

Measuring methods available and examples of their applications

^1H NMR (Proton nuclear magnetic resonance)

The most basic experiment is a simple one-dimensional **proton NMR spectrum**. ^1H NMR is a suitable method for purity control, analysis of mixtures and confirmation of molecular structure. It is widely used in the pharmaceutical, medical, and food industries for quality control. The experiment is highly sensitive and measurement time is short.

Simple NMR spectra are recorded in [solution](#), and [solvent](#) protons must not be allowed to interfere. [Deuterated](#) (symbolized as D) solvents for the specific use in NMR are preferred. The most common solvents used include [deuterated water](#), D_2O , deuterated [acetone](#), $(\text{CD}_3)_2\text{CO}$, deuterated [methanol](#), CD_3OD , [deuterated dimethyl sulfoxide](#), $(\text{CD}_3)_2\text{SO}$, and [deuterated chloroform](#), CDCl_3 . Approximate minimal concentrations of samples are 0.1 mM for ^1H (corresponding 0.015 mg, based on molecular weight 300 and sample volume 0.5 ml). Deuterated solvents permit the use of deuterium frequency-field lock (deuterium lock) to eliminate the effect of the natural drift of the NMR's magnetic field. Proton NMR spectra of most organic compounds are characterized by [chemical shifts](#) in the range +15 to -4 ppm and by [spin-spin coupling](#) between protons. The [integration curve](#) for each proton reflects the abundance of the individual protons.

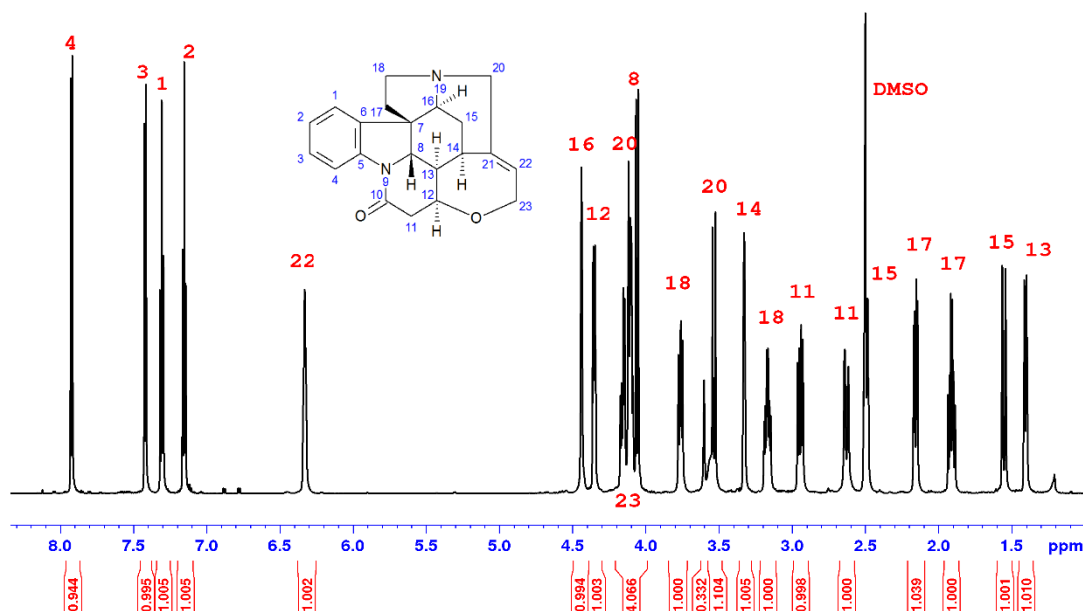


Fig. 1. ^1H NMR spectrum of Strychnine in DMSO-d_6 with assignment

One example of the many applications shows detection of methanol in an alcoholic beverage below. Maximum allowable content of methanol in alcoholic beverages is specified by the Regulation (EC) No. 110/2008; for example, 12 g of methanol per 1 l of ethanol for most fruit distillates.

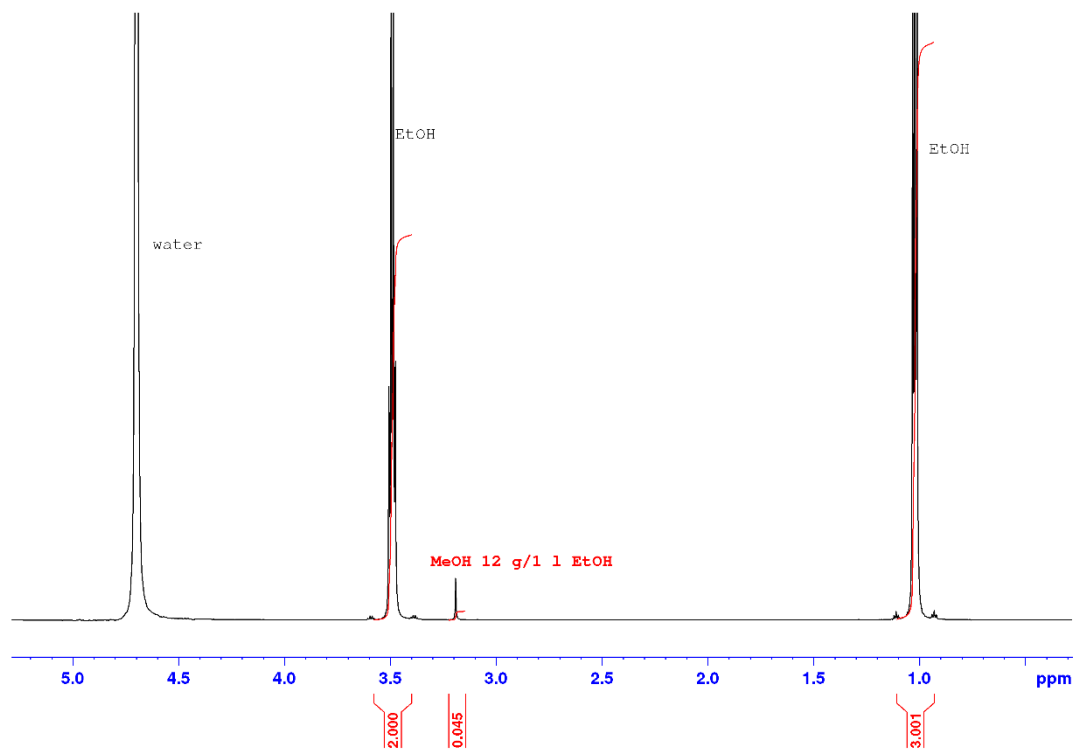


Fig. 2. ^1H NMR spectrum of fruit distillate, time of analysis approx. 5 min.