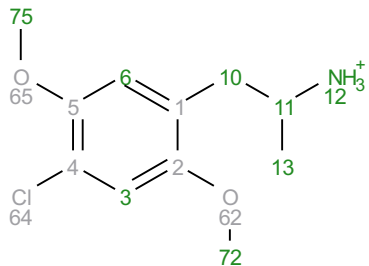
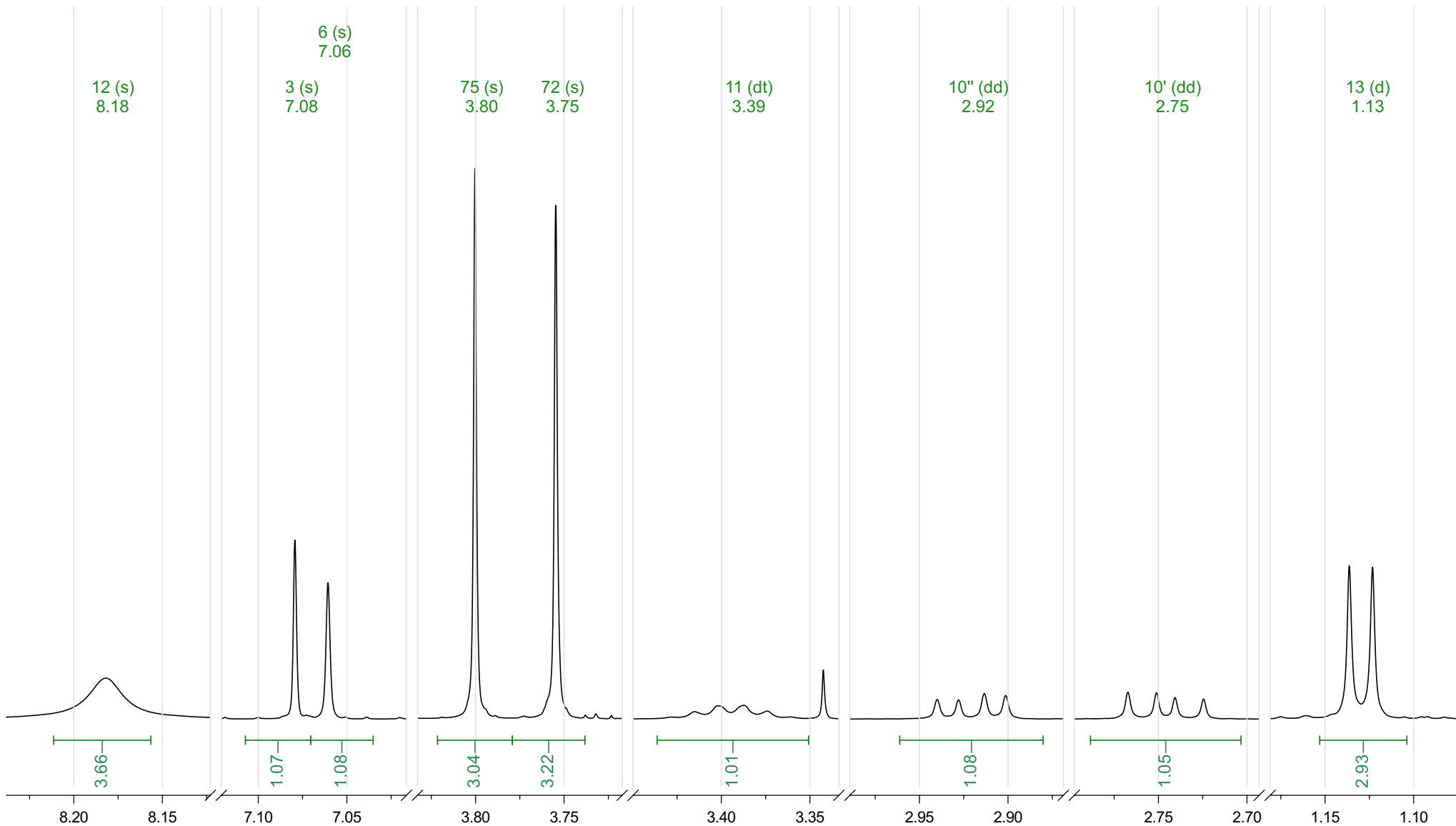


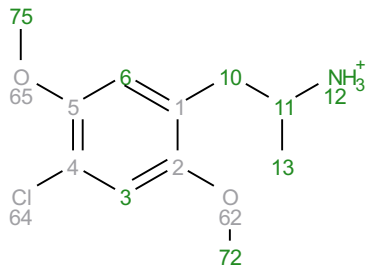
Analyte SB7: DOC H+
 Acquisition Date 2017-06-08T13:10:38
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



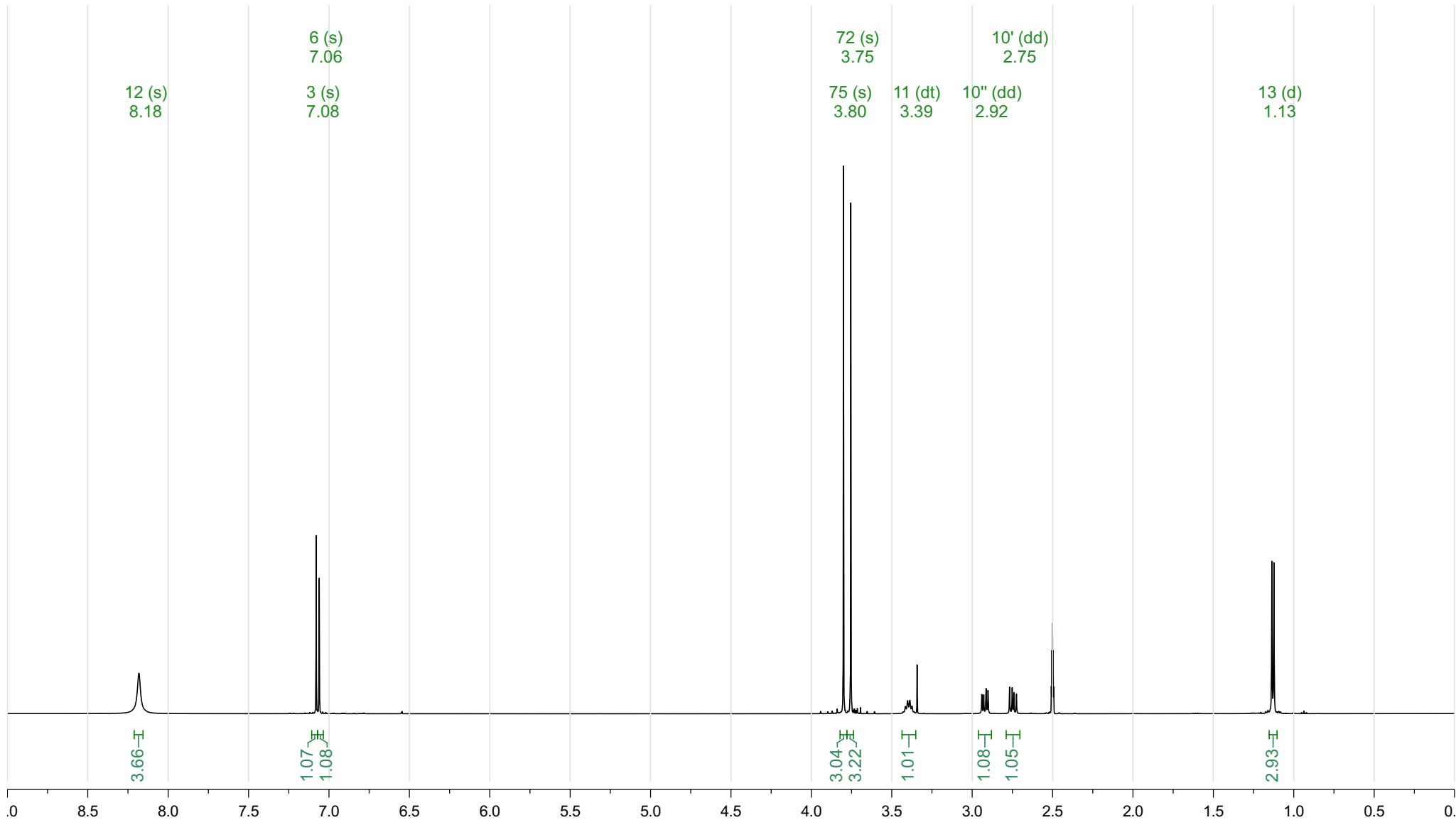
¹H NMR (500 MHz, DMSO-*d*₆) δ 8.18 (s, 3H), 7.08 (s, 1H), 7.06 (s, 1H), 3.80 (s, 3H), 3.75 (s, 3H), 3.39 (dt, *J* = 14.1, 6.5 Hz, 1H), 2.92 (dd, *J* = 13.3, 6.0 Hz, 1H), 2.75 (dd, *J* = 13.3, 8.0 Hz, 1H), 1.13 (d, *J* = 6.5 Hz, 3H).



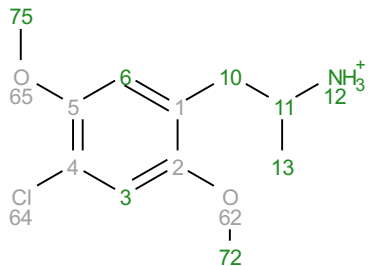
Analyte SB7: DOC H+
 Acquisition Date 2017-06-08T13:10:38
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



¹H NMR (500 MHz, DMSO-*d*₆) δ 8.18 (s, 3H), 7.08 (s, 1H), 7.06 (s, 1H), 3.80 (s, 3H), 3.75 (s, 3H), 3.39 (dt, *J* = 14.1, 6.5 Hz, 1H), 2.92 (dd, *J* = 13.3, 6.0 Hz, 1H), 2.75 (dd, *J* = 13.3, 8.0 Hz, 1H), 1.13 (d, *J* = 6.5 Hz, 3H).



Prediction DOC H+
 Origin Modgraph NMRPredict Desktop
 Solvent DMSO-d6
 Algorithm Best
 GMMX Cycles 5
 Version 15465
 Frequency 500.00
 Nucleus 1H



¹H NMR (500 MHz, DMSO-d₆) δ 8.62 (s, 3H), 7.24 (s, 1H), 6.80 (t, *J* = 1.0 Hz, 1H), 4.06 (q, *J* = 6.3 Hz, 1H), 3.96 (s, 3H), 3.74 (s, 3H), 3.58 (ddd, *J* = 12.4, 6.6, 1.1 Hz, 1H), 3.13 (ddd, *J* = 12.3, 6.4, 0.9 Hz, 1H), 1.45 (d, *J* = 6.0 Hz, 3H).

