# High Resolution NMR Spectroscopy in a Benchtop NMR System





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This compact system combines a permanent magnet generating a very homogeneous 1 Tesla magnetic field with modern electronics and RF technology. Using standard 5 mm NMR sample tubes it offers the highest resolution and sensitivity as well as superb stability in a benchtop NMR system. Its modern lock system and software flexibility make possible the implementation of multidimensional experiments that facilitate structure determination in more complicated samples. In this poster the performance of the benchtop spectrometer is demonstrated using industry standards and other molecules.

#### PRECISE SHIMMING FOR HIGH RESOLUTION

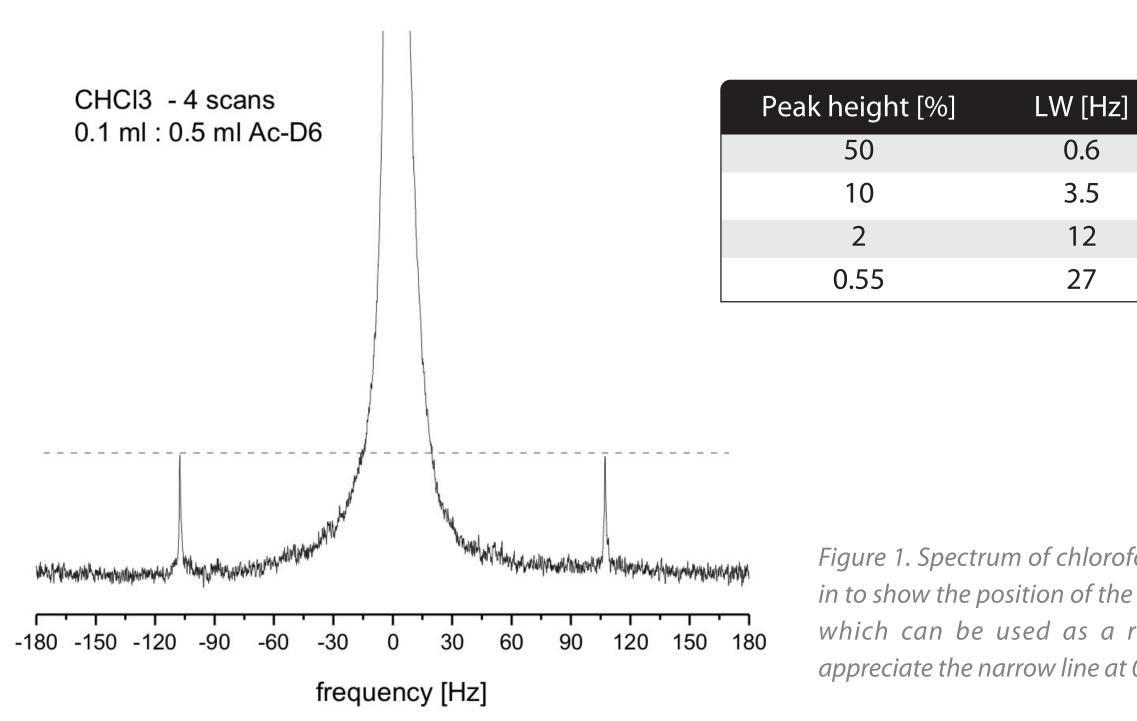


Figure 1. Spectrum of chloroform zoomed in to show the position of the <sup>13</sup>C satellites, which can be used as a reference to appreciate the narrow line at 0.55%.

0.6

3.5

12

27

#### **SUPERB SENSITIVITY**

The sensitivity of NMR spectrometers is typically measured in the quartet of a 0.1% ethyl benzene solution in CDCl<sub>3</sub>. Using this method in this system we measure an SNR of 11.3 in a single scan.

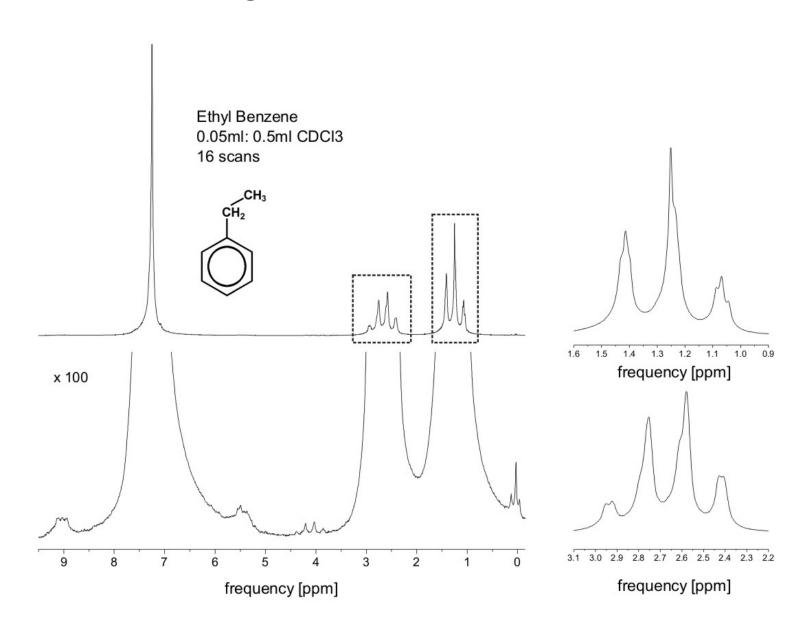


Figure 2. Spectrum of Ethyl benzene (10% concentration) where the high SNR (over 4000 for 16 scans) can be appreciated by zooming verticaly by a factor 100 to observe the structure of the <sup>13</sup>C satellites. Even at this zoom level the noise is hardly observed in the spectrum. The high resolution allows one to resolve the fine structure of the multiplet lines.

## NARROW LINES FOR HIGH RESOLUTION

The high resolution offered by this system makes it possible to resolve not only 2J but also vicinal indirect couplings. This can be appreciated in the spectrum of 4hydroxy-propiophenone shown in Fig. 3. The high SNR in the spectra also opens the door to line-narrowing resolution enhancement techniques. An example is shown below.

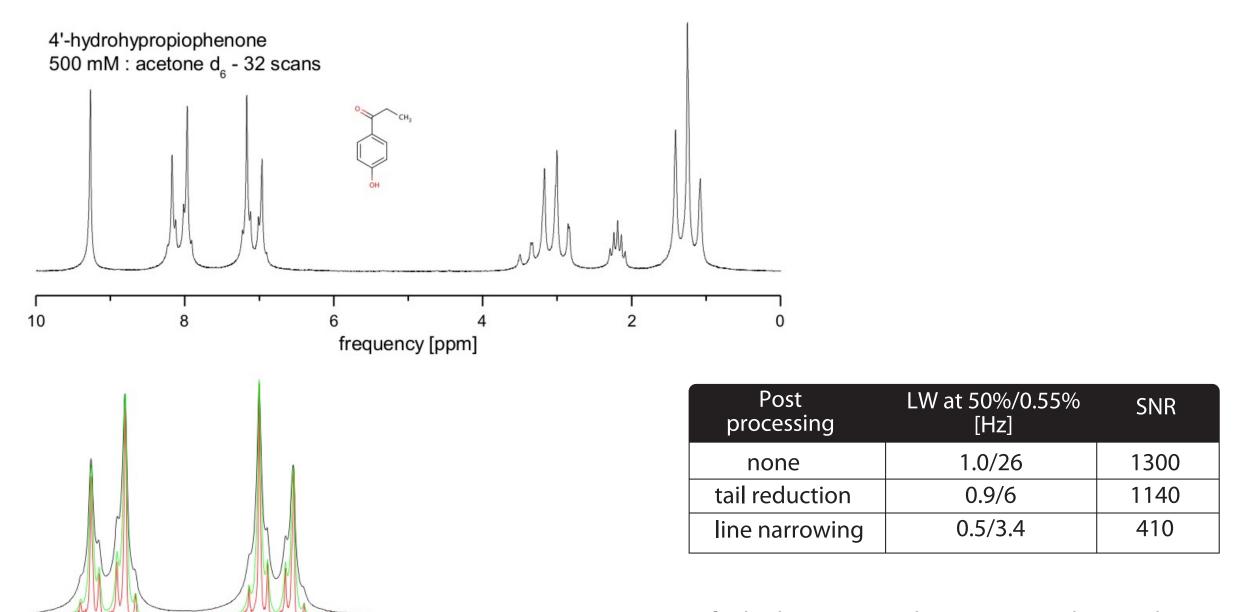


Figure 3. Spectrum of 4-hydroxypropiophenone. Vicinal J-coupling can be clearly resolved. The high sensitivity in the spectrum allows one to apply line narrowing in order to enhance resolution.

#### **RESOLVING MORE COMPLEX STRUCTURES**

Figure 4 shows different spectra of more complicated molecules dissolved at 10% concentration. The spectra are obtained as FT of the raw data, without filtering or additional line broadening or narrowing.

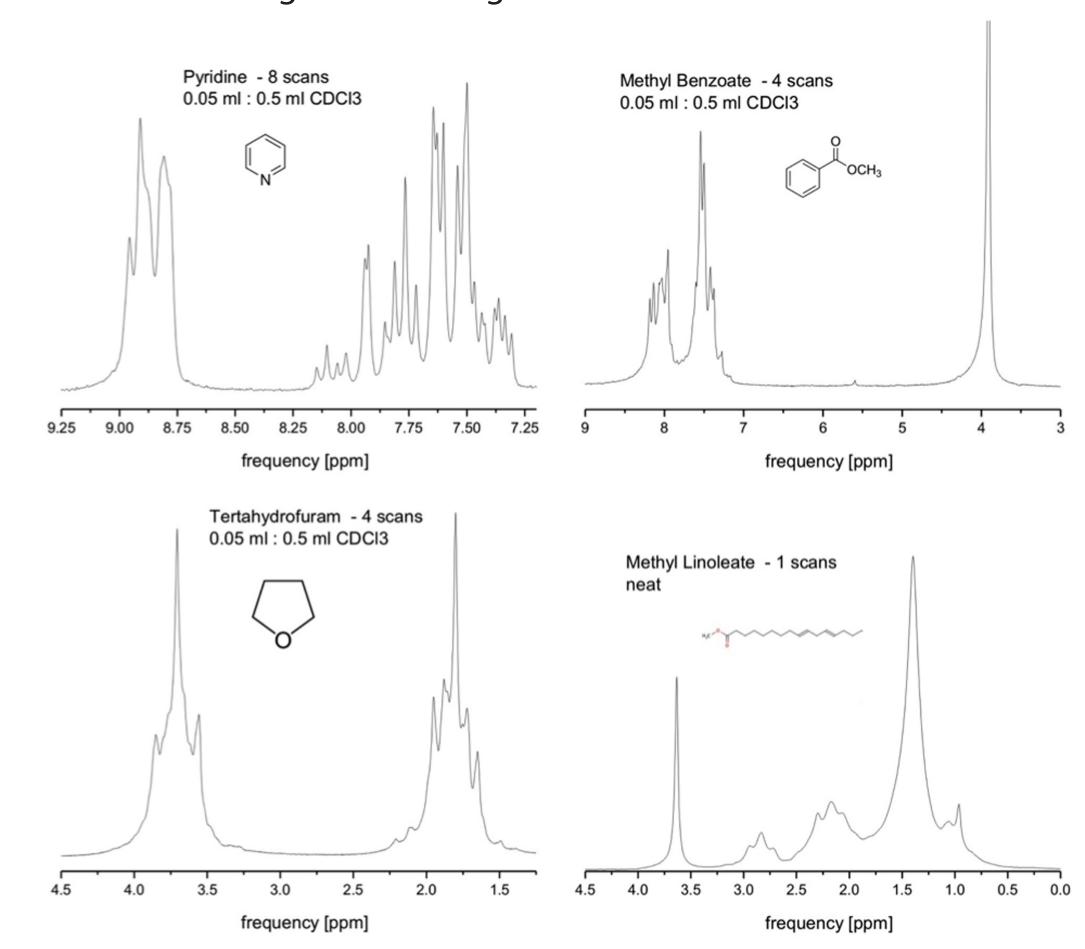


Figure 4. Spectra of more complex structures are shown to illustrate the performance of the system.

## **STABILITY**

The stability of the system was measured by acquiring a spectrum of a sample of neat ethanol every 30 s over a period of 24 hours. No room temperature control was applied. Figure 5 below shows that day/night temperature fluctuations of ±2 °C do not affect the NMR frequency or linewidth.

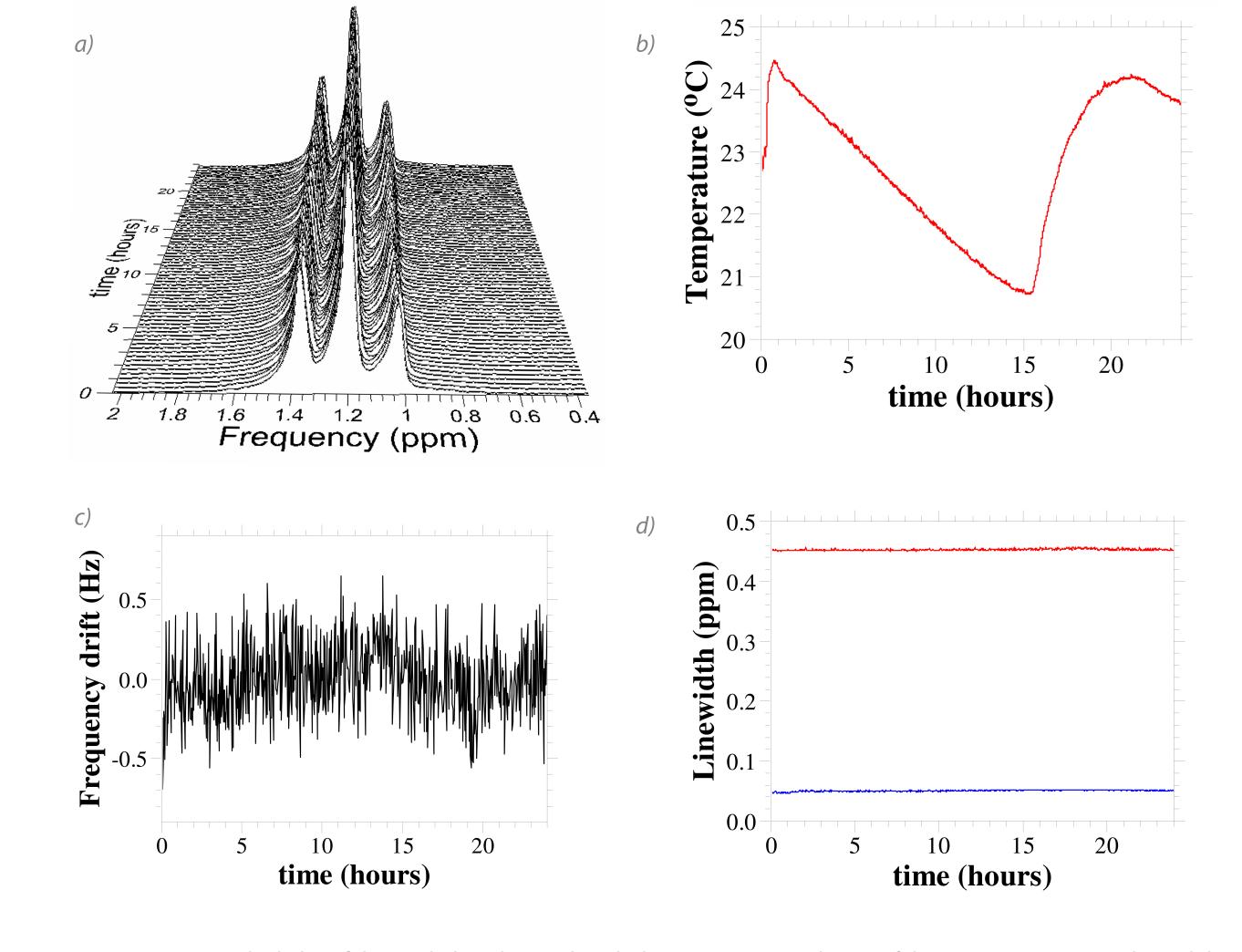


Figure 5. (a) A stacked plot of the methyl peak over the whole experiment. Evolution of the room temperature (b) and the centre frequency of the methyl peak (c) during the experiment. (d) There is no measureable variation in the peak widths at 50 % (blue) and 10 % (red), showing that there is no drift in field homogeneity.

## **CONCLUSION**

8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 frequency [ppm]

The outstanding resolution, sensitivity and stability provided by this benchtop NMR system means that for the first time truly high performance NMR is accesible to all users.

