S4: Median network statistics values across all KEGG networks for the carbon filtered networks.

	AP		
	25th Percentile	Median	75th Percentile
Number of Nodes	494.00	655.00	836.50
Number of Edges	1095.00	1469.00	1884.00
Average Degree	4.32	4.43	4.56
Density	0.01	0.01	0.01
Transitivity	0.05	0.05	0.06
Degree Assortativity	-0.18	-0.16	-0.15
Average Betweenness			
Centrality	685.28	910.10	1165.47
Average Closeness Centrality	0.27	0.27	0.28
Diameter	11.00	12.00	13.00
Average Shortest Path			
Length	3.70	3.77	3.84

	AP-Filtered		
	25th Percentile	Median	75th Percentile
Number of Nodes	434.00	571.00	722.00
Number of Edges	743.00	991.00	1246.00
Average Degree	3.29	3.39	3.48
Density	0.00	0.01	0.01
Transitivity	0.05	0.05	0.06
Degree Assortativity	-0.05	-0.04	-0.02

Average Betweenness			
Centrality	886.91	1146.38	1452.10
Average Closeness Centrality	0.20	0.21	0.21
Diameter	14.00	15.00	16.00
Average Shortest Path			
Length	4.92	5.06	5.21

	FPP		
	25th Percentile	Median	75th Percentile
Number of Nodes	285.00	367.00	477.00
Number of Edges	356.00	478.00	622.00
Average Degree	2.52	2.60	2.66
Density	0.01	0.01	0.01
Transitivity	0.05	0.06	0.06
Degree Assortativity	-0.09	-0.07	-0.05
Average Betweenness			
Centrality	669.26	876.86	1292.81
Average Closeness Centrality	0.17	0.18	0.19
Diameter	16.00	18.00	26.00
Average Shortest Path			
Length	5.63	5.90	6.35

Supplemental Table S5: Median network statistics values across all KEGG networks for the nitrogen filtered networks.

	AP		
	25th Percentile	Median	75th Percentile
Number of Nodes	318.00	433.00	540.75
Number of Edges	663.00	909.50	1154.00
Average Degree	4.07	4.21	4.33
Density	0.01	0.01	0.01
Transitivity	0.06	0.07	0.08
Degree Assortativity	-0.18	-0.17	-0.16
Average Betweenness			
Centrality	423.57	569.78	701.18
Average Closeness Centrality	0.28	0.29	0.29
Diameter	9.00	10.00	11.00
Average Shortest Path			
Length	3.53	3.59	3.66

	A	AP-Filtered		
	25th Percentile	Median	75th Percentile	
Number of Nodes	279.00	379.00	487.00	
Number of Edges	425.00	581.00	747.00	
Average Degree	2.97	3.07	3.17	
Density	0.01	0.01	0.01	
Transitivity	0.05	0.05	0.06	
Degree Assortativity	-0.11	-0.09	-0.06	

Average Betweenness			
Centrality	531.11	714.76	902.13
Average Closeness Centrality	0.21	0.22	0.22
Diameter	12.00	13.00	15.00
Average Shortest Path			
Length	4.62	4.72	4.84

	FPP		
	25th Percentile	Median	75th Percentile
Number of Nodes	207.00	249.00	302.00
Number of Edges	339.00	409.00	481.00
Average Degree	3.11	3.23	3.33
Density	0.01	0.01	0.02
Transitivity	0.06	0.06	0.07
Degree Assortativity	-0.19	-0.17	-0.16
Average Betweenness			
Centrality	310.91	376.59	612.01
Average Closeness Centrality	0.23	0.26	0.27
Diameter	15.00	16.00	23.00
Average Shortest Path Length	3.94	4.13	4.71

Supplemental Table S6: Median network statistics values across all KEGG networks for the phosphorus filtered networks.

	AP		
	25th Percentile	Median	75th Percentile
Number of Nodes	226.00	288.00	342.00
Number of Edges	525.00	668.00	800.00
Average Degree	4.55	4.68	4.77
Density	0.01	0.02	0.02
Transitivity	0.07	0.07	0.08
Degree Assortativity	-0.23	-0.22	-0.21
Average Betweenness			
Centrality	241.66	307.35	377.91
Average Closeness Centrality	0.32	0.32	0.33
Diameter	8.00	9.00	10.00
Average Shortest Path Length	3.12	3.18	3.23

	A	AP-Filtered		
	25th Percentile	Median	75th Percentile	
Number of Nodes	206.00	257.00	313.00	
Number of Edges	352.25	437.00	524.00	
Average Degree	3.32	3.38	3.44	
Density	0.01	0.01	0.02	
Transitivity	0.05	0.06	0.07	
Degree Assortativity	-0.16	-0.15	-0.14	
Average Betweenness				
Centrality	278.14	354.36	443.73	

Average Closeness Centrality	0.27	0.27	0.28
Diameter	10.00	11.00	11.00
Average Shortest Path Length	3.70	3.81	3.90

Supplemental Table S7: Results of Multi-way ANOVA analysis of the effects of database, network representation, and phylum on network metrics. The degrees of freedom are provided for each factor in the DF column, the Sum of Squares and Mean Squares values are provided in the Sum Sq and Mean Sq columns. The F-statistic is provided in the F-value column and the P-value is provided in the p-value column. The results are shown for all three factors as well as the residuals.

Average Degree							
	DF	Sum Sq	Mean Sq	F-Value	p-value		
Network	2	16860	8430	201085.46	< 0.001		
Database	1	3	3	59.85	< 0.001		
Phylum	31	476	15	366.52	< 0.001		
Residuals	16759	703	0				

Density							
	DF	Sum Sq	Mean Sq	F-Value	p-value		
Network	2	0.03735	0.018674	1848.8	< 0.001		
Database	1	0.00941	0.00941	931.6	< 0.001		
Phylum	31	0.21009	0.006777	670.9	< 0.001		
Residuals	16759	0.16928	0.00001				

Transitivity							
	DF	Sum Sq	Mean Sq	F-Value	p-value		
Network	2	0.3278	0.16388	1415	< 0.001		
Database	1	0.1492	0.14921	1288.4	< 0.001		
Phylum	31	0.8232	0.02655	229.3	< 0.001		
Residuals	16759	1.9409	0.00012				

Degree Assortativity							
	DF	Sum Sq	Mean Sq	F-Value	p-value		
Network	2	68.93	34.47	49901.9	< 0.001		
Database	1	4.62	4.62	6694.8	< 0.001		
Phylum	31	2.88	0.09	134.6	< 0.001		
Residuals	16759	11.58	0				

Log(Average Detweenness Centranty)							
	DF	Sum Sq	Mean Sq	F-Value	p-value		
Network	2	775.3	387.7	4374.7	< 0.001		
Database	1	307.9	307.9	3474.2	< 0.001		
Phylum	31	1625.2	52.4	591.6	< 0.001		
Residuals	16759	1485.1	0.1				

Log(Average Betweenness Centrality)

	DF	Sum Sq	Mean Sq	F-Value	p-value
Network	2	48.76	24.38	366486.08	< 0.001
Database	1	2.2	2.204	33135.01	< 0.001
Phylum	31	0.18	0.006	88.53	< 0.001
Residuals	16759	1.11	0		

Average Closeness Centrality

	Dianititi							
	DF	Sum Sq	Mean Sq	F-Value	p-value			
Network	2	175448	87724	53848.67	< 0.001			
Database	1	4266	4266	2618.51	0.002			
Phylum	31	1025	33	20.29	< 0.001			
Residuals	16759	27302	2					

Diameter

Average Shortest Path Length

	DF	Sum Sq	Mean Sq	F-Value	p-value
Network	2	11598	5799	130712.39	< 0.001
Database	1	623	623	14037	< 0.001
Phylum	31	61	2	44.32	< 0.001
Residuals	16759	743	0		

Supplemental Table S8: Eta Square values for each factor in multi-way ANOVA analysis between KEGG and MetaCyc across three network types, representing the proportion of variance in the model explained by each of the factors.

Statistic	Network	Database	Phylum
Average Degree	0.943	0.000	0.026
Density	0.082	0.022	0.493
Transitivity	0.096	0.046	0.254
Degree Assortativity	0.791	0.053	0.033
Average Betweenness Centrality	0.166	0.073	0.388
Average Closeness Centrality	0.935	0.042	0.003
Diameter	0.841	0.021	0.005
Average Path Length	0.893	0.048	0.005

Supplemental Table S9: Genome-scale models used in the analysis of network metric differences between the KEGG, MetaCyc, and GEM based networks.

Organism	Model Name	KEGG Genome ID	MetaCvc ID	Excluded Reactions for FPP Prediction	Reference PMID
				biomass_iRR	
				1083_metals,	
				1083	
Salmonella				Ec biomass	
typhimurium			sent99287cy	iAF1260_cor	
LT2	STM_v1.0	stm	c	e_59p81M	21244678
Escherichia				Ec_biomass_	
coli K-12	A E1200			1AF1260_cor	17502000
MG1055 Mathanasara	1AF1260	eco	ecocyc	e_39p81M	1/593909
ina harkeri	iAF692	mha		30	16738551
Clostridium		liiou			10750551
beijerinckii					
NCIMB			cbei290402c		
8052	iCB925	cbe	yc	biomass	21846360
				Ec_biomass_	
				SynHetero,	
Svnechocvsti				SvnAuto.	
s sp.			ssp1080229c	Ec biomass	
PCC6803	iJN678	sys	yc	SynMixo	22308420
Pseudomona					
s putida			pput160488c	BiomassKT_	
KT2440	iJN746	ppu	yc	TEMP	18793442
Escherichia				Ec_biomass_	
MG1655	iIO1366	eco	ecocyc	$1JO1300_cor$ e 53p95M	21988831
	1501500			BiomassEcol	21700051
				i, LPLIPA3,	
				LPLIPA4,	
				LPLIPA5,	
				LPLIPA6,	
				LPSSYN_E	
				C, PLIPA1,	
Fachanishia				PLIPA2,	
<i>Escherichia</i> coli K_12				$\frac{\Gamma \Gamma \Gamma A3}{\Gamma P \Gamma P \Lambda 2}$	
MG1655	iJR904	eco	ecocyc	LPLIPA1	12952533

ina acetivorans C2A iMB745 mac cyc overall 22139506 SO_BIOMA SSMACRO_ DM_NOAT P2, RNASYN_S ON, DNASYN_S ON, LPSSYN_S O, PASYN_SO _AEROBIC, PLIPPE_SO, PLIPPE_SO, PLIPPE_SO,	Methanosarc					
acetivorans C2AiMB745macmace18893722139506C2AiMB745maccycoverall22139506SO_BIOMA SSMACRO_ DM_NOAT P2, RNASYN_S ON, DNASYN_S ON, DNASYN_S ON, DNASYN_S ON, LPSSYN_S O, PASYN_SO AEROBIC, PLIPPE_SO, PLIPPG_SO,acetwork PLiPPG_SO, PLIPPG_SO,	ina					
C2AiMB745maccycoverall22139506SO_BIOMA SSMACRO_ DM_NOAT P2, RNASYN_S ON, DNASYN_S ON, LPSSYN_S O, PASYN_SO AEROBIC, PLIPPE_SO, PLIPPG_SO,S0_BIOMA SSMACRO_ DM_NOAT P2, RNASYN_S ON, DNASYN_S O, PASYN_SO AEROBIC, PLIPPG_SO,	acetivorans			mace188937		
SO_BIOMA SSMACRO_ DM_NOAT P2, RNASYN_S ON, DNASYN_S ON, LPSSYN_S O, PASYN_SO _AEROBIC, PLIPPE_SO, PLIPPG_SO,	C2A	iMB745	mac	cyc	overall	22139506
1 Ell 1 0_50;					SO_BIOMA SSMACRO_ DM_NOAT P2, RNASYN_S ON, DNASYN_S ON, LPSSYN_S O, PASYN_SO _AEROBIC, PLIPPE_SO, PLIPPE_SO,	22139300
	<u>C1</u>				PLIPPG_SO,	
Snewanella PROISYN_	Snewanella			22115962	PROISYN_	
Oneldensis Sone211380C SON_AERO MB 1 iMB1 700 son	oneidensis	MD1 700		sone211580c	SUN_AEKU	24621204
Mikel notari	Mik-1	IIVIK1_/99	son	ye	BIC	24021294
um tuberculosis biomass Mt	um tuberculosis				biomass Mt	
H37Rv iNJ661 mtv mtbrvcyc b 9 60atp 17555602	H37Rv	iNJ661	mtv	mtbrvcyc	b 9 60atp	17555602
Mycoplasma mgen243273	Mycoplasma			mgen243273		
genitalium iPS189 mge cyc Biomass 19214212	genitalium	iPS189	mge	cyc	Biomass	19214212
SA_biomass _1a, biomass_SA _2a, biomass_SA _2b, biomass_SA _3a, biomass_SA _3b, biomass_SA _4a, biomass_SA _5a, biomass_SA _6a,					SA_biomass _1a, biomass_SA _2a, biomass_SA _2b, biomass_SA _3a, biomass_SA _3b, biomass_SA _4a, biomass_SA _5a, biomass_SA _5a, biomass_SA _6a,	
Staphylococc biomass_SA	Staphylococc			anum150070-	blomass_SA	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	N315	iSB619	sau	saur1388/90	biomass SA	15752426

				_7a, biomass_SA _7b, biomass_SA _8a, biomass_SA _lipids_only, biomass_SA _nuc_only,	
				biomass_SA _only_AA, PASYN_SA	
				BiomassEcol i_TM, GLSe, GLS2e, AMYe, PULLe, GLYCOe, GLCMAN60 0a_e, GLCMAN60	
Thermotoga			tmar243274c	0b_e, GLCMAN60 0c e,	
maritima	iTZ479	tmw	yc	AMYLe	19762644
				Core_Bioma ss, PASYN_WP 3 20C,	
Shewanella				DNASYN,	
piezotolerans			spie225849c	RNASYN,	
WP3	GEM-iWP3	swp	yc	PROTSYN	28382331

	FPP	AP	AP-Filtered
All-elements	100.0%	99.9%	99.8%
Carbon	99.7%	99.9%	99.8%
Nitrogen	98.8%	99.9%	99.2%
Phosphorus	100.0%	99.9%	99.9%

Supplemental Table S10: Summary of the percentage of networks from each category that have small world properties.

Compound ID	Lower Limit	Ilmnou I imit	Compound Name	Compound
cpd_pro-L[e]	0	1000	L-Proline	Amino Acid
cpd_met-L[e]	0	1000	L-Methionine	Amino Acid
cpd_indole[e]	0	1000	Indole	Amino Acid
cpd_ala-D[e]	0	1000	D-Alanine	Amino Acid
cpd_ala-L[e]	0	1000	L-Alanine	Amino Acid
cpd_asp-L[e]	0	1000	L-Aspartate	Amino Acid
cpd_glu-L[e]	0	1000	L-Glutamate	Amino Acid
cpd_gly[e]	0	1000	Glycine	Amino Acid
cpd_gly-asp-			glycyl-L-	
L[e]	0	1000	aspartic acid	Amino Acid
cpd_gly-glu-	0	1000	glycyl-L-	1
	0	1000	glutamic acid	Amino Acid
cpd_1le-L[e]	0	1000	L-Isoleucine	Amino Acid
cpd_leu-L[e]	0	1000	L-Leucine	Amino Acid
cpd_ptrc[e]	0	1000	Putrescine	Amino Acid
cpd_ser-L[e]	0	1000	L-Serine	Amino Acid
cpd_thr-L[e]	0	1000	L-Threonine	Amino Acid
cpd_tyr-L[e]	0	1000	L-Tyrosine	Amino Acid
cpd_val-L[e]	0	1000	L-Valine	Amino Acid
cpd_lys-L[e]	0	1000	L-Lysine	Amino Acid
cpd_trp-L[e]	0	1000	L-Tryptophan	Amino Acid
cpd_akg[e]	0	1000	2-Oxoglutarate	Amino Acid
cpd_gln-L[e]	0	1000	L-Glutamine	Amino Acid
cpd_asn-L[e]	0	1000	L-Asparagine	Amino Acid
cpd_glyc-R[e]	-1000	1000	(R)-Glycerate	Carbohydrate
cpd_ac[e]	-1000	1000	Acetate	Carbohydrate
			N-Acetyl-D-	
cpd_acgam[e]	-1000	1000	glucosamine	Carbohydrate
cpd_bgl[e]	-1000	1000	cellobiose	Carbohydrate
cpd_for[e]	-1000	1000	Formate	Carbohydrate
cpd_fum[e]	-1000	1000	Fumarate	Carbohydrate
cpd_galactan[e]	-1000	1000	Galactan	Carbohydrate
cpd_gal[e]	-1000	1000	D-Galactose	Carbohydrate
cpd_glc-D[e]	-1000	1000	D-Glucose	Carbohydrate
cpd_glyc[e]	-1000	1000	Glycerol	Carbohydrate

Supplemental Table S11: Table showing media constraints used in random deletion simulations for the GEM-iWP3 GEM.

cpd_glyclt[e]	-1000	1000	Glycolate	Carbohydrate
cpd_lac-D[e]	-1000	1000	D-Lactate	Carbohydrate
cpd_lac-L[e]	-1000	1000	L-Lactate	Carbohydrate
cpd_lami[e]	-1000	1000	laminarin	Carbohydrate
cpd_mal-L[e]	-1000	1000	L-Malate	Carbohydrate
cpd_panose[e]	-1000	1000	Panose	Carbohydrate
cpd_malt[e]	-1000	1000	Maltose	Carbohydrate
cpd_malthp[e]	-1000	1000	Maltoheptaose	Carbohydrate
cpd_malthx[e]	-1000	1000	Maltohexaose	Carbohydrate
cpd_maltpt[e]	-1000	1000	Maltopentaose	Carbohydrate
cpd_malttr[e]	-1000	1000	Maltotriose	Carbohydrate
cpd maltttr[e]	-1000	1000	Maltotetraose	Carbohydrate
cpd_pyr[e]	-1000	1000	Pyruvate	Carbohydrate
cpd_succ[e]	-1000	1000	Succinate	Carbohydrate
cpd_ppa[e]	-1000	1000	Propionate	Carbohydrate
cpd chitin[e]	-1000	1000	chitin	Carbohydrate
cpd etoh[e]	-1000	1000	Ethanol	Carbohydrate
				Ions and Small
cpd_na1[e]	-1000	1000	Sodium	Molecules
	1000	1000	Hydrogen	Ions and Small
cpd_h2o2[e]	-1000	1000	peroxide	Molecules
end CrOH3[e]	-1000	1000	Cr(OH)3	Ions and Small Molecules
	1000	1000	01(011)5	Ions and Small
cpd ca2[e]	-1000	1000	Calcium	Molecules
				Ions and Small
cpd_cl[e]	-1000	1000	Chloride	Molecules
1 25 1	1000	1000	CO3	Ions and Small
cpd_co2[e]	-1000	1000	02	Molecules
cpd_cobalt3[e]	-1000	1000	Co3+	Molecules
	1000	1000		Ions and Small
cpd_cobalt2[e]	-1000	1000	Co2+	Molecules
				Ions and Small
cpd_cro4[e]	-1000	1000	chromate	Molecules
and au2[a]	1000	1000	$C_{\rm H}2\pm$	Ions and Small
cpu_cu2[e]	-1000	1000	Cu∠⊤ Dimethyl	Ins and Small
cpd dms[e]	-1000	1000	sulfide	Molecules
1L*J	1000		Dimethyl	Ions and Small
cpd_dmso[e]	-1000	1000	sulfoxide	Molecules

				Ions and Small
cpd_fe2[e]	-1000	1000	Fe2+	Molecules
				Ions and Small
cpd_fe3[e]	-1000	1000	Fe3+	Molecules
				Ions and Small
cpd_h[e]	-1000	1000	H+	Molecules
				Ions and Small
cpd_h2o[e]	-1000	1000	H2O	Molecules
11051	1000	1000	Hydrogen	Ions and Small
cpd_h2s[e]	-1000	1000	sulfide	Molecules
and 1-[a]	1000	1000	V	Ions and Small
сра_к[е]	-1000	1000	Κ +	Molecules
and ma2[e]	1000	1000	Ma	Ions and Small
cpu_mg2[c]	-1000	1000	Wig	Ions and Small
cnd_mn2[e]	-1000	1000	Mn2+	Molecules
	1000	1000	Manganese(IV)	Ions and Small
cpd_mn4o[e]	-1000	1000	oxide	Molecules
	1000	1000		Ions and Small
cpd nh4[e]	-1000	1000	Ammonium	Molecules
				Ions and Small
cpd_no2[e]	-1000	1000	Nitrite	Molecules
				Ions and Small
cpd_no3[e]	-1000	1000	Nitrate	Molecules
				Ions and Small
cpd_o2[e]	-1000	1000	O2	Molecules
				Ions and Small
cpd_pi[e]	-1000	1000	Phosphate	Molecules
1 05 1	1000	1000	a 10.	Ions and Small
cpd_so3[e]	-1000	1000	Sulfite	Molecules
1 45 1	1000	1000	G 16 4	Ions and Small
cpa_so4[e]	-1000	1000	Sullate	Molecules
and tmo[o]	1000	1000	Trimothylomino	Ions and Small
cpu_una[e]	-1000	1000	Trimethylamine	Inforcences
and tmao[e]	-1000	1000	N-ovide	Molecules
	-1000	1000		Ions and Small
cnd_tsul[e]	-1000	1000	Thiosulfate	Molecules
	1000	1000	mosunate	Ions and Small
cpd tttnt[e]	-1000	1000	tetrathionate	Molecules
_r · · · · · L *]	1000	1000	Uranium	Ions and Small
cpd urdio[e]	-1000	1000	dioxide	Molecules
· _ · · J				Ions and Small
cpd_urnyl[e]	-1000	1000	Uranyl	Molecules

				Ions and Small
cpd_mobd[e]	-1000	1000	Molybdate	Molecules
				Ions and Small
cpd urea[e]	-1000	1000	Urea	Molecules
			Dodecanoic	
cpd_dodcan[e]	0	1000	acid (neutral)	Lipid
			hexadecanoate	
			(n-C16:0)	
cpd_hdcan[e]	0	1000	(neutral)	Lipid
			octadecanoate	
			(n-C18:0)	
cpd_ocdcan[e]	0	1000	neutral	Lipid
			tetradecanoate	
			(C14:0)	
cpd_ttdcan[e]	0	1000	(neutral)	Lipid
				Nucleic Acids
cpd_damp[e]	0	1000	dAMP	and Derivatives
				Nucleic Acids
cpd_dcmp[e]	0	1000	dCMP	and Derivatives
				Nucleic Acids
cpd_dgmp[e]	0	1000	dGMP	and Derivatives
				Nucleic Acids
cpd_dtmp[e]	0	1000	dTMP	and Derivatives
				Nucleic Acids
cpd_adn[e]	0	1000	Adenosine	and Derivatives
			Deoxyadenosin	Nucleic Acids
cpd_dad-2[e]	0	1000	e	and Derivatives
			Deoxyguanosin	Nucleic Acids
cpd_dgsn[e]	0	1000	e	and Derivatives
				Nucleic Acids
cpd_ura[e]	0	1000	Uracil	and Derivatives
				Nucleic Acids
cpd_cytd[e]	0	1000	Cytidine	and Derivatives
				Nucleic Acids
cpd_dcyt[e]	0	1000	Deoxycytidine	and Derivatives
				Nucleic Acids
cpd_dna[e]	0	1000	DNA	and Derivatives
				Nucleic Acids
cpd_duri[e]	0	1000	Deoxyuridine	and Derivatives
				Nucleic Acids
cpd_uri[e]	0	1000	Uridine	and Derivatives
				Nucleic Acids
cpd_thymd[e]	0	1000	Thymidine	and Derivatives
				Nucleic Acids
cpd_xan[e]	0	1000	Xanthine	and Derivatives

				Nucleic Acids
cpd_ins[e]	0	1000	Inosine	and Derivatives
				Nucleic Acids
cpd_thym[e]	0	1000	Thymine	and Derivatives
				Nucleic Acids
cpd_hxan[e]	0	1000	Hypoxanthine	and Derivatives
cpd_pmcoa[e]	-1000	1000	Pimeloyl-CoA	Vitamins
cpd_cbl1[e]	-1000	1000	Cob(I)alamin	Vitamins

	T T • • •	TT T • •/	Compound	Compound
Compound ID	Lower Limit	Upper Limit	Name	Category
ala_L	0	1000	L-Alanine	Amino Acid
ile_L	0	1000	L-Isoleucine	Amino Acid
leu_L	0	1000	L-Leucine	Amino Acid
ptrc	0	1000	Putrescine	Amino Acid
spmd	0	1000	Spermidine	Amino Acid
thr_L	0	1000	L-Threonine	Amino Acid
val_L	0	1000	L-Valine	Amino Acid
ac	-1000	1000	Acetate	Carbohydrate
amylose300	-1000	1000	amylose (n=300 repeat units, alpha-1 4-glc)	Carbohydrate
amylose500	-1000	1000	I Ambinaga	Carbohydrate
	-1000	1000	cellulose (n=4	Carbonydrate
cell4	-1000	1000	repeating units)	Carbohvdrate
cell500	-1000	1000	celluose (n=500 repeating units, beta-1,4 glc)	Carbohydrate
11.6	1000	1000	cellulose (n=6	
cell6	-1000	1000	repeating units)	Carbohydrate
cellb	-1000	1000	cellobiose	Carbohydrate
fru	-1000	1000	D-Fructose	Carbohydrate
gal	-1000	1000	D-Galactose	Carbohydrate
galman4	-1000	1000	galactomannan(n=4 repeat units mannose, alpha- 1,4 man)	Carbohydrate
galman6	-1000	1000	galactomannan(n=6 repeat units mannose, alpha- 1.4 man)	Carbohvdrate
			galactomannan (n=600 repeat units mannose,	
galman600	-1000	1000	alpha-1,4 man)	Carbohydrate
glc_D	-1000	1000	D-Glucose	Carbohydrate
glcman4	-1000	1000	glucomannan (n=4 repeat units, glc beta- 1,4 man)	Carbohydrate

Supplemental Table S12: Table showing media constraints used in random deletion simulations for the iTZ479 GEM.

			glucomannan	
			(n=6 repeat	
1 (1000	1000	units, glc beta-	0 1 1 1 4
glcmanb	-1000	1000	1,4 man)	Carbohydrate
			glucomannan	
			(n=000 repeat	
aleman600	1000	1000	1 4 man)	Carbobydrate
giemanooo	-1000	1000	heta-1 $3/1 4$	Carbonyurate
			olucan (Barley	
			n=1500. Glc	
glucan1500	-1000	1000	beta1->3,4 Glc)	Carbohydrate
8			beta-1,3/1,4-	
			glucan (Barley,	
			n=4, Glc beta1-	
glucan4	-1000	1000	>3,4 Glc)	Carbohydrate
			beta-1,3/1,4-	
			glucan (Barley,	
			n=6, Glc beta1-	
glucan6	-1000	1000	>3,4 Glc)	Carbohydrate
glyc	-1000	1000	Glycerol	Carbohydrate
			Glycerol 3-	
glyc3p	-1000	1000	phosphate	Carbohydrate
			glycogen (n=1500 repeat	
			units) (glc alpha	
glycogen1500	-1000	1000	1,4/6 glc)	Carbohydrate
inost	-1000	1000	myo-Inositol	Carbohydrate
lac_L	-1000	1000	L-Lactate	Carbohydrate
lcts	-1000	1000	Lactose	Carbohydrate
lmn2	-1000	1000	Laminaribiose	Carbohydrate
			laminarin (n=30	
			repeat units,	
lmn30	-1000	1000	beta -1,3 glc)	Carbohydrate
malt	-1000	1000	Maltose	Carbohydrate
malttr	-1000	1000	Maltotriose	Carbohydrate
maltttr	-1000	1000	Maltotetraose	Carbohydrate
man	-1000	1000	D-Mannose	Carbohydrate
			Mannobiose	
manb	-1000	1000	(beta-1,4)	Carbohydrate
			mannotriose	
mantr	-1000	1000	(beta-1,4)	Carbohydrate
manttr	-1000	1000	mannotetraose	Carbohydrate
melib	-1000	1000	Melibiose	Carbohydrate

			pullulan (n=1200 repeat	
			units, alpha-1,4	
pullulan1200	1000	1000	and alph-1,6	Carbohydrate
pullularit200	-1000	1000	Doulius)	Carbohydrate
	-1000	1000		Carboliydiate
rib_D	-1000	1000	D-Ribose	
rmn	-1000	1000	L-Rhamnose	Carbonydrate
			repeat units (300 repeat units amylose, 900 repeat units	
			amylopectin,	
starsh 1200	1000	1000	corresponds to	Carbohydrata
starch1200	-1000	1000	Sucross	Carbohydrate
suci	-1000	1000	Trahalaga	Carbohydrate
	-1000	1000		Carboliydiate
xyl3	-1000	1000	D Value	Carbonydrate
xyl_D	-1000	1000	D-Aylose Vylop (12	Carbonydrate
			backbone units, 3 glcur side	
xylan12	-1000	1000	chain)	Carbohydrate
xylan4	-1000	1000	Xylan (4 backbone units, 1 glcur side chain)	Carbohydrate
xvlan8	-1000	1000	Xylan (8 backbone units, 2 glcur side chain)	Carbohvdrate
xvlb	-1000	1000	Xvlobiose	Carbohydrate
	2000	2000	J	Ions and Small
co2	-1000	1000	CO2	Molecules
	1000	1000	T. O.	Ions and Small
te2	-1000	1000	Fe2+	Molecules
fe3	-1000	1000	Fe3+	ions and Small Molecules
	-1000	1000	1.00 '	Ions and Small
h	-1000	1000	H+	Molecules
h2	-1000	1000	H2	Ions and Small Molecules

				I 10 11
				Ions and Small
h2o	-1000	1000	H2O	Molecules
			Hydrogen	Ions and Small
h2s	-1000	1000	sulfide	Molecules
				Ions and Small
hco3	-1000	1000	Bicarbonate	Molecules
				Ions and Small
mg2	-1000	1000	magnesium	Molecules
-0			2	Ions and Small
nal	-1000	1000	Sodium	Molecules
				Ions and Small
nh4	-1000	1000	Ammonium	Molecules
	1000	1000		Ions and Small
pi	-1000	1000	Phosphate	Molecules
<u>r -</u>			F	Ions and Small
S	-1000	1000	Sulfur	Molecules
	1000	1000		Ions and Small
zn?	-1000	1000	Zinc	Molecules
	1000	1000	21110	Nucleic Acids
csn	0	1000	Cytosine	and Derivatives
	0	1000	Cytosine	Nucleic Acids
11179	0	1000	Uracil	and Derivatives
uia		1000		Nucleic Acids
Von	0	1000	Vonthing	and Dorivativas
Xall	0	1000	лапиппе	
		1000	X7 .1	Nucleic Acids
xtsn	0	1000	Xanthosine	and Derivatives

Compound ID	I	I	Compound	Compound
Compound ID	Lower Limit	Opper Limit		Category
			_ ^{1,5-} Diaminopentan	
15dap	0	1000	e	Amino Acid
akg	0	1000	2-Oxoglutarate	Amino Acid
ala-D	0	1000	D-Alanine	Amino Acid
ala-L	0	1000	L-Alanine	Amino Acid
arg-L	0	1000	L-Arginine	Amino Acid
asn-L	0	1000	L-Asparagine	Amino Acid
asp-L	0	1000	L-Aspartate	Amino Acid
crn	0	1000	L-Carnitine	Amino Acid
cys-L	0	1000	L-Cysteine	Amino Acid
gbbtn	0	1000	gamma- butyrobetaine	Amino Acid
gln-L	0	1000	L-Glutamine	Amino Acid
glu-L	0	1000	L-Glutamate	Amino Acid
gly	0	1000	Glycine	Amino Acid
his-L	0	1000	L-Histidine	Amino Acid
ile-L	0	1000	L-Isoleucine	Amino Acid
indole	0	1000	Indole	Amino Acid
leu-L	0	1000	L-Leucine	Amino Acid
lys-L	0	1000	L-Lysine	Amino Acid
met-D	0	1000	D-Methionine	Amino Acid
met-L	0	1000	L-Methionine	Amino Acid
orn	0	1000	Ornithine	Amino Acid
			L-	
phe-L	0	1000	Phenylalanine	Amino Acid
pro-L	0	1000	L-Proline	Amino Acid
ptrc	0	1000	Putrescine	Amino Acid
ser-D	0	1000	D-Serine	Amino Acid
ser-L	0	1000	L-Serine	Amino Acid
spmd	0	1000	Spermidine	Amino Acid
tartr-L	0	1000	L-tartrate	Amino Acid
taur	0	1000	Taurine	Amino Acid
thr-L	0	1000	L-Threonine	Amino Acid
trp-L	0	1000	L-Tryptophan	Amino Acid
tyr-L	0	1000	L-Tyrosine	Amino Acid

Supplemental Table S13: Table showing media constraints used in random deletion simulations for the iJR904 GEM.

val-L	0	1000	L-Valine	Amino Acid
			(S)-Propane-	
12ppd-S	-1000	1000	1,2-diol	Carbohydrate
			_2-Dehydro-3-	
	1000	1000	deoxy-D-	a 1 1 1
2ddglcn	-1000	1000	gluconate	Carbohydrate
			$\frac{3}{1}$	
2h simme	1000	1000	nydroxycinnami	Carbahydrata
Shehim	-1000	1000	$\frac{1}{3}$ (3 bydroxy)	Carbonyurate
3hpppn	-1000	1000	ate	Carbohydrate
	1000	1000	4-	
			Aminobutanoat	
4abut	-1000	1000	e	Carbohydrate
ac	-1000	1000	Acetate	Carbohydrate
acac	-1000	1000	Acetoacetate	Carbohydrate
acald	-1000	1000	Acetaldehyde	Carbohydrate
			N-Acetyl-D-	
acgam	-1000	1000	glucosamine	Carbohydrate
			N-Acetyl-D-	
acmana	-1000	1000	mannosamine	Carbohydrate
			N-	
			Acetylneuramin	
acnam	-1000	1000	ate	Carbohydrate
arab-L	-1000	1000	L-Arabinose	Carbohydrate
	1000	1000	Butyrate (n-	~ 1 1 1
but	-1000	1000	C4:0)	Carbohydrate
cit	-1000	1000	Citrate	Carbohydrate
for	-1000	1000	Formate	Carbohydrate
fru	-1000	1000	D-Fructose	Carbohydrate
fuc-L	-1000	1000	L-Fucose	Carbohydrate
			L-Fucose 1-	
fuc1p-L	-1000	1000	phosphate	Carbohydrate
fum	-1000	1000	Fumarate	Carbohydrate
			D-Glucose 6-	
дбр	-1000	1000	phosphate	Carbohydrate
gal	-1000	1000	D-Galactose	Carbohydrate
galct-D	-1000	1000	D-Galactarate	Carbohydrate
galctn-D	-1000	1000	D-Galactonate	Carbohydrate
galt	-1000	1000	Galactitol	Carbohydrate
			D-	
galur	-1000	1000	Galacturonate	Carbohydrate

gam	-1000	1000	D-Glucosamine	Carbohydrate
glc-D	-1000	1000	D-Glucose	Carbohydrate
glcn	-1000	1000	D-Gluconate	Carbohydrate
glcr	-1000	1000	D-Glucarate	Carbohydrate
glcur	-1000	1000	D-Glucuronate	Carbohydrate
_			D-	
glyald	-1000	1000	Glyceraldehyde	Carbohydrate
glyc	-1000	1000	Glycerol	Carbohydrate
1 2	1000	1000	Glycerol 3-	0 1 1 1
glyc3p	-1000	1000	phosphate	Carbohydrate
glyclt	-1000	1000	Glycolate	Carbohydrate
idon-L	-1000	1000	L-Idonate	Carbohydrate
lac-D	-1000	1000	D-Lactate	Carbohydrate
lac-L	-1000	1000	L-Lactate	Carbohydrate
lcts	-1000	1000	Lactose	Carbohydrate
mal-L	-1000	1000	L-Malate	Carbohydrate
malt	-1000	1000	Maltose	Carbohydrate
malthx	-1000	1000	Maltohexaose	Carbohydrate
maltpt	-1000	1000	Maltopentaose	Carbohydrate
malttr	-1000	1000	Maltotriose	Carbohydrate
maltttr	-1000	1000	Maltotetraose	Carbohydrate
man	-1000	1000	D-Mannose	Carbohydrate
			D-Mannose 6-	
man6p	-1000	1000	phosphate	Carbohydrate
melib	-1000	1000	Melibiose	Carbohydrate
mnl	-1000	1000	D-Mannitol	Carbohydrate
	1000	1000	Phenylpropanoa	C 1 1 1
pppn	-1000	1000	te	Carbohydrate
pyr	-1000	1000	Pyruvate	Carbohydrate
rıb-D	-1000	1000	D-Ribose	Carbohydrate
rmn	-1000	1000	L-Rhamnose	Carbohydrate
sbt-D	-1000	1000	D-Sorbitol	Carbohydrate
succ	-1000	1000	Succinate	Carbohydrate
sucr	-1000	1000	Sucrose	Carbohydrate
tre	-1000	1000	Trehalose	Carbohydrate
xyl-D	-1000	1000	D-Xylose	Carbohydrate
			meso-2,6-	
26 day M	0	1000	Diaminoheptan	Call Wall
	0	1000	euloate	Lell Wall
co2	-1000	1000	CO2	Molecules
	1000	1000		

				Ions and Small
cynt	-1000	1000	Cyanate	Molecules
			Dimethyl	Ions and Small
dms	-1000	1000	sulfide	Molecules
			Dimethyl	Ions and Small
dmso	-1000	1000	sulfoxide	Molecules
				Ions and Small
etoh	-1000	1000	Ethanol	Molecules
				Ions and Small
fe2	-1000	1000	Fe2+	Molecules
				Ions and Small
h	-1000	1000	H+	Molecules
				Ions and Small
h2o	-1000	1000	H2O	Molecules
			_	Ions and Small
k	-1000	1000	potassium	Molecules
				Ions and Small
nal	-1000	1000	Sodium	Molecules
	1000	1000		Ions and Small
nh4	-1000	1000	Ammonium	Molecules
	1000	1000	A . T ¹ . 1 .	Ions and Small
no2	-1000	1000	Nitrite	Molecules
2	1000	1000	A T [•] <i>i i</i>	Ions and Small
no3	-1000	1000	Nitrate	Molecules
	1000	1000	00	Ions and Small
02	-1000	1000	02	Molecules
	1000	1000	D1 1 4	Ions and Small
p1	-1000	1000	Phosphate	Molecules
aa.1	1000	1000	Sulfata	Ions and Small
804	-1000	1000	Sullate	Violecules
tmo	1000	1000	trimathylomina	Moloculos
ulla	-1000	1000	Trimothylamino	Inforcences
tmao	-1000	1000	N-oxide	Molecules
	-1000	1000		Ions and Small
tsul	-1000	1000	Thiosulfate	Molecules
	1000	1000	Thiosultate	Ions and Small
urea	-1000	1000	Urea	Molecules
	1000	1000	Hexadecanoate	Wieleeules
hdca	0	1000	(n-C16:0)	Lipid
		1000	octadecanoate	
ocdca	0	1000	(n-C18:0)	Lipid
		1000	tetradecanoate	- I
ttdca	0	1000	(n-C14:0)	Lipid
	· · · · · ·		× /	1

				Nucleic Acids
ade	0	1000	Adenine	and Derivatives
				Nucleic Acids
adn	0	1000	Adenosine	and Derivatives
				Nucleic Acids
alltn	0	1000	Allantoin	and Derivatives
				Nucleic Acids
amp	0	1000	AMP	and Derivatives
				Nucleic Acids
csn	0	1000	Cytosine	and Derivatives
				Nucleic Acids
cytd	0	1000	Cytidine	and Derivatives
			Deoxyadenosin	Nucleic Acids
dad-2	0	1000	e	and Derivatives
				Nucleic Acids
dcyt	0	1000	Deoxycytidine	and Derivatives
			Deoxyguanosin	Nucleic Acids
dgsn	0	1000	e	and Derivatives
			Dihydroxyaceto	Nucleic Acids
dha	0	1000	ne	and Derivatives
				Nucleic Acids
din	0	1000	Deoxyinosine	and Derivatives
				Nucleic Acids
duri	0	1000	Deoxyuridine	and Derivatives
				Nucleic Acids
gsn	0	1000	Guanosine	and Derivatives
				Nucleic Acids
gua	0	1000	Guanine	and Derivatives
				Nucleic Acids
hxan	0	1000	Hypoxanthine	and Derivatives
				Nucleic Acids
ins	0	1000	Inosine	and Derivatives
				Nucleic Acids
thymd	0	1000	Thymidine	and Derivatives
				Nucleic Acids
ura	0	1000	Uracil	and Derivatives
				Nucleic Acids
uri	0	1000	Uridine	and Derivatives
				Nucleic Acids
xan	0	1000	Xanthine	and Derivatives
				Nucleic Acids
xtsn	0	1000	Xanthosine	and Derivatives
cbl1	-1000	1000	Cob(I)alamin	Vitamins
chol	-1000	1000	Choline	Vitamins
glyb	-1000	1000	Glycine betaine	Vitamins
xtsn cbl1 chol glyb	0 -1000 -1000 -1000	1000 1000 1000 1000	Xanthosine Cob(I)alamin Choline Glycine betaine	Nucleic Acids and Derivatives Vitamins Vitamins Vitamins

nac	-1000	1000	Nicotinate	Vitamins
			Nicotinamide	
			adenine	
nad	-1000	1000	dinucleotide	Vitamins
nmn	-1000	1000	NMN	Vitamins
			(R)-	
pnto-R	-1000	1000	Pantothenate	Vitamins
thm	-1000	1000	Thiamin	Vitamins