Global profiling of metabolites, the small molecules produced by living things, provides one of the most powerful strategies for learning about gene and protein functions. This approach, known as metabolomics, is generating information that will serve as the foundation for engineering of plants and microbes to produce renewable feedstocks for high-value bioactive chemicals and biofuels. Metabolite profiles also are important indicators of health and disease, and many metabolites serve important signaling functions that regulate physiological states ranging from inflammation to resolution of tissue damage.

Research in the Jones laboratory is driven by a desire to understand how genetics and environment combine to influence biological chemistry by: (1) developing analytical and biochemical tools for deep profiling and spatial localization of specialized metabolites, (2) developing experimental and data mining approaches to accelerate discoveries of natural products in medicinal and non-model plants and the genes involved in their accumulation, (3) deployment of mass spectrometry strategies to identify and quantify byproducts generated during processing of lignocellulosic biomass for conversion into renewable fuels and chemicals, and (4) measurements of metabolic biomarkers of inflammation, analgesia, and resolution of disease.

Many plants accumulate large quantities of bioactive phytochemicals in specialized epidermal cells known as glandular trichomes, which are prolific biochemical factories. Our laboratory has pioneered rapid metabolite profiling protocols based on ultrahigh performance liquid chromatography (UHPLC) coupled to time-of-flight mass spectrometry (MS). By employing rapid gradients and by multiplexing collision potentials across a lens between the mass spectrometer ion source and mass analyzer, ~500 metabolites are measured in a 5-minute analysis. This allows for large-scale screening of genetic variants to guide gene function discoveries. Trichomes are also amenable to mass spectrometry imaging, allowing for extensive chemical interrogation of individual trichomes across plant tissues. Ongoing research involves labeling metabolites using $^{13}$C to investigate metabolic dynamics coupled with elucidation of metabolite structures using MS and NMR.

We also investigate whether inflammatory, anti-inflammatory, and analgesic metabolite biomarkers in the blood and urine of human patients indicate mechanisms underlying the effectiveness of various treatments of COPD and traumatic brain injury. In addition, since more diseases are associated with environment and lifestyle than specific genetic factors, our lab is adapting our analytical methods to investigate the exposome, which is the entire range of molecules (e.g. from foods, environment, gut microbes) to which individuals are exposed.

Laser desorption ionization mass spectrometry imaging of two insecticidal acylsugar metabolites in leaf trichomes of the wild tomato relative Solanum habrochaites LA1777.