COMPREHENSIVE DATA ANALYSIS: UNTARGETED METABOLITE DISCOVERY IN TIME-SERIES GC-MS DATA

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Metabolomics is an emerging field in life-sciences research involving the comprehensive identification and quantification of (small molecule-) metabolites present in biological systems such as plants, animals or humans. Since it is often not known a-priori which metabolites change due to an intervention, profiling methods based on chromatographic or spectroscopic (or combinations thereof) is often applied in order to obtain maximum information on the metabolomics samples. When chromatographic profiling is performed on kinetic studies, *i.e.* metabolomics studies in which the time response is monitored after an intervention, complex data seta are obtained. Obviously, only the combination of advanced analytical techniques and sophisticated data analytical tools will allow the extraction of useful information from the huge quantity of data in a timely manner.
In kinetic studies, the interesting metabolites are those that exhibit certain behaviour versus time following an intervention. For example, they will first be formed and then excreted, i.e. their metabolic profile will first increase and then decrease. This type of information can be used to distinguish the more relevant metabolites from those not following a kinetic curve profile pre-defined as “of interest”.
We present a new strategy for metabolite discovery based on univariate techniques to check whether a detected chromatographic peak shows a reasonable profile versus sampling time. Applying these techniques, new metabolites may be discovered in kinetic data usually only used for target-compound analysis. The new strategy will be demonstrated on a sample set obtained from a polyphenols gut fermentation study.