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# CRITICAL EVALUATION OF GC-MS AND COMPREHENSIVE GC-MS FOR TOTAL METABOLITE PROFILING

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Total profiling techniques are very popular in metabolite studies. GC-MS and, more recently GCxGC-MS are extensively used for this purpose. The availability of broad spectrum derivatisation strategies like oximation and silylation allows the derivatisation of large amounts of the, often very polar, metabolites in e.g. plant extracts, bacteria or yeast samples resulting in complex chromatograms containing a lot of biochemical information. The parallel development of many software programs allows for fast data processing which is mainly based on peak alignment and comparison algorithms. The resulting peaks for which the highest deviation of the mean value is measured can subsequently be identified or targeted by the MS. The data can also be treated by multivariate statistical analysis techniques such as principal component analysis to differentiate samples from various origins or conditions. This approach is typical in biomarker discovery programs whereby e.g. samples from ‘healthy’ and ‘unhealthy’ subjects are compared. The main difficulty with this broad spectrum non targeted analysis is, however, that many causes of variability can originate from reasons other than the one which is aimed at in a particular study. Many of those can be of biological origin (age, gender, time of sampling, diet, smoking, history of the patient, etc.) requiring particular care during sampling as has been observed numerous times before. Even the best profiling techniques, however, also still suffer from high analytical variabilities. In this study the use of GC-MS, and various forms of GCxGC-MS have been evaluated for the analysis of total profiles of plant, bacteria and yeast extracts. The possibilities of oximation, silylation, methylation and esterification are critically compared and the deleterious effects of sample stability, column degradation because of the use of excessive and aggressive reagents are demonstrated. The goal is thereby to ensure that the important aspect of having a much lower analytical variability as compared to the biological one is more easily ensured. The benefits of more targeted group type profiling are demonstrated for the analysis of various plant hormones from plants of different type, origin, age and which have been exposed to various conditions.