GLOBAL METABOLOMICS

MUAL Multi-User Analytical Lab and Metabolomics Core — Clemson® University

SECONDARY METABOLITES

What is being measured: This approach is geared towards identifying the suite of small molecules in a biological system (plants, microbes, animals, etc.) in a single instrument analysis. The samples are screened for 1000's of potential compounds that comprise of products and intermediaries of secondary metabolic pathways in these systems including polyphenols, flavonoids, alkaloids, terpenes, hormones, etc.

How it is done: The samples are analyzed using liquid chromatograph coupled to an ultra-high resolution mass spectrometer. Putative IDs of compounds are generated through the matching of accurate mass (<2 ppm error) and fragmentation pattern with online, in silico, and in-house mass spectral libraries. Absolute quantitation is possible when the authentic standards are available. Relative quantitation is determined by normalization with isotope-labeled internal standards.

SAMPLE RESULTS

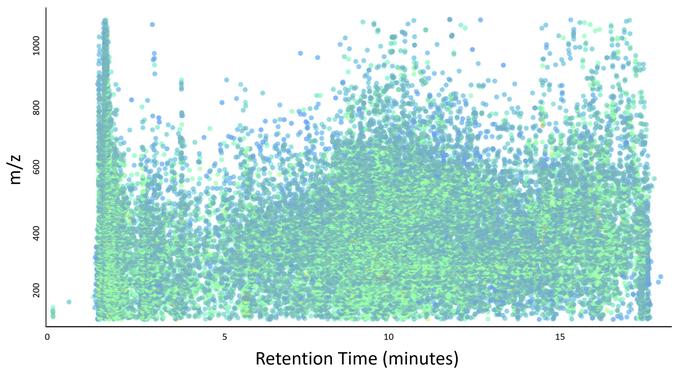
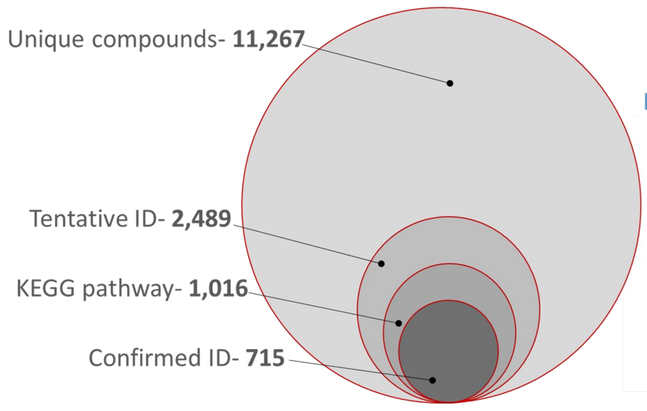


Figure 1. Total mass features detected in plant leaf tissue (x-axis is retention time (minutes) and y-axis is m/z) showing the chemo-diversity within a single plant matrix (MUAL data).



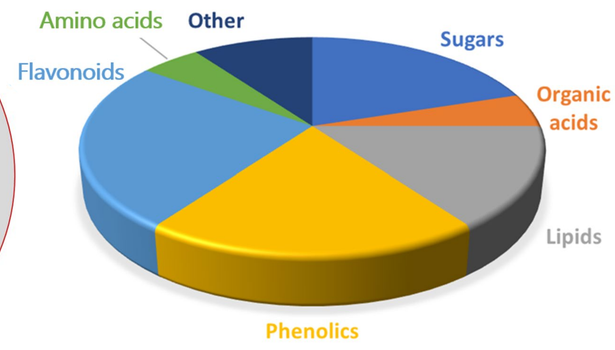


Figure 2. Global metabolome compound identification coverage. Total unique mass features detected in *Amaranthus palmeri* and total confirmed IDs using accurate mass and fragmentation pattern match scoring against mass spectral libraries (MUAL data).

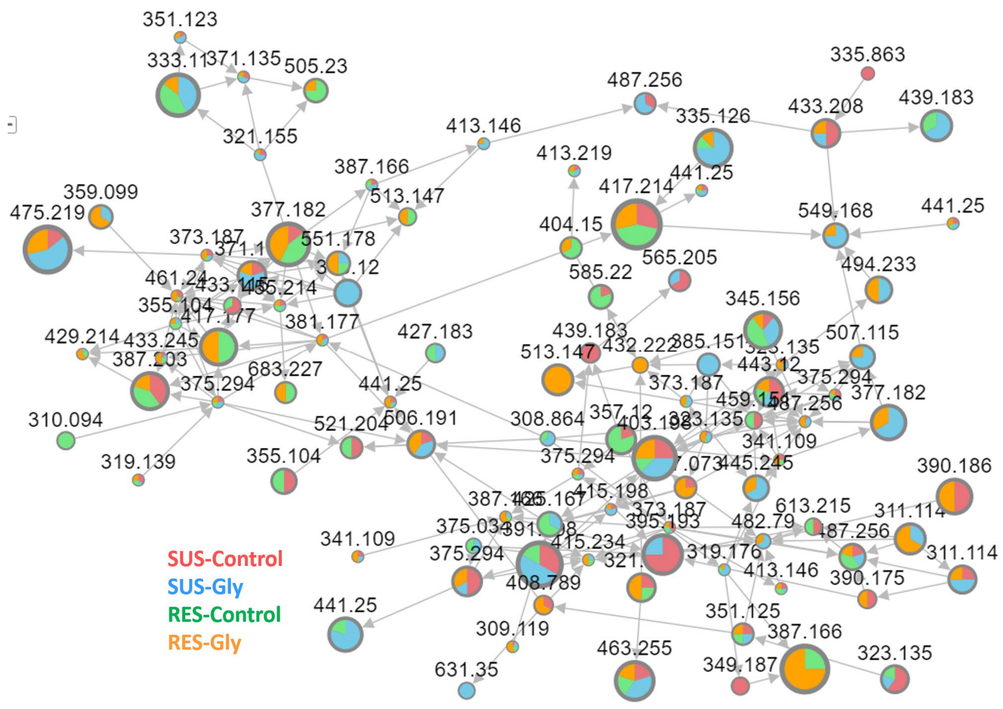


Figure 3. Subset of a molecular ion network linking structurally similar compounds detected using ultra-high resolution tandem mass spectra for identification of unknowns (MUAL data).

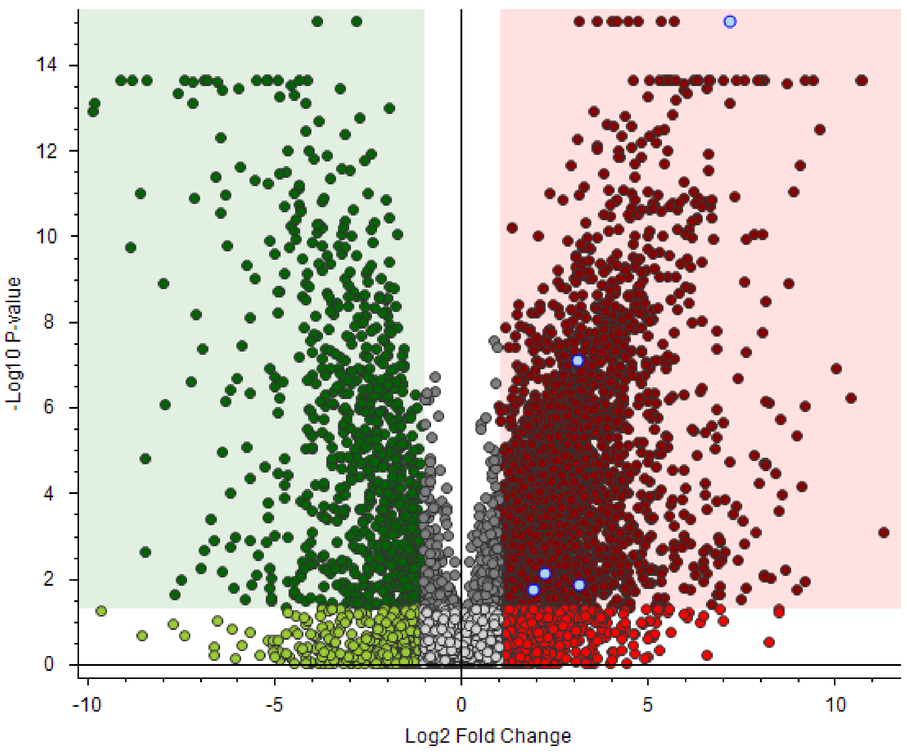


Figure 4. Volcano plot showing the fold change of significant up/down-regulation of metobolites captured through global metabolomic analysis (MUAL data).

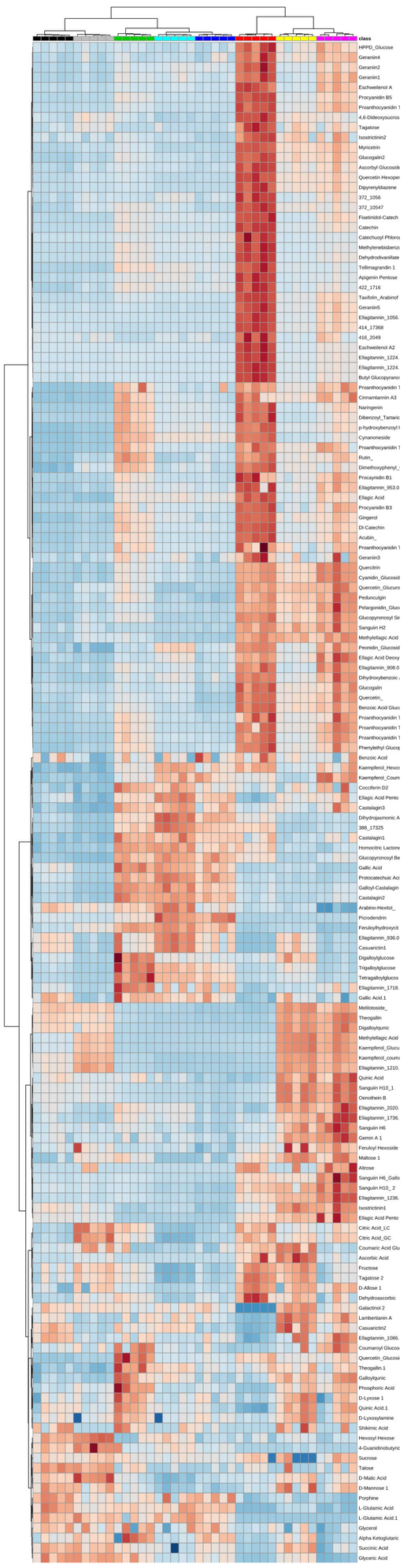


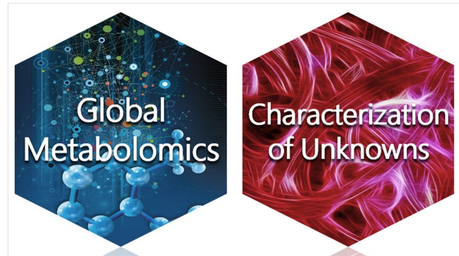
Figure 5. Hierarchical clustering analysis and 2-way heat map of 150 metabolites identified in strawberry leaves as a function of various N treatments (Narvekar, 2017).

INSTRUMENTATION

Thermo Orbitrap Fusion™ Tribrid™ Mass Spectrometer

- Combines quadrupole, ion trap and Orbitrap mass analysis in Tribrid architecture
- Ultrahigh resolution up to 500,000 FWHM
- Sub ppm mass accuracy
- Multiple dissociation techniques—CID, HCD, ETD
- ID-X capability for small molecule identification
- Coupled to HESI and nano-ESI interfaces
- UltiMate 3000 RS UHPLC & UltiMate 3000 RSLCnano

Primary applications



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