NMR-based Metabolomics of Coral with Resistance to Bleaching

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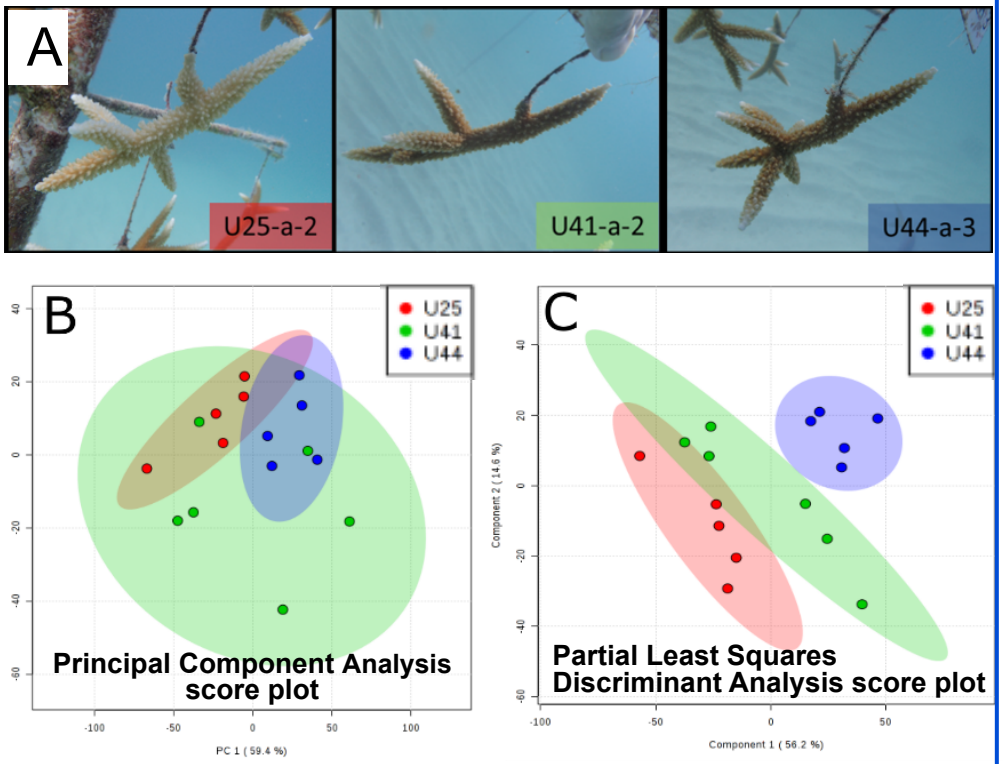
NMR-based metabolite profiling of bio fluids is exquisitely sensitive to changes in metabolism, including coral samples used in this study **[A]**. High-resolution ^{1}H spectra can generate a significant amount of metabolic data and, in conjunction with multivariate analysis, can be effective for determining variability of metabolomic profiles among unique coral genotypes. *^{1}H NMR spectra revealed unique metabolomic profiles for multiple samples from three genetically distinct variants (U25, U41, and U44) of the coral Acropora cervicornis living in a common coral nursery.*

^{1}H NMR spectra from methanol extracted *A. cervicornis* metabolite samples were collected at 14.1T. Fifty-nine chemical shifts that significantly differed between genotypes of *A. cervicornis* were identified with analysis of variance (ANOVA). Principal Component Analysis (PCA) **[B]** and Partial Least Squares Discriminant Analysis (PLS-DA) **[C]** found 72.8% and 70.8%, respectively, of total variance among genotypes in components 1 and 2. Clusters for genotypes U25 (red) and U44 (blue) are relatively separated while U41 (green) is not. *Trimethyl-amine-N-oxide, a molecule that protects against nitrogen overload, is a primary driver of species differences*.

These data provide insights into the previously unknown metabolism of corals that have a superior survivability in the face of increased coral bleaching.



[A] *Three genotypes of* Acropora cervicornis *from an established coral nursery near Tavernier, FL used in this study;*
[B] *PCA score plot with explained variances enclosed in brackets,*
[C] *PLS-DA score plot with explained variances enclosed in brackets.*

Facilities and instrumentation used: Bruker 600 MHz NMR system with 5 mm cryoprobe at the MagLab's AMRIS Facility.

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