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The Characterization of a New Metabolite from a Trichodesmium Bloom

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The goal of my honors project was to carry out a natural products isolation work flow from start to finish. This process includes extraction, fractionation, high-performance liquid chromatography (HPLC), mass spectrometry (MS), and nuclear magnetic resonance (NMR). Ultimately, the end goal is the purification and characterization of a new metabolite. The sample I worked with was from a *Trichodesmium thiebautii* bloom, a species of cyanobacteria that is scientifically underexplored. Cyanobacteria as a taxa are known to produce chemically diverse secondary metabolites and over twenty new to science compounds had already been isolated from this bloom by The Bertin Lab.

The fraction I worked with over the course of my project, "I1," was amongst the most polar fractions. This fraction was obtained following silica gel vacuum liquid chromatography of the total crude extract, which was separated into 9 fractions, A-I, from least to most polar. Fraction I was then passed over a C18 column using solid phase extraction chromatography to obtain 4 further fractions, 1-4, from most polar to least polar. Fraction I1 was then further fractionated by passing over a C18 column using solid phase extraction chromatography to obtain five fractions (I1A-I1E). Our previous analysis of this bloom utilized bioassay guided isolation (neuro-2A cytotoxicity), however, this study utilized UV and MS-based isolation.

Three HPLC methods were developed and used to isolate one pure compound. Refer to attached poster for chromatograms and methods. The UV/Vis spectra of the purified peak shows absorbance at 196nm, 236nm, and 300nm. An absorbance at 300nm provides evidence for a highly conjugated system. An absorbance at 236nm provides evidence for a conjugated lactone ring as seen in another molecule isolated by The Bertin Lab, trichophycin F. However, we did not see the 300nm absorbance in F.

High resolution mass spectrometry (HRMS) of the purified compound can be seen on the attached poster. The m/z shown, 456, is the $M + Na^+$. The molecular weight of the molecule is 433 and the HRMS measurement supports a formula of $C_{25}H_{39}NO_5$. When comparing the MS/MS of the purified molecule to similar molecule trichophycin F, many fragment peaks from the new compound are two fewer than trichophycin F which is evidence of the similarity of the two compounds and suggests one extra unsaturation in the new metabolite's core structure.

Three NMR experiments were run on the pure compound including 1H NMR, COSY and TOCSY (500 MHz, $DMSO-d_6$). These experiments were analyzed and compared to NMR data from trichophycin F. The compounds share many similar proton shifts including the O-methyl proton signal, N-methyl proton signals, and proton signals on the lactone ring. The structure of this molecule is not being revealed because it is not yet published. This molecule will be published in the future along with other trichophycin molecules which still remain unpublished.