

## Supporting Information

Suppression of Protonated Organic Solvents in NMR Spectroscopy using a DISPEL Pulse Sequence

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## Table of Contents

S1 Experimental conditions .....	S2
Figure S2: Spectra with and without PFG inversion.....	S3
Figure S3: Comparison of NOESY-PRESAT and DISPEL with presaturation .....	S3
Figure S4: Comparison of NOESY-PRESAT and DISPEL with presaturation .....	S4
Figure S5: Enlargement of the alkene resonance of Linalool .....	S5
Figure S6: DISPEL spectra of Chlorsulfuron in protonated THF.....	S6

## S1 Experimental conditions

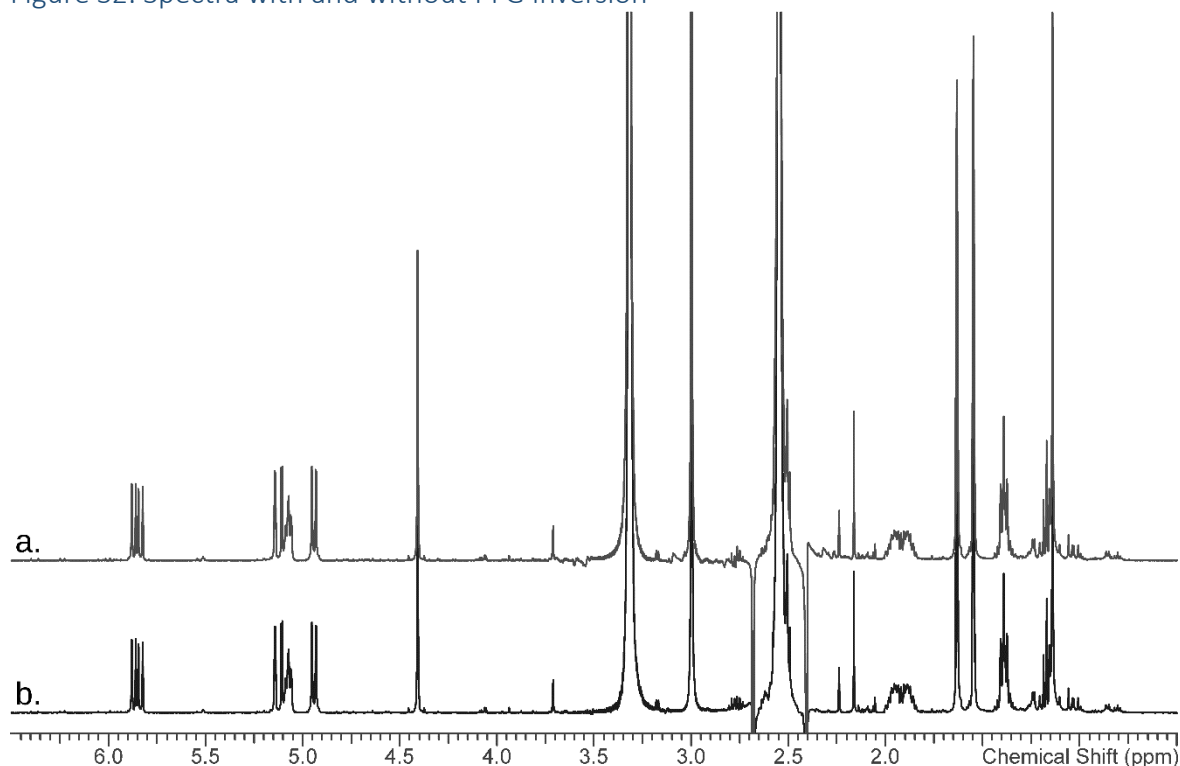
Linalool was obtained from Lancaster Synthesis and Chlorsulfuron was obtained from Syngenta's internal chemical collection. Samples were prepared using reagent grade THF and DMSO from Fisher Chemicals and deuterated DMSO and acetonitrile from Cambridge Isotope Limited.

All NMR spectra were acquired at 298K on a Bruker Avance III 500MHz spectrometer fitted with a nitrogen cooled 5mm H/F{X} PFG Prodigy probe and operating with Topspin 3.2 software. RF pulses were applied using the following RF field strengths: high power proton pulses at 21.27kHz; presaturation of the DMSO resonance at 30Hz; presaturation of the THF resonances at 20Hz; and high power  $^{13}\text{C}$  pulses at 21.73kHz.  $^{13}\text{C}$  inversion pulses were replaced by composite  $90_x240_y90_x$  pulses and were applied at 40ppm (DMSO) or 50ppm (THF).

The two-stage DISPEL sequence of Moutzouri *et al* was used with the following modifications. A presaturation pulse was applied with phase y, the final z-filter was omitted (except where stated) and the phase cycle was  $\Phi_1$ : x,x,x,x,-x,-x,-x,-x;  $\Phi_2$ : y,y,y,y,y,y,y,-y,-y,-y,-y,-y,-y,-y;  $\Phi_3$ : y;  $\Phi_4$ : x,y,-x,-y;  $\Phi_5$ : x,x,-x,-x;  $\Phi_r$ : x,-x,x,-x,-x,x,-x, x. After completion of the phase cycle, polarities of all PFG were inverted. Optimum results were obtained with the full 16-step phase cycle and PFG inversion, although reasonable results can be obtained using 8 steps.

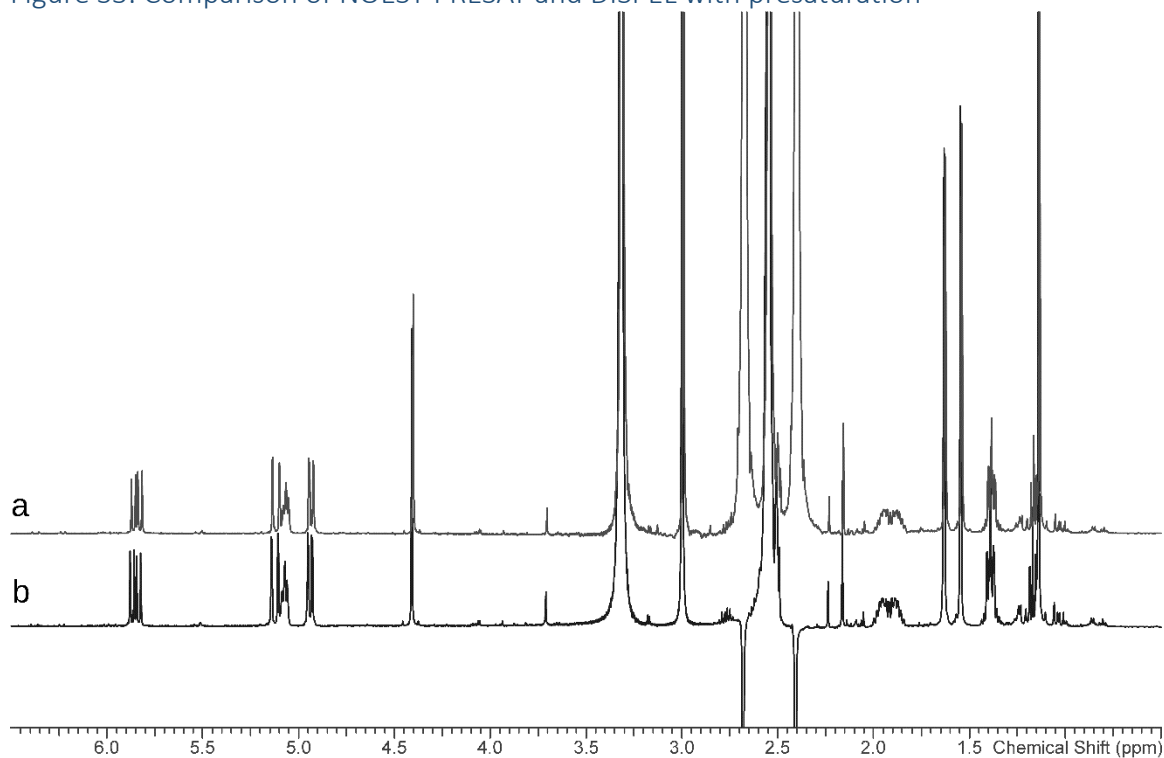
The delays of the DISPEL-2 sequence were optimised for the solvent being suppressed. For the DMSO sample,  $2 \times \tau = \tau_1 = \tau_2 = 3.649\text{ms}$ . For the THF sample,  $2 \times \tau = \tau_1 = 3.759\text{ms}$ ,  $\tau_3 = 3.448\text{ms}$ . The relaxation delay was 4.97s and presaturation was applied for 4.9s. For THF, presaturation was applied using 100ms rectangular pulses phase-modulated to excite both solvent resonances simultaneously. 8192 complex points were acquired giving an acquisition time of 1.02s for a spectral width of 16ppm.

Figure S2: Spectra with and without PFG inversion



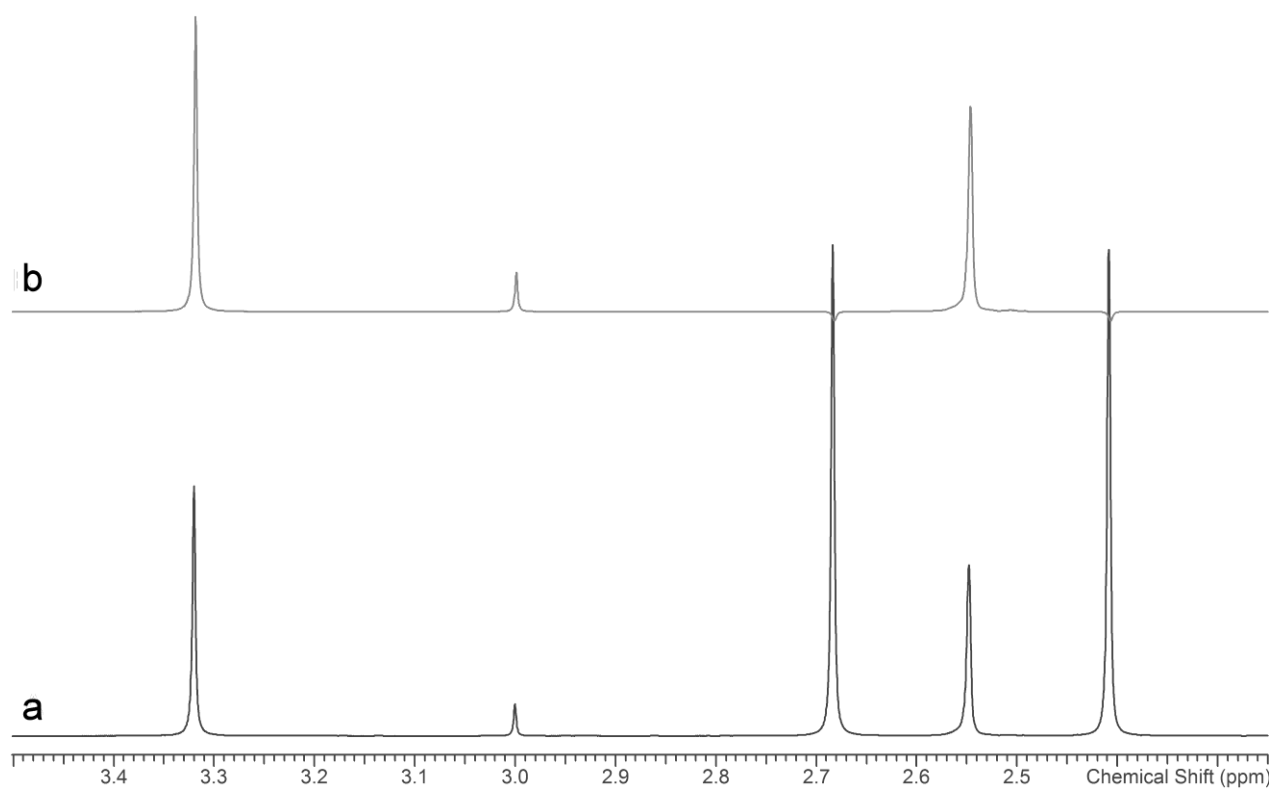
DISPEL-2 spectra of Linalool in 90% protonated DMSO a) with and b) without PFG inversion after 16 transients.  $2 \times 16$  transients were acquired.

Figure S3: Comparison of NOESY-PRESAT and DISPEL with presaturation



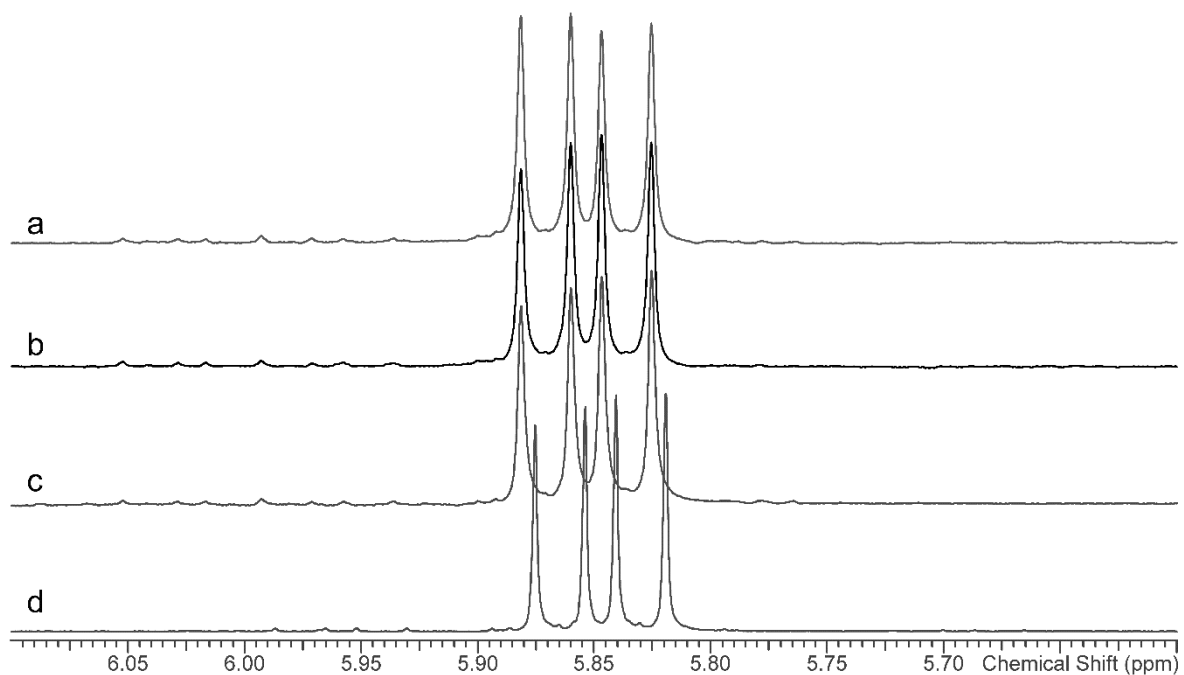
a) NOESY-PRESAT (noesygprr1d) and b) DISPEL-2 spectra of Linalool in 90% protonated DMSO. Note the minor baseline distortions in a.

Figure S4: Comparison of NOESY-PRESAT and DISPEL with presaturation



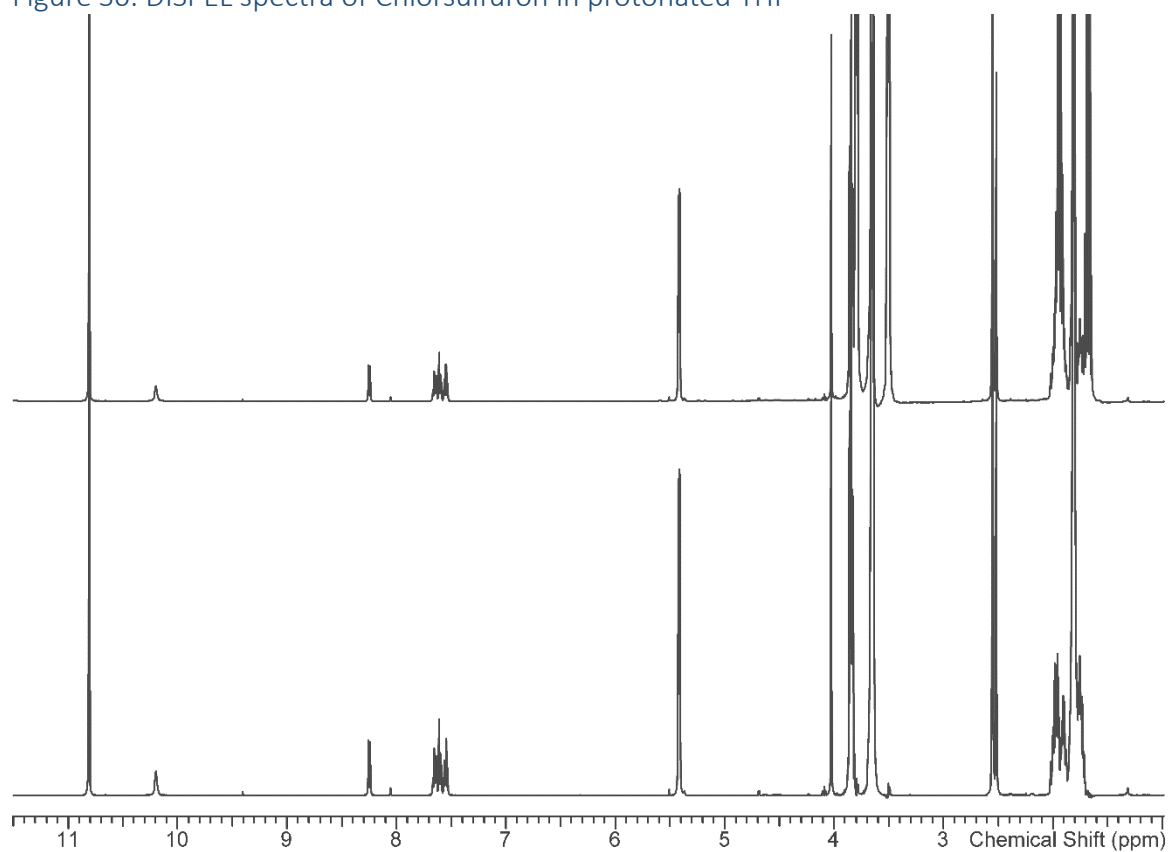
a) NOESY-PRESAT (noesygppr1d) and b) DISPEL-2 spectra of Linalool in 90% protonated DMSO, enlarged to show the similar quality of solvent suppression. Note the order of the spectra is reversed compared to Figure S3

Figure S5: Enlargement of the alkene resonance of Linalool



The alkene resonance of Linalool at 5.7ppm in spectra acquired using presaturation and DISPEL-2 with a) no z-filter, b) a  $\pi/2$  y-pulse, and c) a final z-filter immediately prior to acquisition. d) reference spectrum acquired using pulse-acquire in deuterated DMSO.

Figure S6: DISPEL spectra of Chlorsulfuron in protonated THF



DISPEL-2 spectrum of Chlorsulfuron in 90% protonated THF (upper) without and (lower) with application of  $^{13}\text{C}$  pulses. The resonance at 10.8ppm is the peroxide resonance of THF peroxide.