
HYPHENATED AND MULTIDIMENSIONAL ANALYTICAL METHODOLOGIES FOR METABOLONOMICS

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Metabolomics aims at the comprehensive quantitative analysis of all metabolites in a biological system and describes metabolic changes caused by disease, environmental, nutritional, or genetic factors in an organism. Typically, the goal is to identify metabolites that can be used as specific biomarkers of a certain disease. Since the metabolome comprises thousands of small molecules, this constitutes a huge analytical challenge. To obtain this goal, highly efficient tools are required for sample preparation, analysis and data processing of the samples. Due to the large diversity of the metabolites, several analytical techniques are utilised in the characterisation of the metabolites. For polar and nonvolatile species, such as lipids, liquid chromatography-mass spectrometry (LC-MS) is an appropriate choice. For the analysis small, volatile metabolites, comprehensive two-dimensional gas chromatography-time-of-flight mass spectrometry allows a very high separation efficiency. Typically, the number of samples is very large, and thus, also the development of efficient tools for the data analysis is crucial in metabolomics. In this study, LC-MS, GC-MS and GCxGC-TOFMS systems together with several in-house developed data analysis methodologies were utilised in the search of biomarkers for selected chronic diseases. The sample matrices included serum and different types of tissue samples. The data-analysis methods allow processing and visualizing both LC-MS and GCxGC-TOFMS data and they have capability to perform batch processing for large number of files, support for parallel processing.