NMR SPECTRA AS WINE FINGERPRINTS

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Various NMR techniques and their application in determining various parameters influencing a wine's quality will be discussed, such as the investigation on geographical origin, variety and vintage. Ranging from one-dimensional ^1H NMR with solvent suppression for water and ethanol signals, quantitative inverse-gated ^{13}C NMR, to the other less represented nuclei such as ^{31}P NMR, which can be used to determine glycerol content in wine. NMR spectroscopy has several advantages over other conventional techniques such as simple sample preparation and the absence of need for calibration standards. ^1H NMR can be used in both targeted and untargeted analysis, as well as for quantitative determination of wine metabolites.[1-3] Lastly, the vast amount of information contained within a single NMR spectrum of a wine can act as a fingerprint when coupled with advanced statistical methods such as deep reinforcement learning.[4]

A selected example of using DOSY (Diffusion-ordered) NMR spectroscopy in the investigation of sparkling wines will be presented. It can provide information on hydrodynamic radii, which in turn gives insight into the molecule size, and can aid in the analysis of complex mixtures. In sparkling wine investigation, DOSY NMR can help better resolving signal overlapping observed in ^1H NMR, which usually hinders useful information.

The potential of NMR spectroscopy in wine analysis even further increases by using modern statistical approaches like deep reinforcement learning protocols for analyzing experimental data providing reliable models for wine classifications, sensory property determination and fraud detection.

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