Many organometallic complexes contain paramagnetic ions. These extend the chemical shift range of proton spectra to hundreds of ppm. At high field, such large bandwidths are very challenging to achieve. The Magritek Spinsolve benchtop NMR spectrometer has a special Paramagnetic protocol designed to scan such samples. The acquisition bandwidth is 20 kHz corresponding to 480 ppm frequency range. Since paramagnetic ions also reduce the $T_1$ relaxation time of the sample, the repetition time between scans is reduced to 3 seconds resulting in faster scan times. The examples in this note demonstrate the ability of the Paramagnetic protocol to resolve peaks which are not visible in the standard 1D Proton protocol.
Bis(N-2'‐Butylsalicylicylaldiminato)Nickel(II)

In order to demonstrate how paramagnetic ions can extend the spectral range, a sample of bis(n-2'-butylsalicylicylaldiminato)nickel(II) from a third-year chemistry teaching lab was dissolved in CDCl₃ and analysed.

Figure 1 shows the spectrum of the sample using the 1D Proton (red spectrum) and Paramagnetic (blue line) protocols. The bandwidth of the 1D Proton protocol is not sufficient to cover the entire spectral range of the sample while the Paramagnetic protocol tells the full story.

Figure 1: 1H NMR spectrum of bis(n-2'-butylsalicylicylaldiminato)nickel(II) dissolved in CDCl₃ using the 1D Proton (red spectrum) and Paramagnetic (blue line) protocols. Note that the bandwidth of the 1D Proton protocol is insufficient to cover the entire spectrum of the sample.
This example from a third-year chemistry experiment demonstrates the reaction of coordinated ligands using the conversion of paramagnetic [Co(phen)$_3$]$^{2+}$ to diamagnetic [Co(phen)$_3$]$^{3+}$ complexes.

Figure 2 shows how the chemical shift range differs dramatically between the paramagnetic and diamagnetic cobalt complexes.

Figure 2: NMR spectrum of diamagnetic and paramagnetic Co(phen)$_3$ dissolved in D$_2$O, using the Paramagnetic protocol. Note how the chemical shift range extends dramatically for the paramagnetic complex. Spectra courtesy of Paul S Donelly, University of Melbourne.
Conclusion

Paramagnetic samples are often difficult to obtain NMR spectra from. The specially designed Paramagnetic protocol enables the Spinsolve benchtop NMR spectrometer to resolve peaks in wide line spectra, which cannot be resolved with standard methods.