**Intraspecific variation in polar and nonpolar metabolite profiles of a threatened Caribbean coral**

This project aims to identify differences in metabolomic profiles among seven known, unique genotypes of the threatened staghorn coral Acropora cervicornis.

**Abstract**

Research aimed at understanding intraspecific variation among corals could substantially increase understanding of coral biology and improve outcomes of active restoration efforts. Metabolomics is useful for identifying physiological drivers leading to variation among genotypes and has the capacity to improve our selection of candidate corals that express phenotypes beneficial to restoration. Our study aims to compare metabolomic profiles among known, unique genotypes of the threatened coral *Acropora cervicornis*. In doing so, we seek information related to the physiological characteristics driving variation among genotypes, which could aid in identifying genets with desirable traits for restoration. Significant variation in polar and nonpolar metabolite profiles was found among *A. cervicornis* genotypes. Despite difficulties identifying all significant metabolites driving separation among genotypes, our data support previous findings and further suggest metabolomic profiles differ among various genotypes of the threatened species *A. cervicornis*. The implementation of 1H-NMR and LC-MS analyses allowed identification of several key metabolites driving separation among genotypes and expanded our understanding of the *A. cervicornis* metabolome. Although our research is specific to *A. cervicornis*, these findings have broad relevance for coral biology and active restoration. Furthermore, this study provides specific information on the understudied *A. cervicornis* metabolome and further confirmation that differences in metabolome structure could drive phenotypic variation among genotypes.

**Sample Description:**

Coral colonies were brought to the surface intact, and ~3 cm nubbins were clipped from actively growing branch tips. Nubbins were wrapped in aluminum foil and immediately frozen in liquid nitrogen. Nubbins were then ground down in an ice chilled mortar pastel in 10 mL of 2:1 Chloroform/Methanol solution. Supernatant was then transferred into a test tube labeled with sample I.D. and "Organic" and vortexed for 10 seconds. 2 mL of .9% NaCl was then added to each tube and vortexed for an additional 10 seconds. Samples were then allowed to separate for 15 minutes on ice. After the allotted time, the supernatant was separated and placed in a separate test tube labeled with sample I.D. and "Aqueous". Both test tubes were then stored in a -80°C freezer until processing.

The data obtained for the NMR metabolomics analysis can be found in the accompanying files:

Procedures: 1. Coral Reefs Metabolomics Procedures.docx

Study Design Tables: 2. Coral Reefs Metabolomics Study Design Table.xls

Metadata: 3. Coral Reefs Metabolomics METADATA.xlsm

Processed Data: 4. Coral Reefs Metabolomics.xlsx

Raw Data: 5. Coral Reefs Metabolomics NMR Raw Data.zip

**Notes:**

Full NMR sample preparation and analysis procedures are available in the accompanying document entitled **1. Coral Reefs Metabolomics Procedures**.

The normalized data that was used in Metaboanalyst 3.0 analysis is available in the accompanying files: **4. Coral Reefs Metabolomics.xlsx for binned NMR data.**

The raw fid as well as 1r file can be found in **5. Coral Reefs Metabolomics NMR Raw Data.zip**