

NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA, USA)

Sample Preparation: Sample diluted in deuterated solvent (e.g., DMSO-D₆, CD₃OD)

Instrument: 600 MHz Bruker Avance III Spectrometer

300 MHz INOVA VARIAN Spectrometer

Experiment Types: ¹H-NMR, ¹³C-NMR, DQF-COSY, and/or HSQC

Parameters: 600.1 MHz for proton (¹H) and 150.9 MHz for carbon (¹³C)

Probe: 5 mm TXI H{CN} cryoprobe

Temperature: -1.0 °C

Chemical shifts reported in δ units, ppm, relative to TMS

¹H-NMR: Scans: 16, Spectral window: 12.0 KHz, Spectral offset: 3.7 KHz, Resolution: 0.37 Hz, Acquisition time: 2.7 s, Recycle delay: 1.0 s

¹³C-NMR: Scans: 1024, Spectral window: 36.2 KHz, Spectral offset: 15 KHz, Resolution: 1.1 Hz, Acquisition time: 0.9 s, Recycle delay: 2.0 s

DQF-COSY: Scans: 4, Pulse width: 9.72 μs, Acquisition time: 0.13 s, Spectral window: 7.8 KHz for ¹H in both dimensions

HSQC: Scans: 16, Pulse width: 9.72 μs, Acquisition time: 0.061 s, Spectral window: 8.4 KHz for ¹H and 24.9 KHz for ¹³C

Data Processing: SpinWorks 4.2.10 (2019, Kirk Marat, Univ. of Manitoba, Canada)

**Some parameters and setpoints may vary based on individual sample and experiment type(s).*