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NMR-based metabolomic in study on fruit-oils: Determination of optimal treatment on fruits and differences on oil composition

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Introduction

This research aims to study several vegetable oils (tiger nut, pistachio), to understand how different treatments on the fruit can improve the oil composition. Besides, the major and minor metabolites in walnut oils from different varieties are also included in this study.

Methodology

a) Multinuclear NMR analysis

^{1}H, ^{13}C and ^{31}P NMR experiments were carried out by triplicate on the oil samples.

b) NMR data processing and statistical analysis

After processing each spectrum, the NMR data matrices were used to record statistical analysis in terms of Linear Discriminant Analysis (LDA).

Results and discussion

1H and 31P NMR experiments show differences in the prole of the different oils. On the basis of ^{13}C NMR quantification of the unsaturated fatty acid content in each sample, only the pistachio oil samples from fruits submitted to toasted treatments show a slight decrease in oleic acid and an increase in linoleic acid with temperature and time. To carry out the LDA, groups of samples were generated in terms of the toasted treatments. Using the 1H NMR data, although the separation is not extreme, the distinct groups can be easily differentiated from each other suggesting a correct interpretation of the results on the composition.

The 13C NMR analysis of the different walnut varieties help differentiate the samples by their content in linoleic acid, which is the major component. They can be categorised into four groups according to the decreasing content in linoleic acid and subsequent increase in oleic and linolenic acids. The LDA on the 1H NMR data shows a strong separation between these pre-defined groups.

Conclusion

We herein report an efficient analysis of metabolites of different vegetable oils by NMR spectroscopy and statistical tools, constituting a valid approach for sample characterization in terms of fruit pre-treatment and varieties.