

In-depth analysis of complex VOC mixtures by GC×GC-HRTOFMS

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Comprehensive two-dimensional gas chromatography coupled to mass spectrometry (MS), and especially to a time-of-flight MS (GC×GC-TOFMS) is a powerful Separation Science tool. It combines advantages from the added peak capacity and zone compression of GC×GC and from the deconvolution of mass spectral signals of TOFMS. This can further be completed by accurate mass measurements for proper analyte identity assignments. GC×GC-TOFMS is of particular interest for the study of complex volatile organic compound (VOC) mixtures in biological areas. The collection of exhaustive data sets including first and second retention time values (1t_R and 2t_R), intensities, mass spectra, accurate mass values,... however results in the production of large files that require specific treatment before they can be exploited. On the top of basic spectral alignment and normalization, supervised and non-supervised statistics have to be used to extract the relevant information from the multidimensional perspective. Moreover, because of the biological variation always observed between replicates of similar data sets, because numbers of replicates are often limited by practical issues, and because long lists of analytes are produced for each single sample, the data treatment exercise on such flat tables is even more complicated. Practical examples such as metabolite profiling, breath analyses, cell culture monitoring, cadaveric decomposition studies, combustion processes, beer analyses... will be presented to illustrate various statistical approaches such as Fisher discrimination ratio, principal component analysis (PCA), and profiling of VOC signatures.