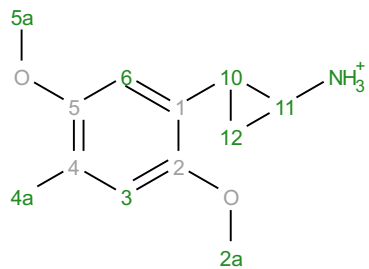
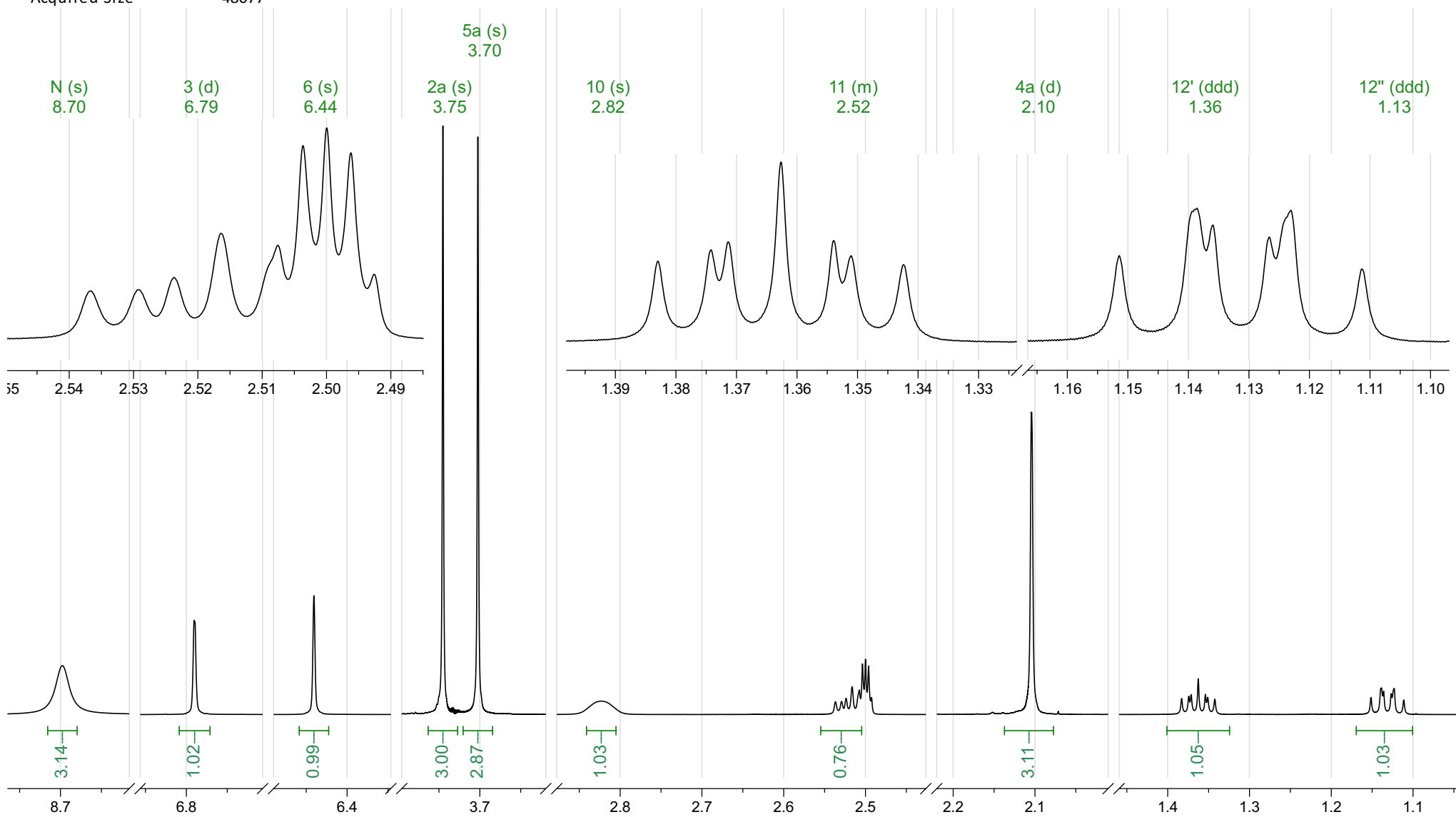


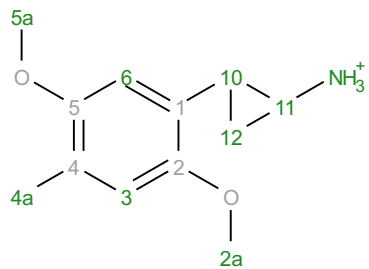
Analyte X61: DMCPA HCl
 Acquisition Date 2019-03-08T15:54:42
 Solvent dms0
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Experiment 1D
 Spectrometer Frequency 499.66
 Spectral Width 8012.8
 Nucleus 1H
 Acquired Size 48077



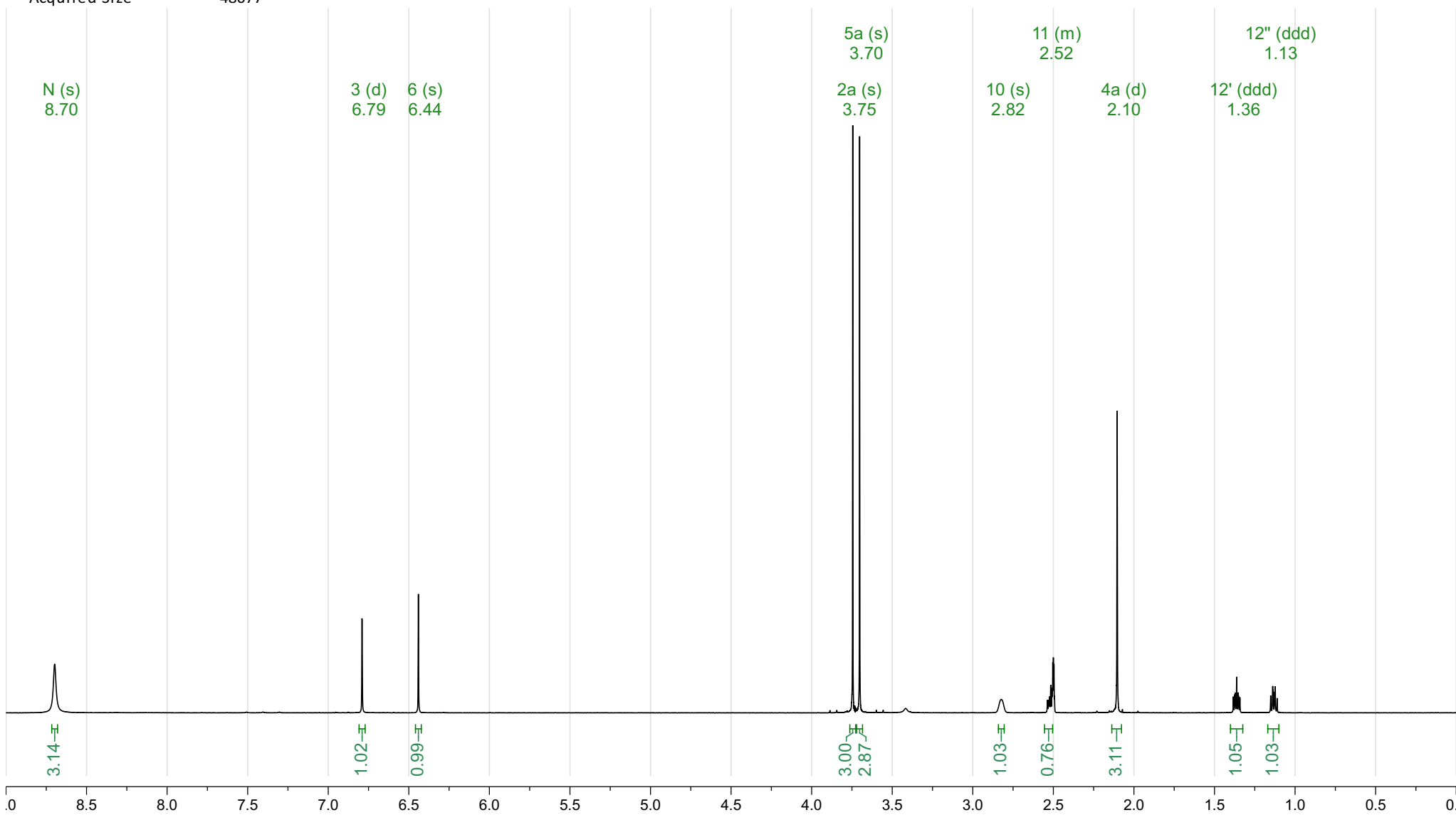
^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 8.70 (s, 3H), 6.79 (d, $J = 0.8$ Hz, 1H), 6.44 (s, 1H), 3.75 (s, 3H), 3.70 (s, 3H), 2.82 (s, 1H), 2.55 – 2.50 (m, 1H), 2.10 (d, $J = 0.7$ Hz, 3H), 1.36 (ddd, $J = 10.1, 5.8, 4.3$ Hz, 1H), 1.13 (ddd, $J = 7.7, 6.5, 5.8$ Hz, 1H).



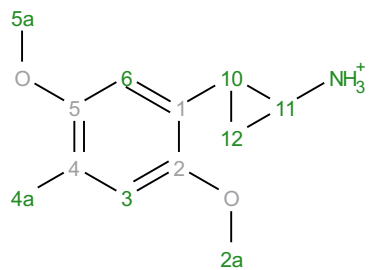
Analyte X61: DMCPA HCl
 Acquisition Date 2019-03-08T15:54:42
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Experiment 1D
 Spectrometer Frequency 499.66
 Spectral Width 8012.8
 Nucleus 1H
 Acquired Size 48077



¹H NMR (500 MHz, DMSO-*d*₆) δ 8.70 (s, 3H), 6.79 (d, *J* = 0.8 Hz, 1H), 6.44 (s, 1H), 3.75 (s, 3H), 3.70 (s, 3H), 2.82 (s, 1H), 2.55 – 2.50 (m, 1H), 2.10 (d, *J* = 0.7 Hz, 3H), 1.36 (ddd, *J* = 10.1, 5.8, 4.3 Hz, 1H), 1.13 (ddd, *J* = 7.7, 6.5, 5.8 Hz, 1H).



Prediction DMCPA H+
Origin Mnova Best
Solvent DMSO-d6
Version 1.0.0
Frequency 500.00
Nucleus 1H



¹H NMR (500 MHz, DMSO-d₆) δ 7.53 (d, *J* = 6.6 Hz, 3H), 6.93 (d, *J* = 0.7 Hz, 1H), 6.75 (s, 1H), 3.82 (d, *J* = 12.9 Hz, 6H), 3.65 – 3.57 (m, 1H), 3.15 (hept, *J* = 6.9 Hz, 1H), 2.39 (dt, *J* = 12.4, 7.0 Hz, 1H), 2.30 (dt, *J* = 12.4, 7.0 Hz, 1H), 2.21 (s, 3H).

