

# Research metabolomics assays

Our research metabolomics assays include:

## **Lipidomics:**

Required sample volume (EDTA plasma): 75  $\mu$ L

**What:** A semi-quantitative HILIC MS/MS method covering more than 1200 targets in 19 lipid classes resolved at the fatty acid chain level has been developed and validated. Electron Activated Dissociation (EAD) methods will be optimised and used to induce more extensive fragmentation of molecular ions than usually obtained by collision-induced dissociation.

**How:** After a liquid-liquid extraction, HILIC chromatography is coupled to a triple quadrupole mass spectrometer which operates at polarity switching mode. Instrumentation used for this assay comprises of a Sciex ExionLC coupled to a Sciex QTRAP 6500+ mass spectrometer.



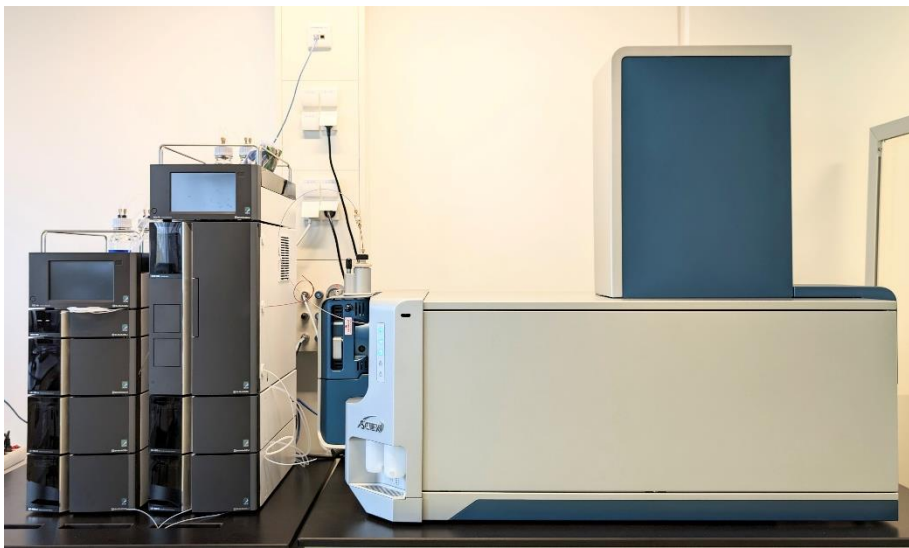
*Instrumentation used for lipidomics assay*

**Global apolar untargeted profiling:**

Required sample volume (EDTA plasma): 150 µL

**What:** This assay reports apolar metabolites including biogenic amines, organic acids, carbohydrates, di-/tri-peptides, bile acids, steroids, free fatty acids, and exposure markers, such as food, drugs, PFAS, pesticides and other pollutants.

**How:** After a protein precipitation step and phospholipid removal, these metabolites are measured by reversed-phase UHPLC-MS after two separate injections: one in positive ionization mode and one in negative ionization mode. Metabolite identification is executed by SWATH-MS analysis based on our in-house spectral library. Instrumentation used for this assay comprises of a Shimadzu UHPLC coupled to a Sciex ZenoTOF 7600 mass spectrometer.



*Instrumentation used for global apolar untargeted profiling assay*

**Live Single Cell metabolomics:**

Required sample volume: single mammalian cells, frozen cell pellet, cells in 2D/3D culture, 10  $\mu$ L of sample

**What:** This assay reports untargeted metabolic measurements of single cells or volume-limited samples. Single cell drug monitoring can also be achieved if the drug can be suitably ionized and detected by mass spectrometry

**How:** Cells are cultured in their optimal environment, and under microscopic observation, sampled using micro glass capillaries. Ionization / extraction solvent is then added to the opposite end of the capillary. The capillary also acts as a nano-ESI source where ionization and spraying into an Orbitrap 480 mass spectrometer occurs. Data is processed and analyzed using our in-house data analysis pipeline and a putatively annotated feature list is generated and reported



*Instrumentation used for single cell metabolomics assay*