

CAN NMR SPECTROSCOPY PAVE THE WAY FOR COMMUNITY-BUILT ANALYTICAL SYSTEMS?

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NMR spectroscopy is gaining ever-growing importance in analytical chemistry. In the last decade, quantitative NMR (qNMR) and non-targeted approaches allowed for great improvements in both quantification of molecules in complex mixtures and identification of product features in suitable sample pools. Metrological traceability of products can be successfully achieved by qNMR even when no certified reference materials are commercially available. Along with quantification and purity assessment of molecules, NMR is emerging also as a powerful tool in food chemistry, especially when searching for product features such as cultivar, geographical origin, typicality of the production process, etc.

The great application potential of NMR spectroscopy derives from the fact that, based on theory, the ratio between a signal generated by the molecule under investigation and the signal of a reference molecule depends exclusively on the corresponding mole ratio. In other words, when a given sample is analyzed by different spectrometers, the same output is obtained in terms of signal ratios independently of the hardware configuration. This offers the unique opportunity to develop community-built analytical systems capable of identifying sample features and quantifying a number of molecules.

In this presentation, based on our previous studies carried out with different NMR spectrometers (300 to 700 MHz),^[1,2] the first examples of community-built analytical systems will be shown. In particular, the case study of a data-driven grape juice identification system will be presented along with the advantages and the limitations of using non-targeted NMR analyses performed at different magnetic fields. Moreover, quantification of metabolites in grape juices by using a community-built calibration tool will be also shown.^[3] The feasibility of NMR spectroscopy to generate statistically equivalent NMR signal ratios from a number of different spectrometers will be demonstrated also for other complex mixtures such as aqueous extracts of wheat and flour.^[4] Finally, potential use of benchtop NMR in both quantification of standard molecules and valorization of food biodiversity will be introduced.

Acknowledgements. This work has been supported by Ministero dell'Università e della Ricerca (Program Agreement ACPR20_00189)

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