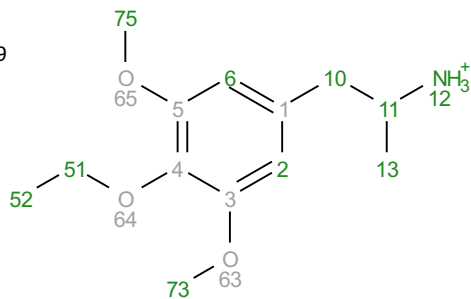
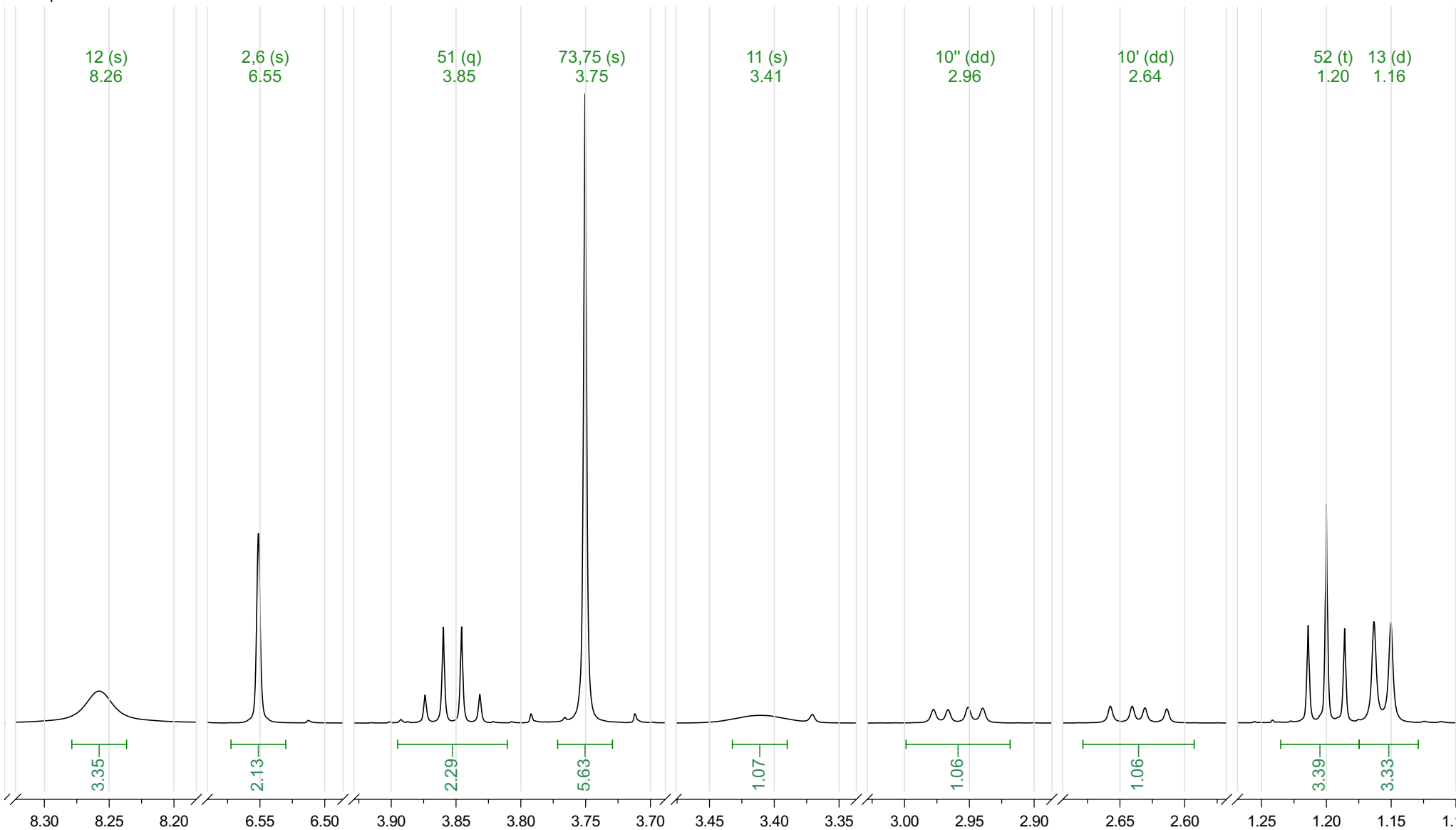


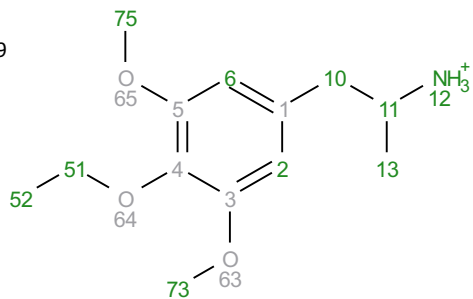
Analyte SB5: 3C-E H+  
Acquisition Date 2017-06-08T12:51:59  
Solvent dmso  
Temperature 25  
Number of Scans 16  
Relaxation Delay 5  
Spectrometer Frequency 499.67  
Spectral Width 10000.0  
Nucleus 1H  
Acquired Size 65536



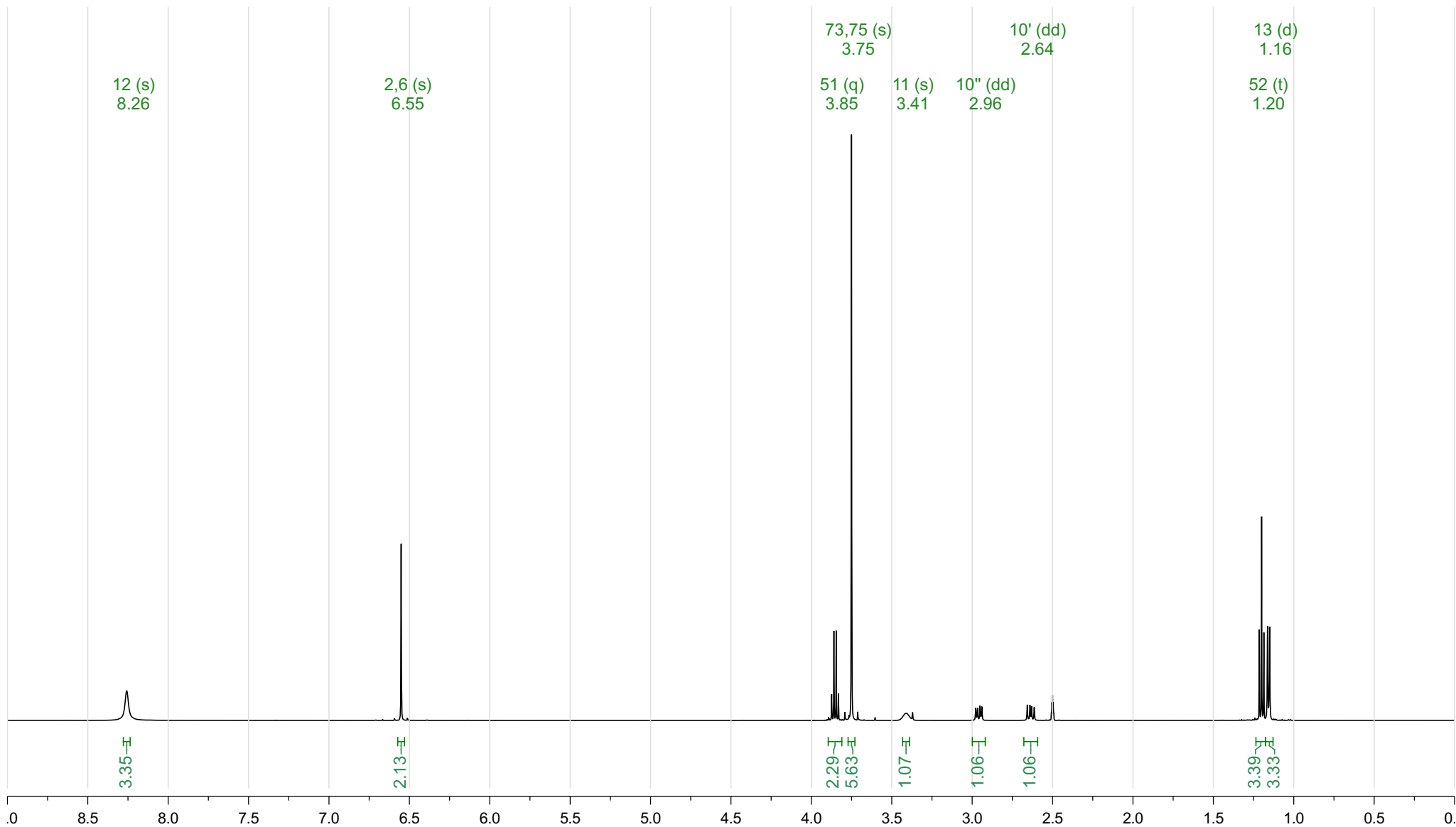
<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 8.26 (s, 3H), 6.55 (s, 2H), 3.85 (q, *J* = 7.0 Hz, 2H), 3.75 (s, 6H), 3.41 (s, 1H), 2.96 (dd, *J* = 13.4, 5.6 Hz, 1H), 2.64 (dd, *J* = 13.3, 8.4 Hz, 1H), 1.20 (t, *J* = 7.0 Hz, 3H), 1.16 (d, *J* = 6.5 Hz, 3H).



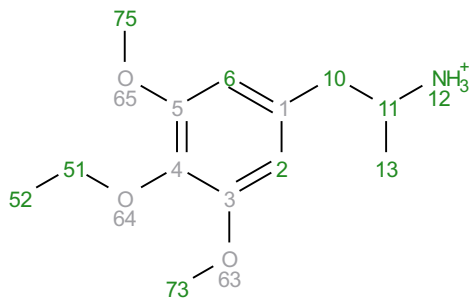
Analyte SB5: 3C-E H+  
 Acquisition Date 2017-06-08T12:51:59  
 Solvent dmso  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 5  
 Spectrometer Frequency 499.67  
 Spectral Width 10000.0  
 Nucleus 1H  
 Acquired Size 65536



<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 8.26 (s, 3H), 6.55 (s, 2H), 3.85 (q, *J* = 7.0 Hz, 2H), 3.75 (s, 6H), 3.41 (s, 1H), 2.96 (dd, *J* = 13.4, 5.6 Hz, 1H), 2.64 (dd, *J* = 13.3, 8.4 Hz, 1H), 1.20 (t, *J* = 7.0 Hz, 3H), 1.16 (d, *J* = 6.5 Hz, 3H).



Prediction SB5: 3C-E H+  
Origin Modgraph NMRPredict Desktop  
Solvent DMSO-d6  
Algorithm Best  
GMMX Cycles 5  
Version 15465  
Frequency 500.00  
Nucleus 1H



$^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  8.62 (s, 3H), 6.48 (t,  $J = 1.0$  Hz, 2H), 4.10 (q,  $J = 5.9$  Hz, 2H), 4.06 (qt,  $J = 6.1, 3.2$  Hz, 1H), 3.70 (s, 6H), 3.58 (ddt,  $J = 12.3, 3.1, 1.0$  Hz, 1H), 3.13 (ddt,  $J = 12.5, 3.1, 0.9$  Hz, 1H), 1.45 (d,  $J = 6.0$  Hz, 3H), 1.34 (t,  $J = 5.9$  Hz, 3H).

