



## Metabolomics and Small Biomolecule Analysis

**Context**—Metabolomics is an analytical profiling technique for measuring and comparing large numbers of metabolites in cells, tissues, biofluids, or organisms. This approach combines high-throughput analytical chemistry and multivariate data analysis and offers a means to understand metabolic mechanisms. The identification and quantification of these trace level, molecules, and metabolites in biological samples represents a considerable challenge. The main methodologies used for metabolite recovery and identification are untargeted and targeted mass spectrometry-based techniques. Untargeted metabolomics aims to measure the broadest range of metabolites present in a sample without a priori knowledge of their chemical identity. Conversely, targeted metabolomics provides higher sensitivity and selectivity than untargeted metabolomics, whereby methods are developed and optimized for the analysis of previously identified specific metabolites and metabolic pathways of interest.

**Resources and Instrumentation**—CESE has extensive analytical expertise and advanced instrumentation in both untargeted identification and targeted quantification of small bioactive molecules and their metabolites in biological matrices. Instrumentation includes:

- Sciex X500R ultra high-performance liquid chromatograph - time-of-flight high resolution mass spectrometer (UHPLC-QToF).
- Ultra performance liquid chromatograph/tandem mass spectrometer (UPLC-MS/MS).
- Ultra performance liquid chromatograph with evaporative light scattering, fluorescence, and photo diode array detectors.
- A variety of sample preparation equipment such as a Genevac centrifugal evaporator.



**Research Capabilities**—CESE has considerable capacity to support a diversity of metabolite and small molecule (< 2000 Da) research projects by providing a quantitative assessment with high precision, for a wide array of small organic bioactive molecules, as well as providing expertise in biostatistical analysis and experimental design.

Examples of projects that CESE can support include:

- Analysis of fatty acids and fatty acid metabolites as indicators in patients with chronic hepatitis.
- Assess metabolic changes of cancerous tissues to identify metabolites as potential biomarkers.
- Quantification biomarkers for diagnostics or potential new drug targets.
- Determining the mechanism of action of small molecule drugs by monitoring the associated metabolic pathways.
- Identification of regulated metabolites in the pathogenesis of disease as potential biomarkers.
- Using untargeted analysis to develop metabolomic models to identify biomarkers of malnutrition in fish.