

## NMR data acquisition method

$^1\text{H}$ -NMR spectroscopy was performed according to the miniaturised method described by Mason *et al.* (2018). Samples were measured at 500 MHz in 2 mm NMR MATCH tubes, with the 5 mm triple-resonance inverse (TXI) probe head optimised for  $^1\text{H}$  observation. The sample temperature was maintained at a constant 300 K.  $^1\text{H}$  spectra were acquired as 128 transients in 32K data points with a spectral width of 6000 Hz (12.0 ppm). The  $\text{H}_2\text{O}$  resonance at 4.70 ppm was suppressed using the pulse sequence program NOESY-presat, which presaturates the  $\text{H}_2\text{O}$  resonance by single-frequency irradiation during a relaxation delay of 4 s, with a  $90^\circ$  excitation pulse of 10  $\mu\text{s}$ . The acquisition time and receiver gain were set for 2.7 s and 64, respectively. The number of dummy scans ( $n=4$ ) and scans ( $n=128$ ) yielded a run time of 15 min and 45 s per sample. Each sample was automatically shimmed on the deuterium signal, locked, probe tuned and matched, and pulse calibrated. NMR analysis and processing were performed using Bruker Topspin (v 3.5), and further processing conducted using Bruker AMIX (v 3.9.14).