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Benchtop NMR Spectroscopy Without Deuterated Solvents

Most discussions on proton NMR spectroscopy are based on the fact that spectra are typically recorded in solutions prepared with deuterated solvents. The reason for this is that a protonated solvent will give rise to large solvent peaks which may obscure spectral features of the solute. Furthermore, most modern NMR spectrometers rely on the solvent's deuterium signal for shimming and locking. Although there are certain advantages in using proton-free solvents, it may be desirable to examine a reaction or a product in its native solution. The Magritek Spinsolve benchtop NMR spectrometer uses a fast external lock and does therefore not require deuterated solvents for high-resolution performance. In this note, we show some representative examples of proton NMR spectra recorded in fully protonated solvents.

Ibuprofen

Two samples of a 200 mM solution of ibuprofen in chloroform were prepared, one in deuterated and one in a protonated solvent. Spectra were recorded with the Quickscan option of the *1D Proton* protocol. Figure 1 shows the spectra for both samples.

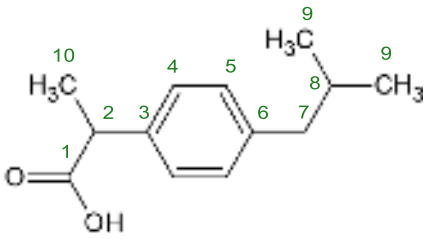


Figure 1

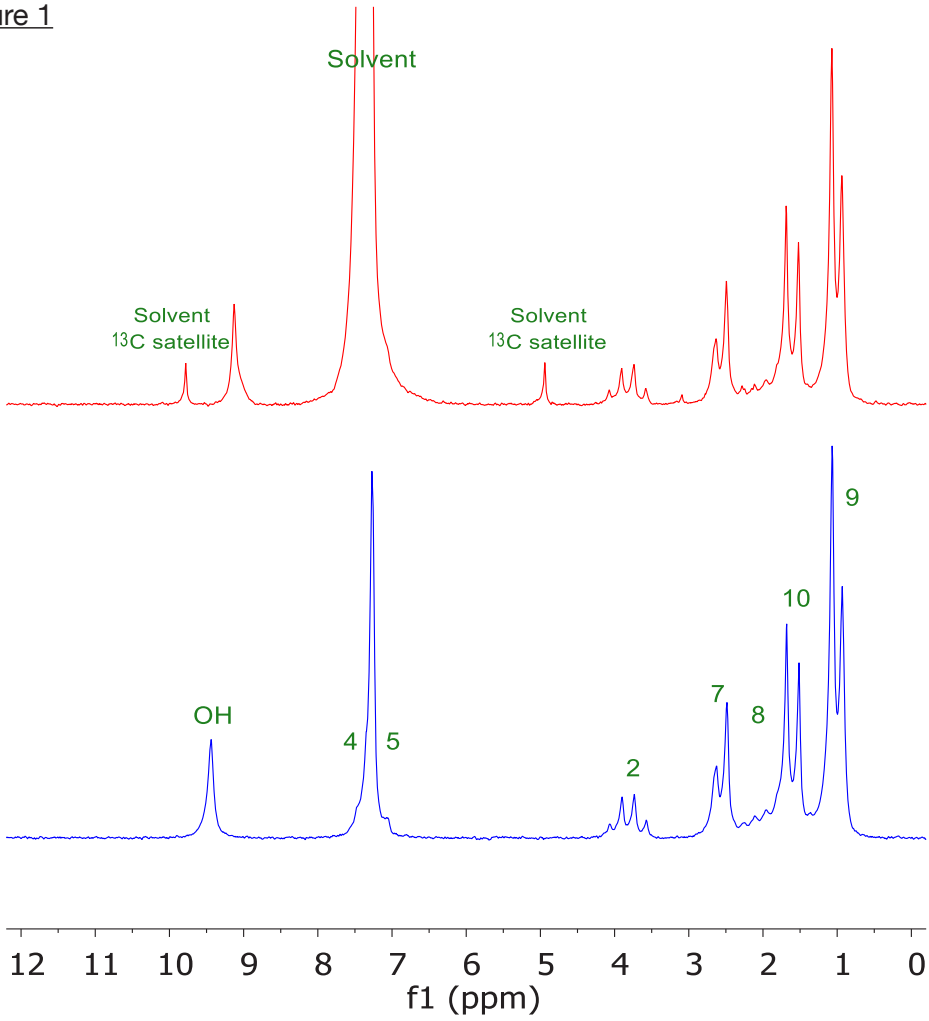


Figure 1: NMR spectrum of 200 mM Ibuprofen in $CHCl_3$ (red) and in $CDCl_3$ (blue). Although the solvent peak overlaps with peaks 4 and 5 of the solute, all other spectral features can be resolved very clearly.

Nitration of AcetanilideILIDE

In this second-year chemistry experiment, students synthesise *p*-nitroacetanilide through the nitration of acetanilide.

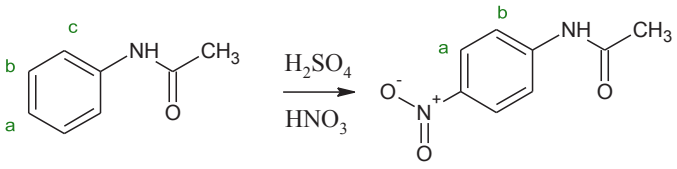


Figure 2

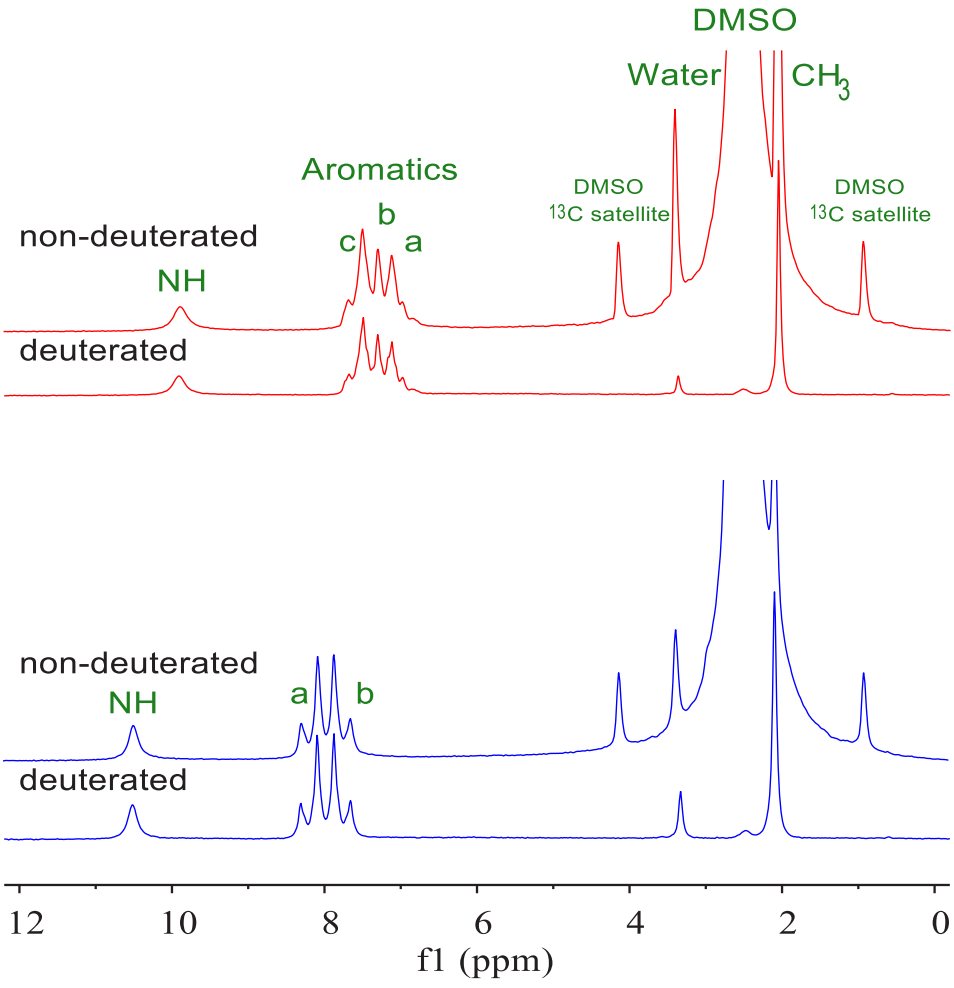
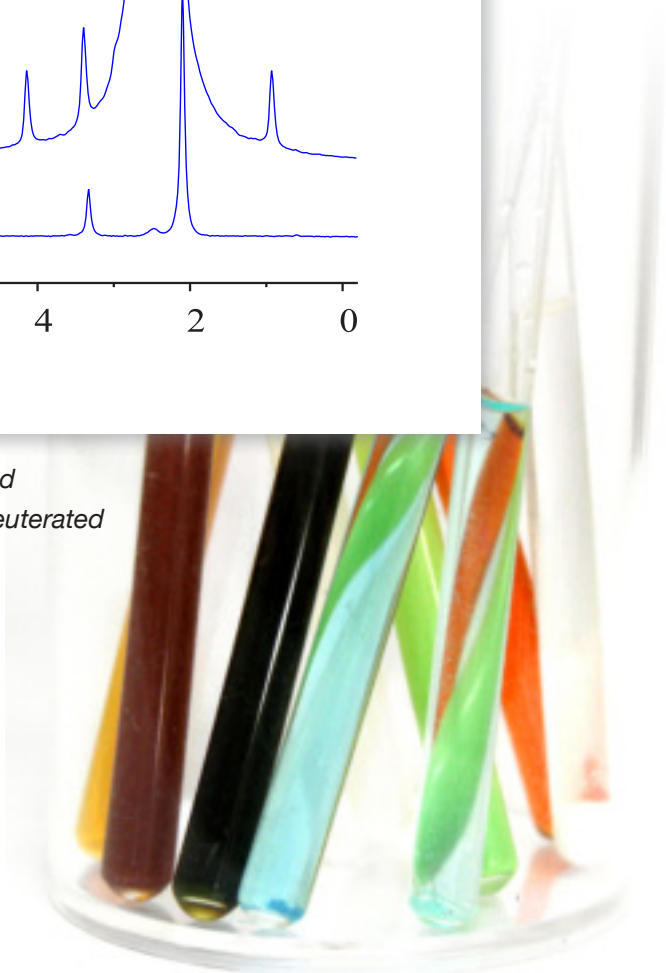


Figure 2: NMR spectra of 200 mM acetanilide (red) and p-nitroacetanilide (blue) in deuterated and non-deuterated DMSO.



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Caffeine

A sample of caffeine dissolved in water was taken from a chromatographic column for benchtop NMR analysis.

No further sample processing or purification was required. The proton NMR spectrum is shown in Figure 3.

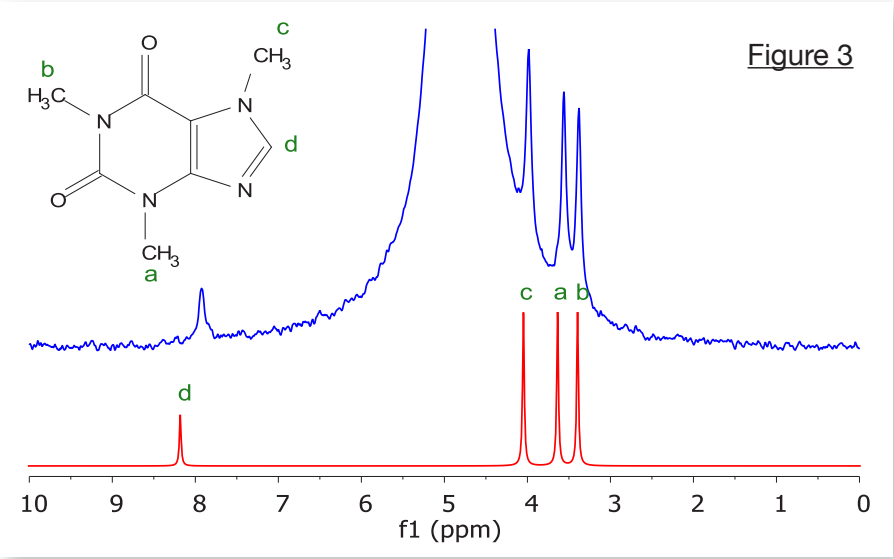

Figure 3: Measured NMR spectrum of caffeine in H_2O (blue) as taken from a HPLC column, and the simulated NMR spectrum of the molecule (red).

Conclusion

The Spinsolve benchtop NMR spectrometer has been used to record proton NMR spectra in deuterated and non-deuterated solvents. Although there may be a slight disadvantage in the large solvent peak obscuring peaks of the solute, the vast benefit in using non-deuterated solvents is that reactions and reagent solutions can be routinely studied in the native solution. Such issues, as well as running costs, become important when using benchtop NMR as an on-line monitoring tool.

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Website: www.magritek.com/contact-us

GERMANY +49 241 9278 7270

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