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Product control using differential GC/MS and comprehensive GCxGC/MS

Marco Ruijken
MsMetrix, Netherlands

During product control or trouble shooting, the investigator is often confronted with two samples; one sample relates to the good quality product, while the other sample can be an out-of-spec batch, or a sample with bad product characteristics, e.g. having a different smell or taste. Typically for the above examples is the limited time available to solve these problems. GC-Analyzer is a software product developed to detect differences between two samples at very low levels. All fragmentation ions are searched for being different between both samples. De-convolution and subsequent identification (NIST) is implemented to quickly identify possible components of interest. Similar algorithms have been developed to handles comprehensive GCxGC-MS data. Certainly, 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.

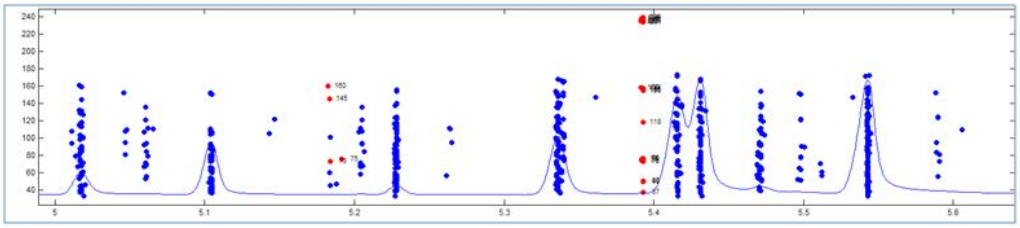

Figure 1: Differential analysis Dot Plot, showing differential peaks in red and similar peaks in blue.

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.

mr@msmetrix.com

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