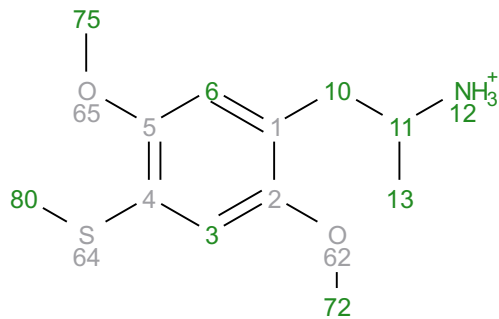
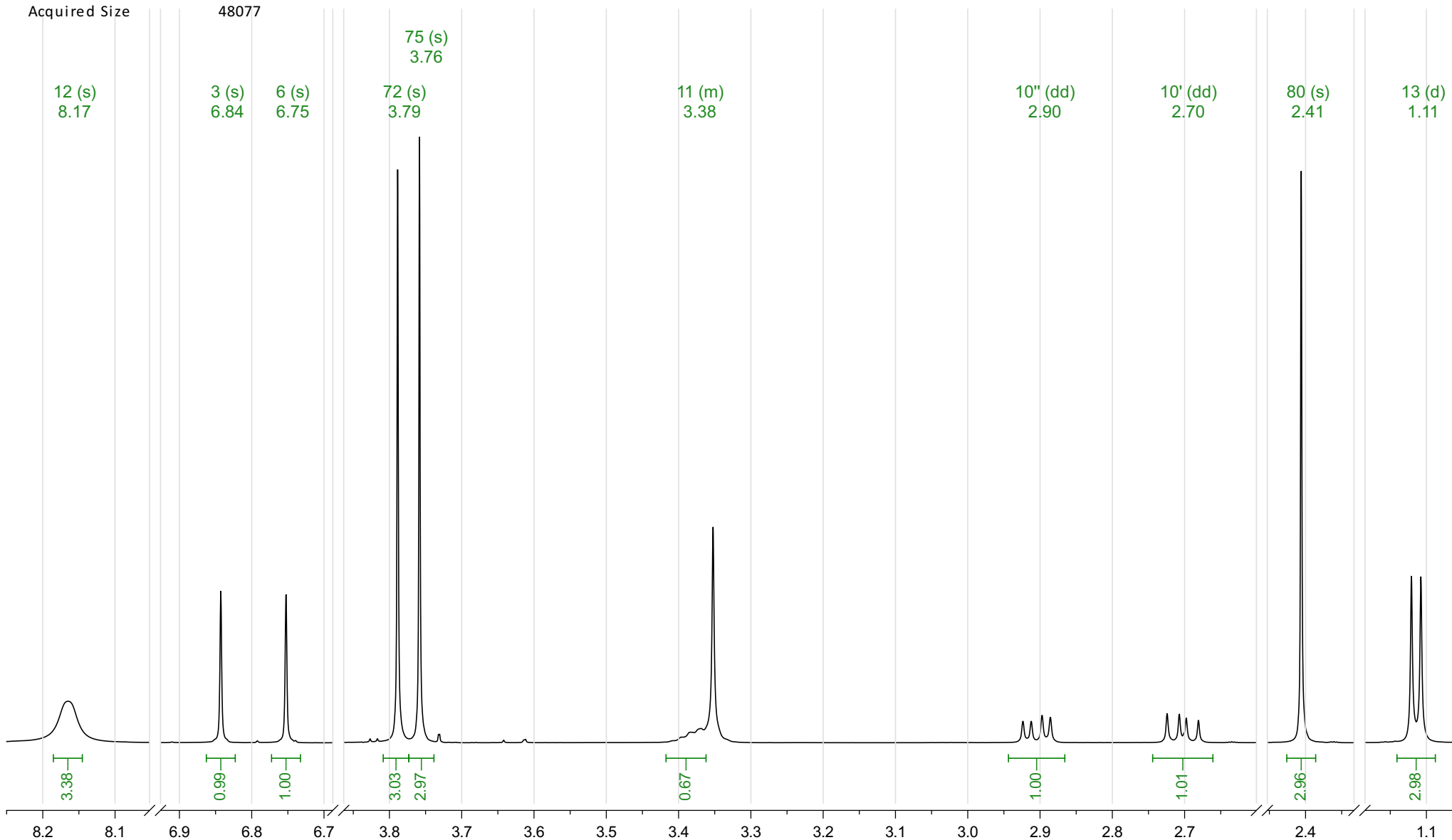


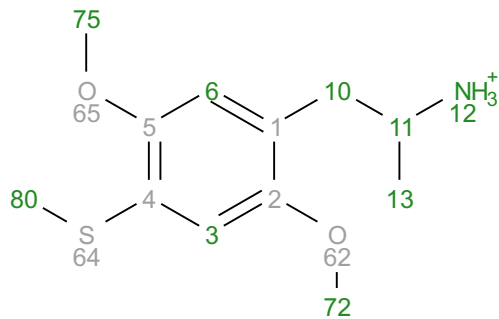
Analyte SB1: ALEPH-1 H+  
 Acquisition Date 2016-12-02T16:35:28  
 Solvent dmso  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 1  
 Spectrometer Frequency 499.66  
 Spectral Width 8012.8  
 Nucleus 1H  
 Acquired Size 48077



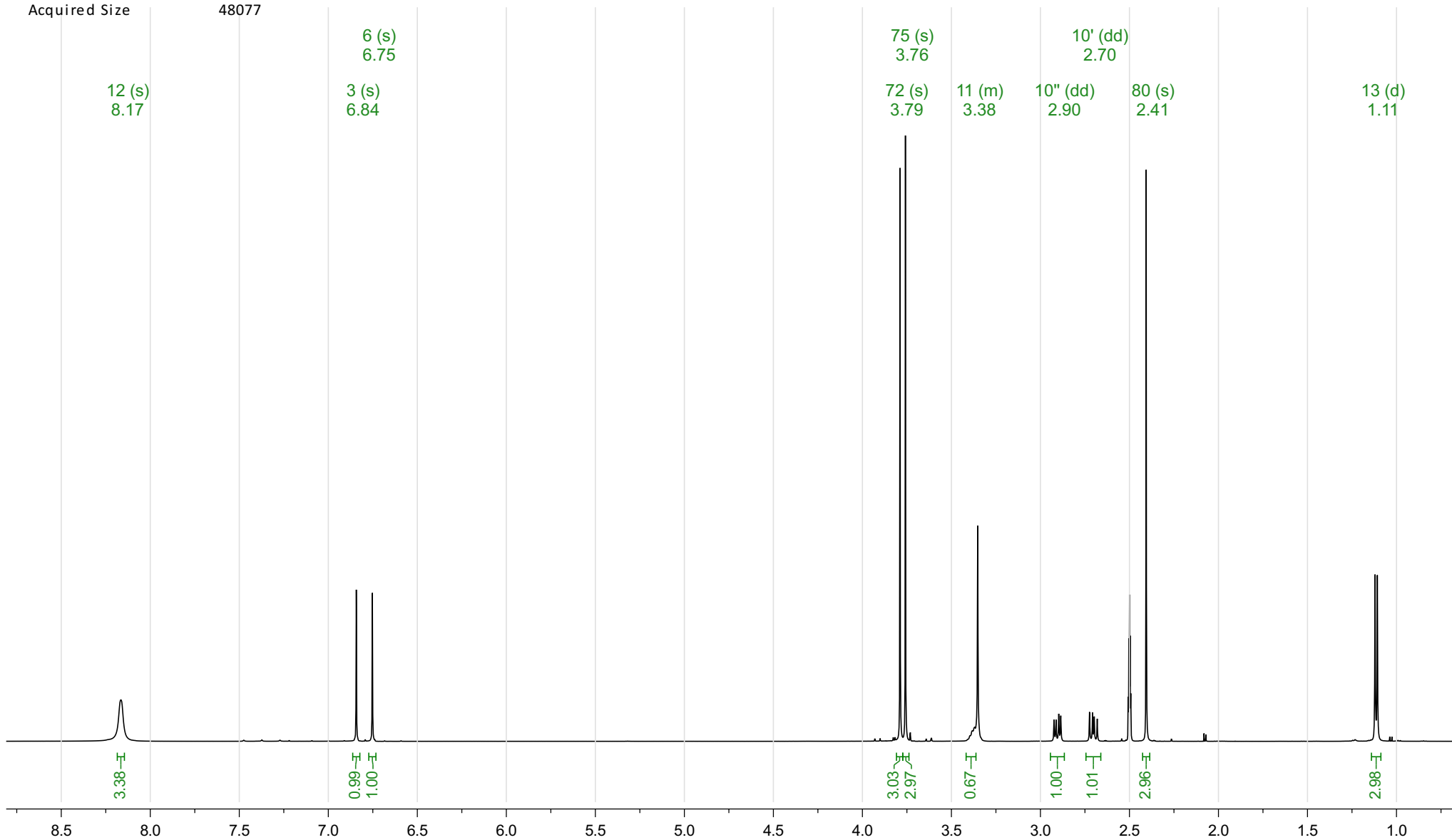
$^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  8.17 (s, 3H), 6.84 (s, 1H), 6.75 (s, 1H), 3.79 (s, 3H), 3.76 (s, 3H), 3.42 – 3.35 (m, 1H), 2.90 (dd,  $J = 13.2, 5.7$  Hz, 1H), 2.70 (dd,  $J = 13.2, 8.4$  Hz, 1H), 2.41 (s, 3H), 1.11 (d,  $J = 6.5$  Hz, 3H).



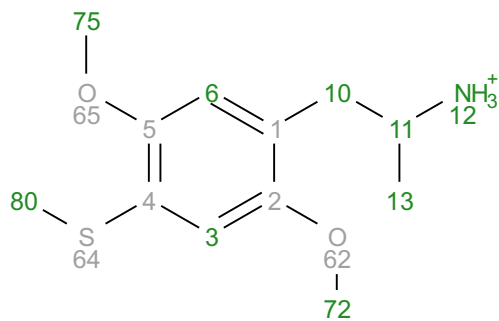
Analyte SB1: ALEPH-1 H+  
 Acquisition Date 2016-12-02T16:35:28  
 Solvent dmso  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 1  
 Spectrometer Frequency 499.66  
 Spectral Width 8012.8  
 Nucleus 1H  
 Acquired Size 48077



<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 8.17 (s, 3H), 6.84 (s, 1H), 6.75 (s, 1H), 3.79 (s, 3H), 3.76 (s, 3H), 3.42 – 3.35 (m, 1H), 2.90 (dd, *J* = 13.2, 5.7 Hz, 1H), 2.70 (dd, *J* = 13.2, 8.4 Hz, 1H), 2.41 (s, 3H), 1.11 (d, *J* = 6.5 Hz, 3H).



Prediction Prediction for ALEPH-1 H+  
 Origin Modgraph NMRPredict Desktop  
 Solvent DMSO-d6  
 Algorithm Best  
 GMMX Cycles 25  
 Version 18153  
 Frequency 500.13  
 Nucleus 1H



<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 8.25 (d, *J* = 5.2 Hz, 3H), 6.89 (s, 1H), 6.78 (t, *J* = 1.0 Hz, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.46 (ddq, *J* = 12.0, 6.5, 5.5 Hz, 1H), 2.99 (ddd, *J* = 15.6, 6.5, 1.0 Hz, 1H), 2.87 (ddd, *J* = 15.6, 6.5, 1.1 Hz, 1H), 2.32 (s, 2H), 1.11 (d, *J* = 5.5 Hz, 3H).

