

Non-target Characterization of Complex Essential Oil and Fragrance Samples with GCxGC-MS/FID for Reliable Identification and Relative Quantitation in a Single Injection

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Abstract

Flavours, just like fragrances, are composed of tens or hundreds of ingredients selected from a palate of thousands. Identifying and quantifying individual species in a fragrance or flavour is challenging, requiring a dual workflow, using MS for identification and FID for quantification. Additionally, due to the complexity of these samples, two analyses are often required to isolate the individual compounds; one using a polar and another using a non-polar GC separation.

Here, we demonstrate a possible improvement to this workflow using a prototype GCxGC-TOFMS/FID instrument applied to essential oils and fragrances. GCxGC provides enhanced chromatographic separation of individual analytes, thus removing the requirement for two separate 1D assays. Using MS and FID, applying dual detection enables both identification from MS data and area % quantification via the FID in one injection. Quantification accuracy, when using area % determinations, can be affected with many fixed or EPC splitters due to variations of the split ratio across the analytical run. The prototype instrument used in this study uses a reverse fill flush modulator, allowing total transfer of the primary effluent to the secondary column and a controlled splitter that maintains a consistent split ratio between the MS and FID. These characteristics help to ensure that biases are not introduced from changing split ratios throughout the chromatographic separation, which could skew quantification. Novel algorithms that align the MS and FID peaks facilitated data interpretation. Various samples were analysed, demonstrating reliable analyte identifications and quantifications from single injections.