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Forensic Isotope Ratio Mass Spectrometry

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Oral

IRMS, SNIF-NMR and Proton NMR in Wine Analysis

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Wine is an important element of world food industry; last year the wine production in EU was over 180 million hl (over 60% share of the world) and contributed over € 7 billion to EU trade balance. Such large markets always attract fraudulency and wine is no exception: in 2012 to 2015 counterfeit goods have cost € 59 billion, of these spirits and wine being € 2.7 billion.
Therefore, effective control of such adulterations requires use of robust and reliable analytical methods for authentication of wines.
One of these is isotope ratio mass spectrometry (IRMS), via which it is possible to measure ratios of nature stable isotopes of carbon, hydrogen and oxygen in wine. They depend on the origin of the compounds containing them and, therefore, allow for determining geographical origin of the samples and addition of water and exogenous sugar.
Another approach is Site-specific Natural Isotopic Fractionation Nuclear Magnetic Resonance Spectroscopy (SNIF-NMR). By this method, the site-specific D/H isotope ratio in methylic and methylenic sites of ethanol is measured, and the values aid in determining the origin of ethyl alcohol in wine. In 1990s European Commission and International Organization of Vine and Wine (OIV) has adopted this method as a certified official method for analysis of wines. It is the only method based on NMR recognized as official standard.
IRMS and SNIF-NMR methods are robust and reliable, but have some disadvantages, such as use of expensive standards, prolonged sample preparation, expensive equipment maintenance; also, the analysis is destructive in many cases.

Over the recent years, a new approach for wine analysis emerged: proton NMR spectroscopy, which can be used for either targeted analysis, or non-targeted profiling. Compared to classical methods, proton NMR requires less sample preparation, less time to record the spectrum and has cheaper equipment maintenance costs. However, it has not yet been officially approved for food authentication.