Comprehensive two-dimensional separation and analysis of plant volatiles using Gas Chromatography and Mass Spectrometry (GCxMS)

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Multidimensional analysis in chromatography can be defined as any technique that combines two or more distinct separation or analysis steps, where at least one of the steps or dimensions involves a chromatographic separation.

The concept of multidimensional chromatography can be extended to some detectors that also have separation capability, such as the mass spectrometer. For Mass Spectrometry (MS) the term "separation" requires a mechanism that is able to produce a "distinguishable label" for the individual components on a mixture. However the mass spectra produced by electron ionization (70 eV EI) cannot meet this requirement, because EI produces multiple fragments and similar classes of compounds will have similar fragmentation patterns. However, when MS is applied using a soft ionization technique, such as field ionization (FI), only one type of ion (parent ions) is produced in the mass spectra of each component allowing this combination of GC and MS to be used as a separation/ identification tool. In fact using MS with FI, the application of the multidimensional separation concept is fulfilled and additionally a two dimensional separation device, GCxMS, is achieved allowing a separation of unknown mixtures through measurement of the exact mass of each component in a comprehensive way.

In this communication, the application of the comprehensive two-dimensional separation using GC and MS (GCxMS) to the study of the volatile fraction composition of pine needles and white clover is demonstrated and compared with comprehensive two-dimensional gas chromatography technique (GCxGC).