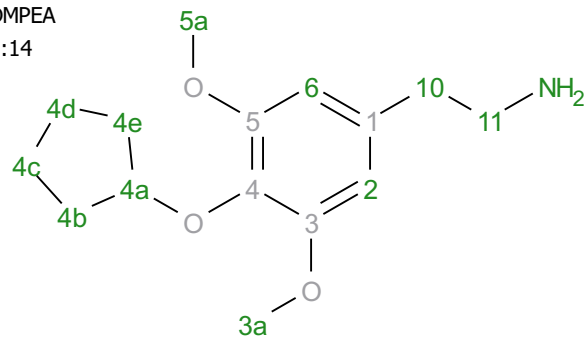
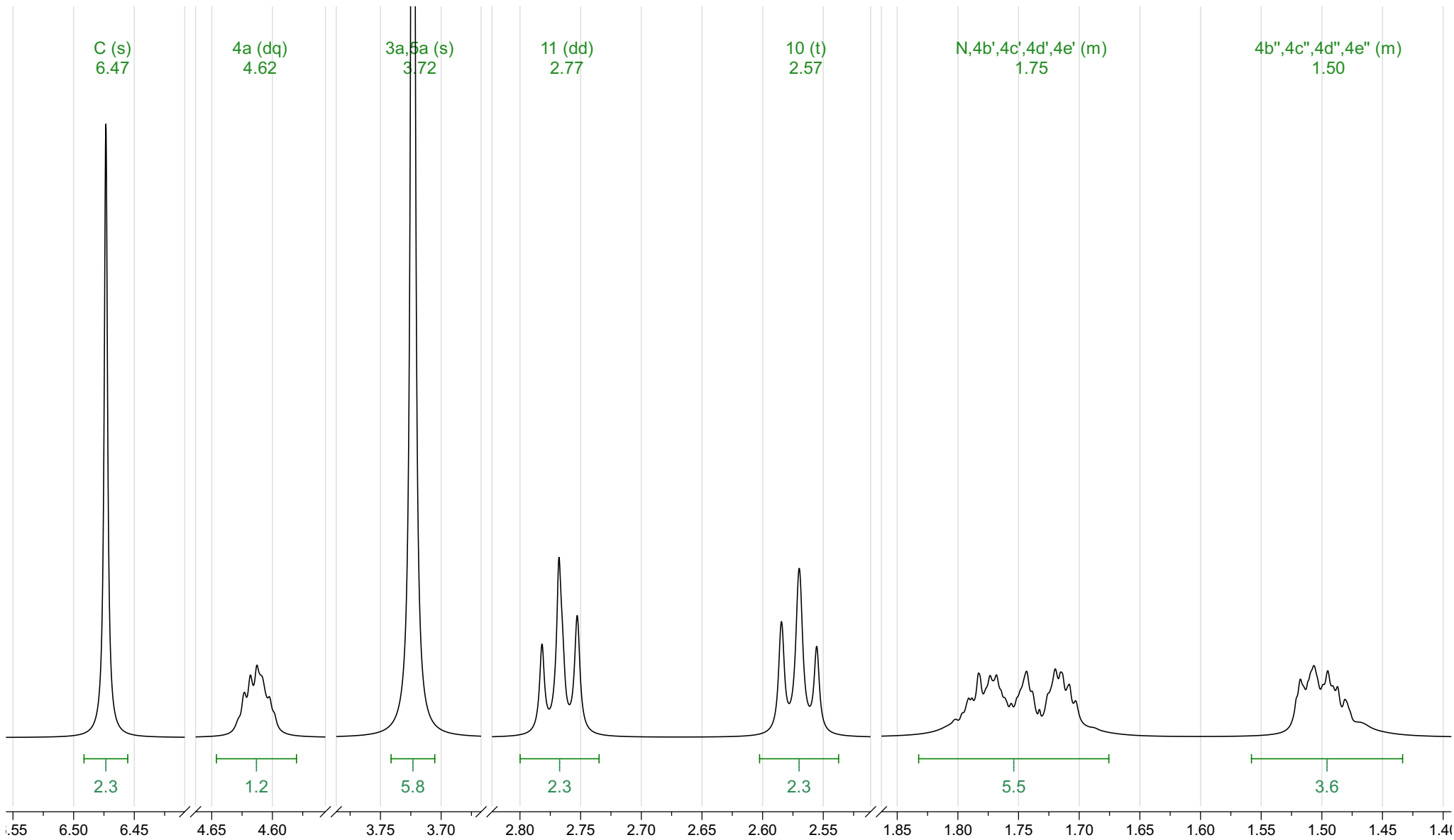


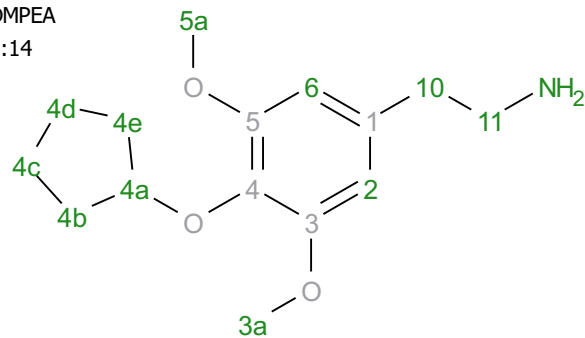
Analyte P30: 4-cPeO-3,5-DMPEA
 Acquisition Date 2019-09-25T17:43:14
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Spectrometer Frequency 499.66
 Spectral Width 8012.8
 Nucleus 1H
 Acquired Size 48077



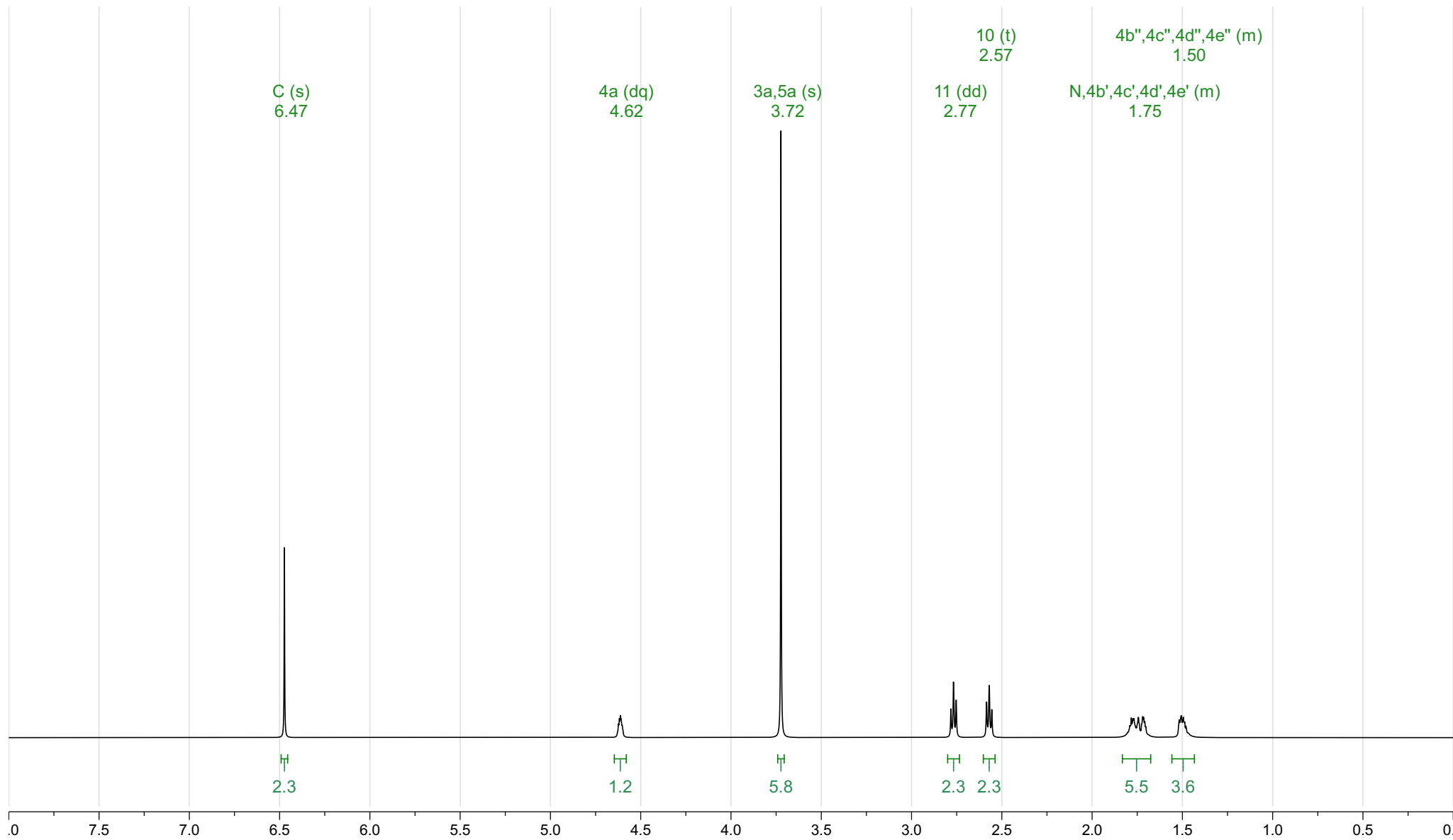
^1H NMR (500 MHz, DMSO- d_6) δ 6.47 (s, 2H), 4.62 (dq, $J = 5.4, 3.6, 3.0$ Hz, 1H), 3.72 (s, 6H), 2.77 (dd, $J = 8.0, 6.6$ Hz, 2H), 2.57 (t, $J = 7.3$ Hz, 2H), 1.83 – 1.68 (m, 6H), 1.56 – 1.43 (m, 4H).



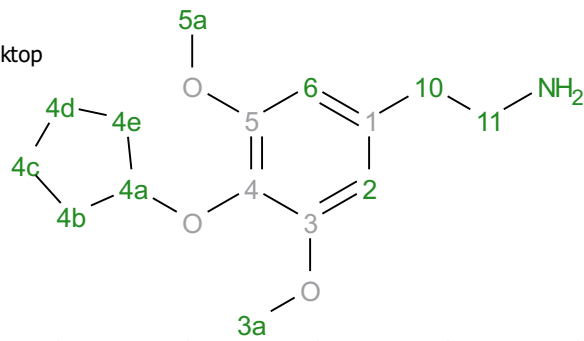
Analyte P30: 4-cPeO-3,5-DMPEA
 Acquisition Date 2019-09-25T17:43:14
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Spectrometer Frequency 499.66
 Spectral Width 8012.8
 Nucleus 1H
 Acquired Size 48077



¹H NMR (500 MHz, DMSO-*d*₆) δ 6.47 (s, 2H), 4.62 (dq, *J* = 5.4, 3.6, 3.0 Hz, 1H), 3.72 (s, 6H), 2.77 (dd, *J* = 8.0, 6.6 Hz, 2H), 2.57 (t, *J* = 7.3 Hz, 2H), 1.83 – 1.68 (m, 6H), 1.56 – 1.43 (m, 4H).



Prediction 4-cPeO-3,5-DMPEA
Origin Modgraph NMRPredict Desktop
Solvent DMSO-d6
Algorithm Best
GMMX Cycles 10
Version 1.15 (5.076)
Frequency 500.00
Nucleus 1H



$^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 6.66 (t, $J = 1.0$ Hz, 2H), 4.58 (t, $J = 6.7$ Hz, 3H), 3.84 (s, 6H), 3.33 – 3.25 (m, 2H), 2.97 (tt, $J = 4.9, 1.0$ Hz, 2H), 1.70 – 1.58 (m, 4H), 1.57 – 1.46 (m, 4H).

