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

Global Metabolomics

CENTRAL CARBON & NITROGEN METABOLISM (PRIMARY METABOLOMICS)

What is being measured: This is an untargeted metabolomic analysis that is geared towards identifying and quantifying the end products and intermediates in C and N metabolism in biological samples as a function of experimental treatments.

How it is done: The analysis is performed using gas chromatography coupled to quadrupole time-of-flight mass spectrometer (GC-QToF), and compound identification are based on accurate mass, fragmentation pattern, and retention index. The mass spectral library resources allow us to identify >1,000 metabolites through this analysis. As needed, absolute quantification of >100 of these metabolites is performed using authentic standards. For compounds without an authentic standard, the relative abundance is reported based on isotope-labeled internal standards.

SAMPLE RESULTS

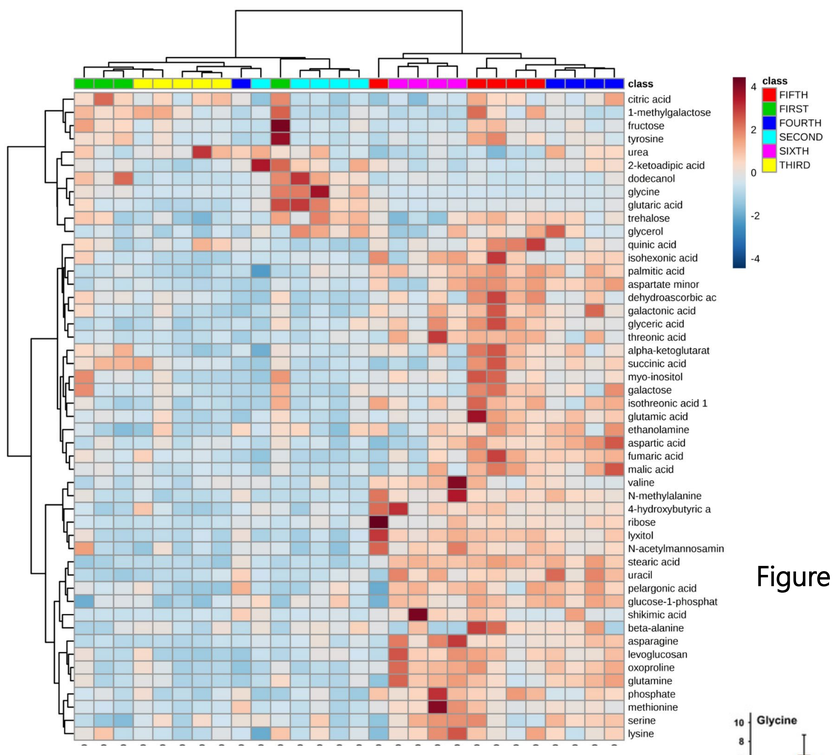


Figure 2. Heatmap and hierarchal clustering of metabolites based on relative abundance.

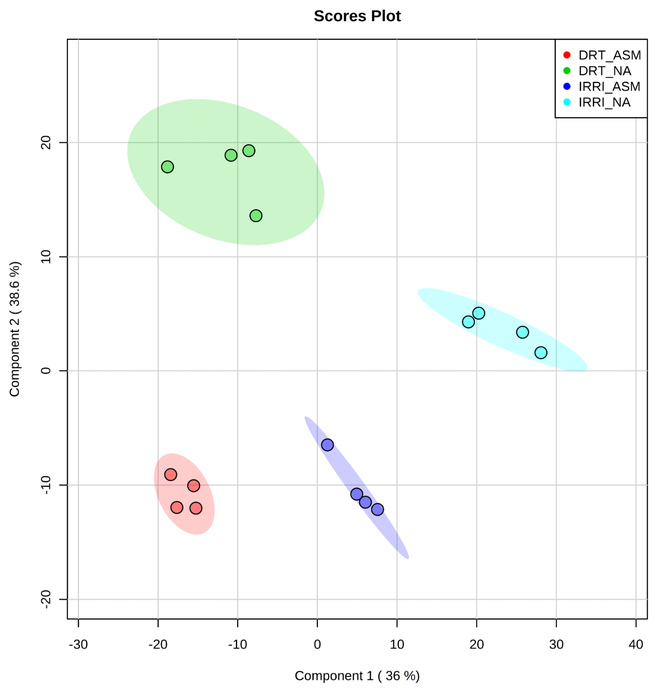


Figure 3. Partial Least Squares- Discriminant Analysis (PLS-DA) elucidating the effect of treatment on carbon and nitrogen metabolism.

Carbon & Nitrogen Metabolism

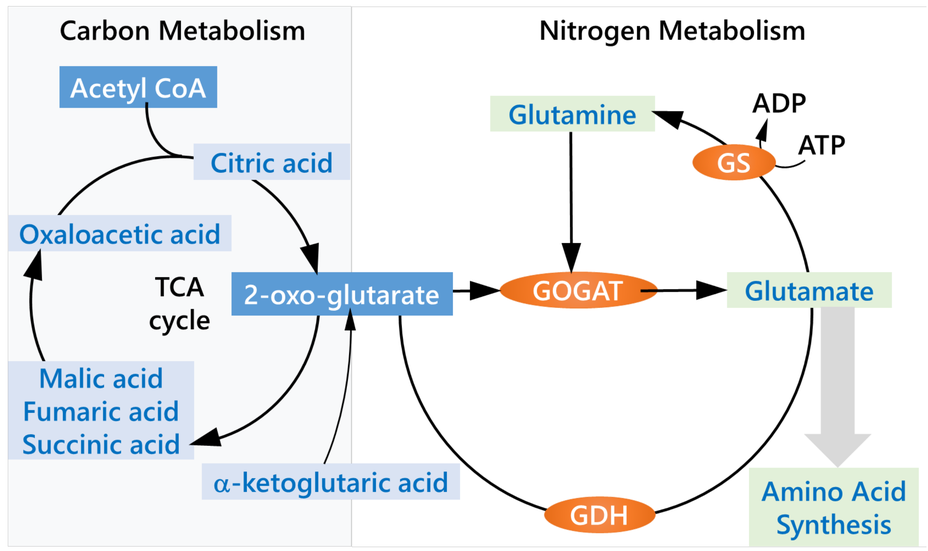


Figure 1. Central carbon and nitrogen metabolic pathways involved in organic acid and amino acid synthesis.

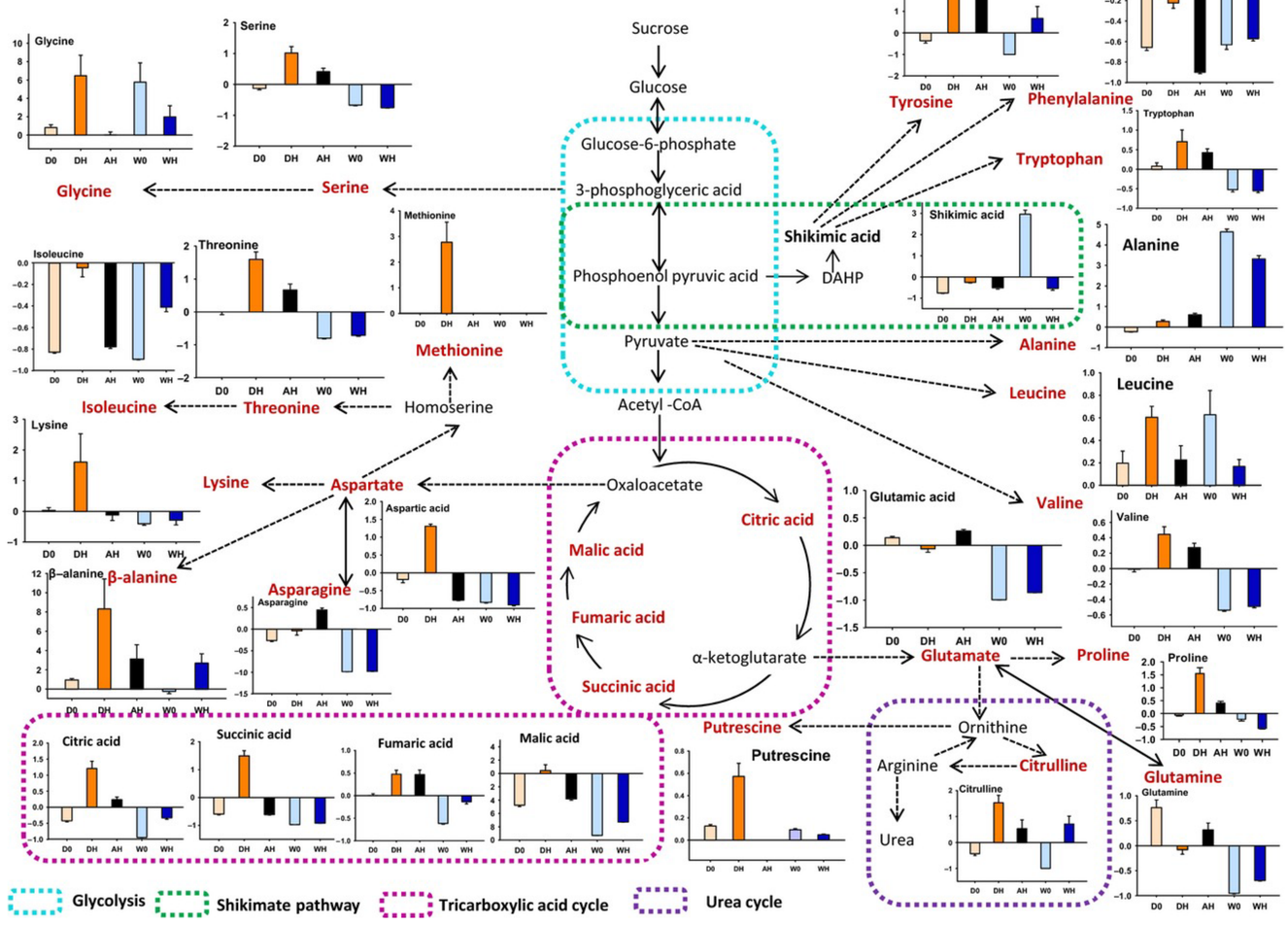


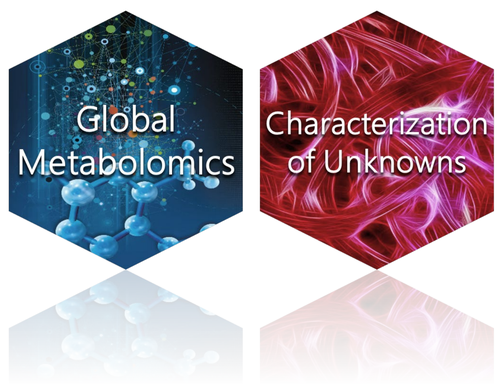
Figure 4. Path-analysis of primary metabolites during leaf senescence as influenced by climate (MUAL-data)

INSTRUMENTATION

Agilent 7250 GC/QTOF

- Quadrupole Time-of-flight mass spectrometer
- Delivers full-spectrum, high-resolution, accurate-mass data
- Low-energy EI for softer ionization and molecular ion enhancement
- Elucidates chemical structures with MS/MS capabilities
- TOF mass accuracy- < 2ppm RMS
- TOF Resolution > 25,000 at m/z 271.896
- Data acquisition rates of up to 50 spectra per second
- Electron Ionization, settable 5-200 eV

Primary applications



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Scan for more information

Amino Acids
Alanine
Alanylalanine
Arginine
Asparagine
Aspartic acid
Citrulline
Cysteine
Glutamic acid
Glutamine
Glycine
Histidine
Homoserine
Hydroxyproline
Isoleucine
Leucine
Lysine
Methionine
Phenylalanine
Proline
Pyroglutamic acid
Serine
Threonine
Tryptophan
Tyramine
Tyrosine
Valine

Phenolic acids
Caffeic acid
Cinnamic acid
Coumaric acid
Ferulic acid
Gallic acid
Hydroxybenzoic acid
Proto-catechuic acid
Salicylic acid
Sinapic acid
Syringic acid
Vanillic acid

Organic Acids
2-Aminobutyric acid
2-deoxytetronic acid
2-Oxoglutaric acid
5-Aminolevulinic acid (ALA)
alpha-Ketoglutaric acid
Ascorbic acid
Chlorogenic acid
Citraconic acid
Citric acid
Cysteine sulfinic acid
Dehydroascorbic acid
Dehydroshikimic acid
Isocitric acid
Erythronic acid
Fumaric acid
Galactonic acid
Gluconic acid
Glutaric acid
Glyceric acid
Glycolic acid
Isohexonic acid
Lactic acid
Lactobionic acid
Linoleic acid
Malic acid
Mannonic acid
Nicotinic acid
Oxalate
Oxaloacetic acid
Oxamic acid
Pyruvic acid
Quinic acid
Shikimic acid
Succinic acid
Tartaric acid
Threonic acid
Xylonic acid

Sugars
1-Kestose
Allose
Arabinose
Erythrose
Fructose
Galactose
Gentiobiose
Glucose
Hexose
Inulotriose
Lactose
Lactulose
Leucrose
Lyxose
Maltose
Mannose
Melibiose
Methylhexose
Psicose
Rhamnose
Ribose
Sorbose
Sucrose
Tagatose
Trehalose
Xylose

Sugar Alcohols
Arabitol
Erythritol
Galactitol
Glycerol
Hexitol
Inositol
Lactitol
Maltitol
Mannitol
Palatinitol
Ribitol
Sorbitol
Xylitol

Other
2-Hydroxypyridine
4-Hydroxypyridine
Adenine
Adenosine
Dihydroxyacetone (DHA)
Dopamine
gamma-Aminobutyric acid (GABA)
Glycerol-3-galactoside
Guanine
Mannosylglycerate
Methionine sulfoxide
N-Acetyl glucosamine
N-Methylnicotinate
Paeoniflorin
Pantothenate
Putrescine
Salicyl alcohol-b-glucoside
Serotonin
Uracil
Urea
Uridine