

HYPHENATED TECHNIQUES IN CLINICAL SCIENCES : GC×GC-HRTOFMS APPROACH IN METABOLOMICS

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For the last decade, metabolomics has been receiving more and more attention in clinical sciences, with multiple applications and challenges. Based on our experience in the field of small molecule separation in complex biological fluids, we developed and validated a 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, the major bottleneck recognized in the field. 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.