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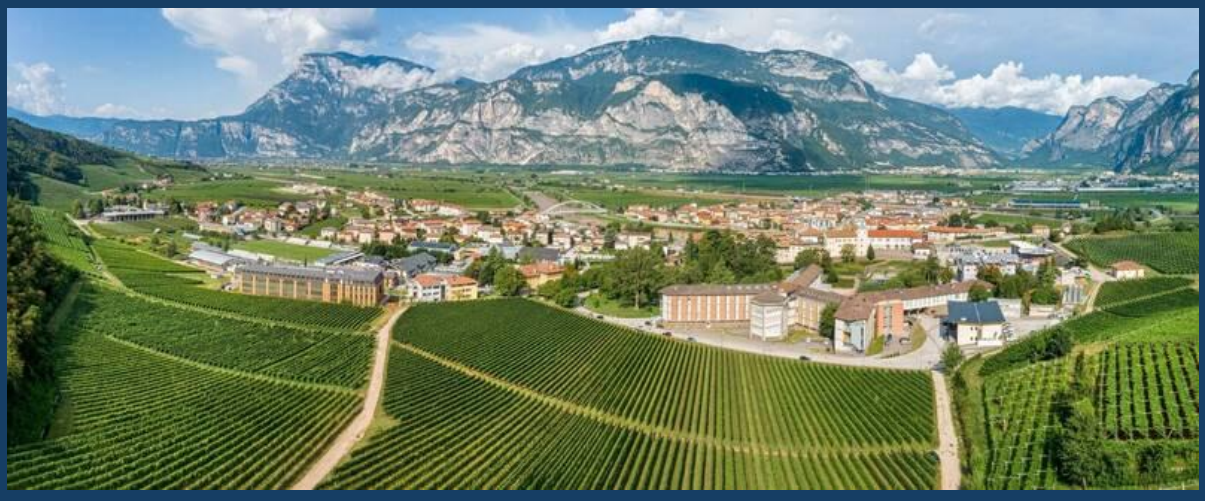
BOOK OF ABSTRACT



O15. Application of NMR spectroscopy and metabolomics in food science

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NMR Spectroscopy, Metabolomics, Food Analysis

Nuclear magnetic resonance (NMR) spectroscopy saw its first use in food analysis very shortly after its discovery, in the early 50s, albeit at a low resolution for determination of water content. In the next decades, as higher resolution fields and especially Fourier transformation and superconductive magnets became available, it entered this area too for determining fat composition in plant and animal oils and similar materials. In the early 80s isotopic fractionation by deuterium NMR entered the scene and has cemented its place and official recognition as a powerful tool in controlling the authenticity of various alcoholic beverages throughout Europe and beyond. Very soon the next milestone was reached, as the development in magnet filed strength and computing power allowed us to utilize NMR for liquid foods such as milk, fruit juices, vinegar and the like, often with the aid of water suppression techniques. At the beginning of this century, chemometric tools began to see wide application for differentiation and authentication of diverse food matrices. As of today, two general strategies have emerged. The first one is called targeted profiling, a quantitative determination of components or metabolites. The second one is called non-targeted profiling, and it consists in viewing the whole NMR spectrum of the food matrix sample and interpreting it as a unique fingerprint of the product. Both approaches imply the use of statistical methods, such as principal component analysis (PCA), partial least squares (PLS), linear discriminant analysis (LDA), factorial discriminant analysis (FDA), and combinations of these.

The last few years have seen rapid development in the so-called artificial intelligence, which is already finding its first uses in this field as well.

Compared to other analytical techniques such as gas or liquid chromatography coupled with mass spectroscopy (MS), infrared (IR) and ultraviolet-visible (UV-VIS) methods, NMR requires less laborious sample preparation, features decreased time in data acquisition and the equipment maintenance costs are significantly lower. Naturally, NMR spectroscopy also has its intrinsic limitations. The sensitivity, when compared to that of MS, is several degrees of magnitude lower, even when cryoprobes are used. The structure of the spectra is in many cases quite complex, which makes interpretation of data very challenging; the initial purchase cost of NMR equipment may also be higher with respect to MS/IR/UV ones.

Various types of NMR analyses, from isotopic to metabolomics have been applied in Edmund Mach foundation over recent years. The lecture will cover these in more detail.

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