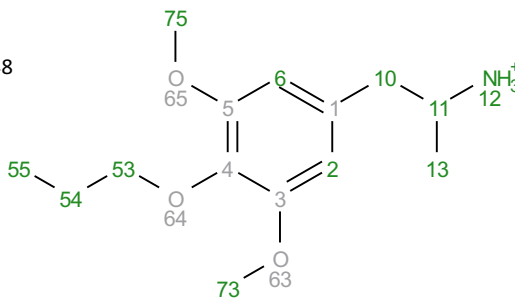
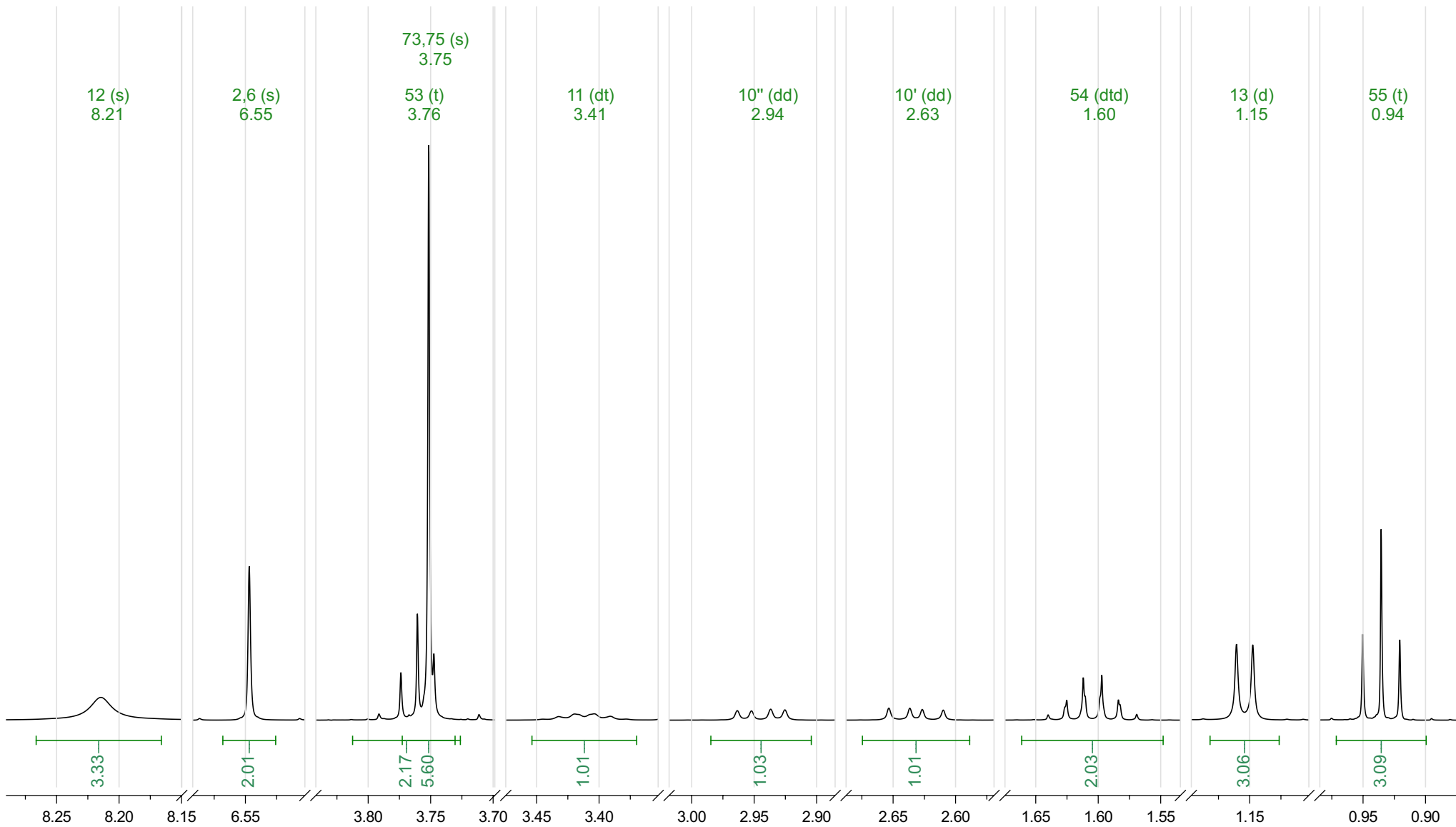


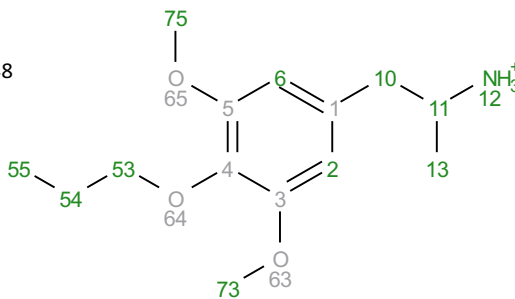
Analyte SB6: 3C-P H+
 Acquisition Date 2017-06-08T13:01:48
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



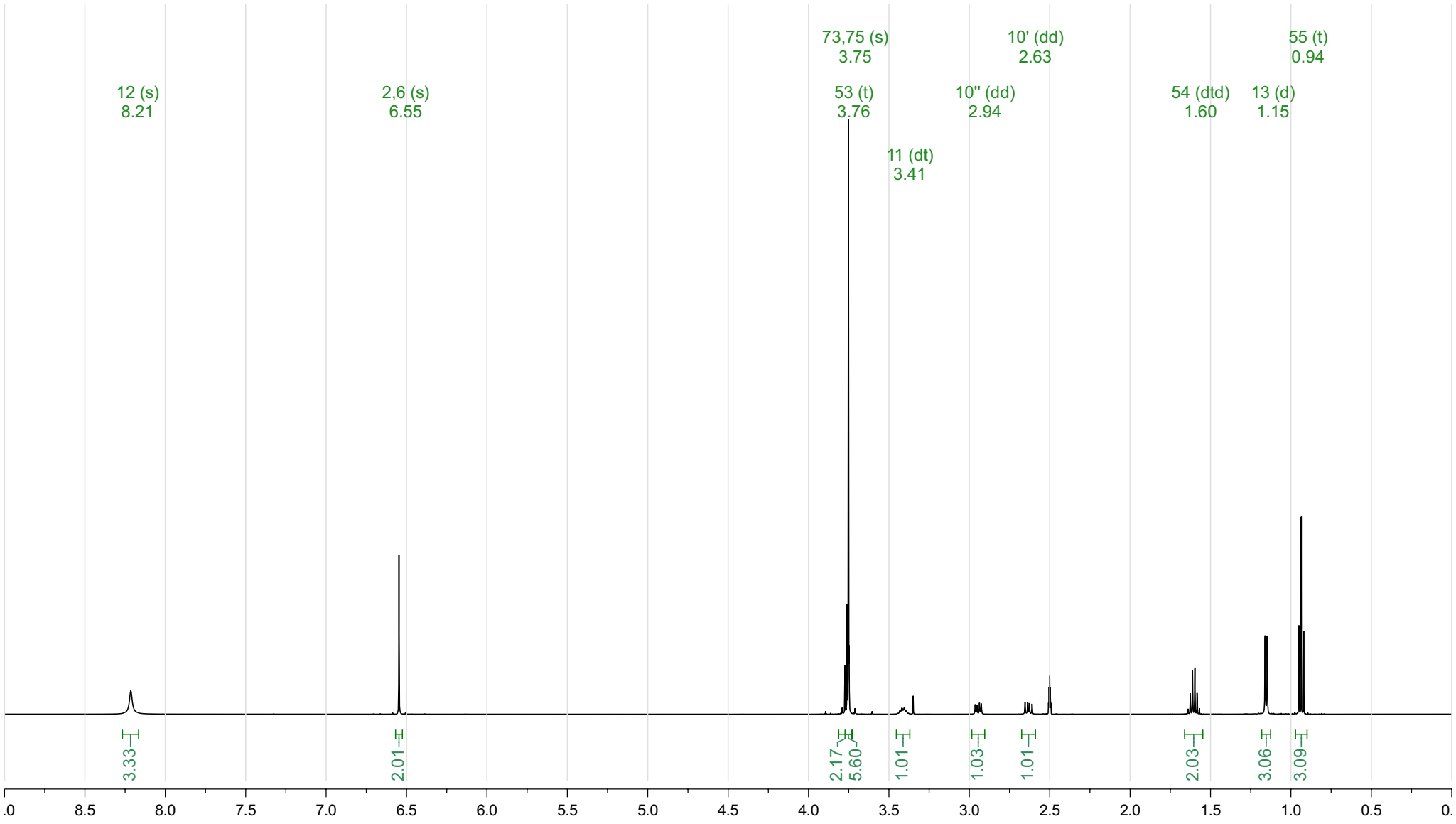
¹H NMR (500 MHz, DMSO-*d*₆) δ 8.21 (s, 3H), 6.55 (s, 2H), 3.76 (t, *J* = 6.6 Hz, 2H), 3.75 (s, 6H), 3.41 (dt, *J* = 8.3, 6.1 Hz, 1H), 2.94 (dd, *J* = 13.4, 5.7 Hz, 1H), 2.63 (dd, *J* = 13.4, 8.4 Hz, 1H), 1.60 (dtd, *J* = 14.0, 7.4, 6.6 Hz, 2H), 1.15 (d, *J* = 6.5 Hz, 3H), 0.94 (t, *J* = 7.4 Hz, 3H).



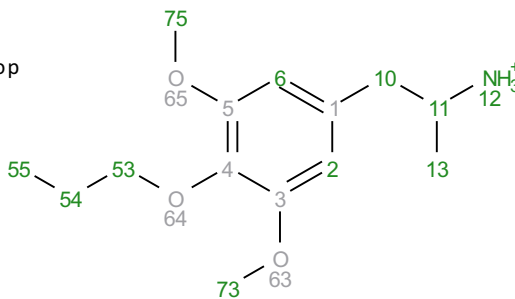
Analyte SB6: 3C-P H+
 Acquisition Date 2017-06-08T13:01:48
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



¹H NMR (500 MHz, DMSO-*d*₆) δ 8.21 (s, 3H), 6.55 (s, 2H), 3.76 (t, *J* = 6.6 Hz, 2H), 3.75 (s, 6H), 3.41 (dt, *J* = 8.3, 6.1 Hz, 1H), 2.94 (dd, *J* = 13.4, 5.7 Hz, 1H), 2.63 (dd, *J* = 13.4, 8.4 Hz, 1H), 1.60 (dtd, *J* = 14.0, 7.4, 6.6 Hz, 2H), 1.15 (d, *J* = 6.5 Hz, 3H), 0.94 (t, *J* = 7.4 Hz, 3H).



Prediction SB6: 3C-P 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-*d*₆) δ 8.62 (s, 3H), 6.48 (t, *J* = 1.0 Hz, 2H), 4.11 – 3.98 (m, 3H), 3.70 (s, 6H), 3.58 (ddt, *J* = 12.5, 6.6, 1.1 Hz, 1H), 3.13 (ddt, *J* = 12.3, 6.6, 0.9 Hz, 1H), 1.80 – 1.68 (m, 2H), 1.45 (d, *J* = 6.0 Hz, 3H), 0.98 (t, *J* = 6.7 Hz, 3H).

