

PT15 Determination of the composition of fatty acid mixtures using gas chromatography combined with field ionisation mass spectrometry: a comprehensive two dimensional separation approach

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Fatty acids are identified by location on a plane defined by mass and relative retention.

Gas chromatography (GC) using a highly polar column combined with field ionisation mass spectrometry (FI-MS) is used as a comprehensive two-dimensional (2D) separation¹⁻³ approach to analyse mixtures of fatty acid methyl esters (FAMES). A unique ordered pattern and classification of FAMES is obtained in a 2D GC×FI-MS separation plot. FAMES are classified based on the number of carbons, the degree of unsaturation and a combination of both by which the geometrical, positional and structural isomers group together. The method also provides sub-classifications such as grouping of the FAMES with different chain length but identical geometry, position and degree of unsaturation. Non-fatty acid compounds and fatty acids with various functional groups are identified using the ordered separation pattern of the FAMES in the GC×FI-MS plot and the exact mass data from the FI-MS mode. The latter also acts as a high resolution separation technique to separate overlapping peaks. The method is illustrated by and applied to samples of fish, canola and biodiesel oils and two standard mixtures of 37 FAMES and linolenic acid methyl ester geometrical isomers. A great wealth of information is achieved in a single run.

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