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All ion differential analysis in product control applications using comprehensive GCxGC/MS

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Many applications in comprehensive GCxGC/MS relate to finding differences between a newly measured sample and a so-called reference sample. These questions may typically arise in application areas like product control or during trouble shooting. Examples are: what are the new impurities present in a new batch compared to a reference batch?; why does this product behave differently compared to our reference batch? And; the comparison of samples in food fraud applications to detect illegally added substances. Typically for the above examples is the limited time available to solve these problems. Furthermore, most of the time only a few samples are available, which excludes the use of statistical comparison tools as applied in the field of metabolomics. Although GCxGC-MS has become an invaluable laboratory analysis tool, the procedure may produce gigabytes of data per sample in four dimensions, which makes data analysis time consuming and complicated. In the presentation, new methods and software tools will be presented to quickly find differential components from a comparison between two samples only. Certainly, comprehensive GCxGC/MS is a technique having superior separation capabilities compared to 1-dimensional GC/MS, but co-elution or near co-elution still might occur, especially in complicated matrices. Whereas most software tools for GCxGC/MS use processing of "TIC" data only, our new methods apply data analysis using the "all ions" approach. The implemented method allows for the detection and de-convolution of differential components that are not or badly separated, even in two dimensions. It will be demonstrated that processing using the "all ion" approach will substantially detect more (differential) components, compared to the analysis using TIC data only. Technical details of the algorithms will be explained and examples will be given from applications like food analysis, product control in flavor & fragrance industry and from base chemistry industry.
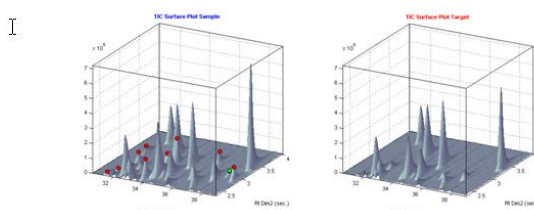
Figure 1: Differential Analysis results between Sample on the left and control on the right. Differential Peaks have been marked in the plot.

Biography

Marco Ruijken is the Owner/ Head of Research of MsMetrix, Maarssen the Netherlands. MsMetrix develops informatics solutions for LC/MS and GC/MS Data Analysis in the area of: Metabolite Profiling, Metabolomics, Proteomics, BioMarker Discovery, and Impurity / Degradation Profiling. Our mission is to be the premier provider of fast, affordable, user-friendly and reliable software in the above application fields. His educational background is in Chemometrics/Statistics and Processing of complex data. Current research topics are advanced deconvolution in GC/MS and GCxGC/MS with the focus on Differential Analysis. Furthermore, we are specialized in implementing ideas or requirements from universities or companies into our existing software tools.

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Page 49