



## Untargeted Analysis – Biomedical and Environmental

**Context**— Analyses of complex mixtures of molecules in biological and environmental samples are an extremely challenging task. Targeted approaches provide good sensitivity, consistent identification, and precise quantification of pre-identified target compounds. However, this traditional approach has a significant drawback as it always will miss compounds that were not pre-identified at the start of the analysis, including unknowns or untargeted substances, even if at high concentrations or with bioactive potential. Over the past decade, new hardware and software tools have been developed that make non-targeted screening approaches reliable and affordable, expanding the depth and breadth of opportunities in research.

Untargeted analytical approaches are being used in support of research in a variety of fields, including, gut microbiota profiling, environmental contaminant and metabolite screening, and natural product and bioactive compound discovery.

**Resources and Instrumentation**—CESE has extensive analytical expertise and advanced instrumentation to support identification and quantification of untargeted and unknown compounds in ground and surface waters, biological tissue, soil, and sediment.

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)
- Custom sample extraction equipment to eliminate contamination of samples with PFAS
- Genevac automated concentrator

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**Research Capabilities**—CESE has considerable capacity to support a diversity of research projects related to the quantitative and qualitative analysis of unknown or unidentified compounds.

Examples of projects that CESE can support include:

- Measurement of the concentrations of cellular metabolites (Metabolomics).
- Quantitative assessment of metabolic responses of living systems to foreign stimuli (Metabonomics).
- Human and ecological risk assessment through the quantification of PFAS and other emerging organic contaminants in biological tissues and the environment.
- Suspect screening of micropollutants in wastewater, surface water, and drinking water.
- Characterization of bioactive phytochemical compounds and natural products.
- Screening of extracts from *Cannabis* spp. for pesticides and other pollutants.