Nuclear Magnetic Resonance and Chromatography Data Fusion approach for authentication and traceability of Italian hazelnuts

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Abstract for **oral communication.**

In the past years, the interest towards metabolomics has been considerably gaining momentum. Its application ranges from medicine to environmental science, also including life science, agriculture, and food science. In the latter, robust and sensitive methodologies need to be developed and continuously updated to assess traceability and to guarantee quality and safety of a huge variety of food products [1].

Accordingly, NMR-based and LC/MS-based approaches have been established as useful tools in Foodomics studies. The high reproducibility of the NMR technique, combined with its low difficulty in the automatization of the entire analytical process, even with very large numbers of samples, makes it suitable for high-throughput analysis [2]. On the other hand, LC/MS combined techniques show a remarkable sensitivity and excellent identification capabilities [3].

In this perspective, the present study proposes a promising NMR–LC/MS combined approach applied to traceability and authenticity of an Italian food excellence, the "Tonda Gentile Trilobata" (TGT) hazelnut variety, which in 1996 obtained the Protected Geographical Indication (PGI) collective label from the European Union [4].

Using ^{1}H solution nuclear magnetic resonance (^{1}H-NMR) spectroscopy and ultra-high-performance liquid chromatography coupled with electrospray ionization quadrupole time-of-

flight mass spectrometry (UHPLC-ESI/QTOF-MS) we analyzed 54 hazelnuts samples of different origin, variety, and production year (2020 and 2021). All samples were finely ground and treated with a methanol extraction process. Then, different volumes of the extracted liquid were submitted to the two analytical techniques.

Data originating from both techniques were imported into MATLAB environment to be analysed with multivariate statistical tools. The two datasets, i.e. the spectral data from NMR analysis and the quantified compounds from LC/MS, were firstly treated separately with different pre-processing methods, mean centering and autoscaling respectively, and then investigated with principal component analysis (PCA). The PCA models of the two separate datasets revealed interesting clusters related to production year, but also groupings referable to Piedmont origin and to the TGT variety. For these reasons, we decided to apply a data fusion approach by creating a new joined dataset containing data from both techniques. Because of the diversity of the PCA results obtained from NMR and LC/MS, we chose a mid-level data fusion approach. The new dataset was therefore obtained combining the scores of the first 10 principal components of each PCA model, i.e., the individual model of each characterization technique.

The new fused dataset was explored with PCA and then used to build three different classification models using partial least square discriminant analysis (PLS-DA). The obtained cross-validated models, with different performances and robustness, were able to distinguish year of harvest, hazelnuts of Piedmont from other origins and TGT variety from other varieties.

References

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