

Metabomeeting

A new comprehensive two-dimensional gas chromatography coupled to high resolution time-of-flight mass spectrometry (GC×GC-HRTOFMS) approach in metabolomics

N. DI GIOVANNI, J.-F. FOCANT, Liège University, Belgium

University of Liège, Chemistry Institute (B6c), Mass Spectrometry Laboratory, Organic & Biological Analytical Chemistry Group, Allée du Six Août, 11, Quartier Agora B-4000 Sart-Tilman, (Liège) – Belgium.

For the last few years, comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (GC×GC-TOFMS) appeared to have high potential in metabolomics. Based on our experience in the field of small molecule separation in complex biological fluids, we developed an innovative GC×GC- high resolution(HR)TOFMS method for the metabolic profiling of biofluids, with a focus on human serum and inflammatory bowel diseases.

State-of-the-art experimental design (ED) and data processing tools have been used for the optimization of this analytical approach. We focused our efforts on the implementation of a strong QA/QC procedure to ensure the integrity of the data produced. Our quality control system is based on the use of internal standards, QC serum aliquots, control charts, and carefully chosen criteria and the validation -accuracy and precision- on the certified reference material (NIST SRM 1950).

We further developed a dedicated data processing strategy based on proper signal alignments, class-to-class comparison, implementation of statistically relevant F_{critical} threshold values to enhance our chances to highlight and uniquely identify analytes expressing the highest degree of influence on statistical segregation of our samples classes.

We hope this method development exercise would contribute to offer better analytical tools for the use of metabolomics in clinical research.