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Poster Session Day 2

Position-Specific Isotopic Analysis (PSIA) by ^{13}C NMR using the intramolecular referencing concept: application to fatty acid methyl esters

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^{13}C-NMR appears as a generic tool for PSIA [1]. Thus, ^{13}C intramolecular isotopic composition can be established with adequate trueness and precision on the δ-scale expressed in ‰ or mUr. For reaching such a performance, all the peaks of the ^{13}C spectrum should be integrated with high accuracy, allowing thus the satellites contribution to be corrected (^{13}C-^{13}C coupling). Then combined with the global $\delta^{13}Cg$ value measured by irm-MS, the calculation of positional $\delta^{13}Ci$ is achieved [2].

However, difficulties arise when analyzing complex molecules such as fatty acids due to signal overlap, which makes the accurate determination of $\delta^{13}Ci$ more complicated. Relative comparisons are still possible, but the "absolute" $\delta^{13}Ci$ are not available [3]. To overcome this limitation, the internal chemical referencing has been proposed, [4]. But these approaches require high level of "know-how" for a routine analysis.

We present a novel methodology that leverages the concept of isotopic intramolecular referencing, specifically applied to the position-specific ^{13}C isotope analysis of saturated fatty acid methyl esters. This method uses the methoxy signal (O-CH_3) as an internal standard, which is a robust isotopic reference. For this purpose, we have shown that the $\delta^{13}Cg$ of the methanol used for (trans)esterification of the fatty acids is stable and exempt of isotope fractionation. The whole methodology is repeatable allowing the expression of $\delta^{13}Ci$ on the classical δ-scale. As an illustration, the method was applied on FAMEs from several sources as butter and coconut oil.

References

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