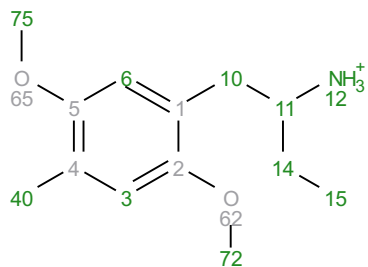
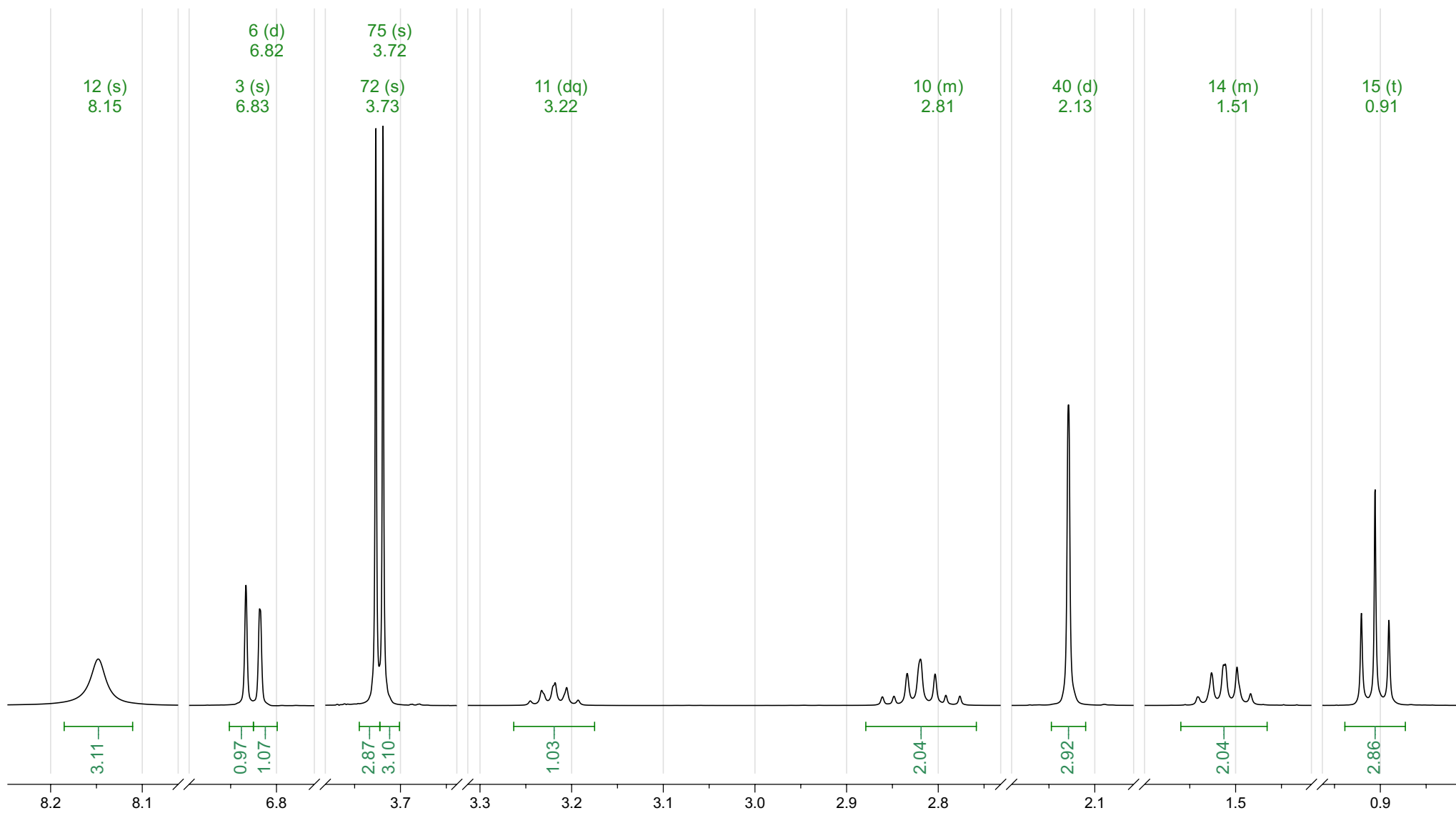


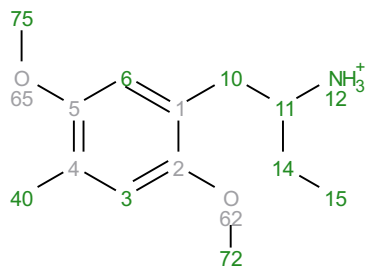
Analyte X60: 4C-D H+  
 Acquisition Date 2019-01-08T12:58:49  
 Solvent dmso  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 5  
 Experiment 1D  
 Spectrometer Frequency 499.67  
 Spectral Width 10000.0  
 Nucleus 1H  
 Acquired Size 65536



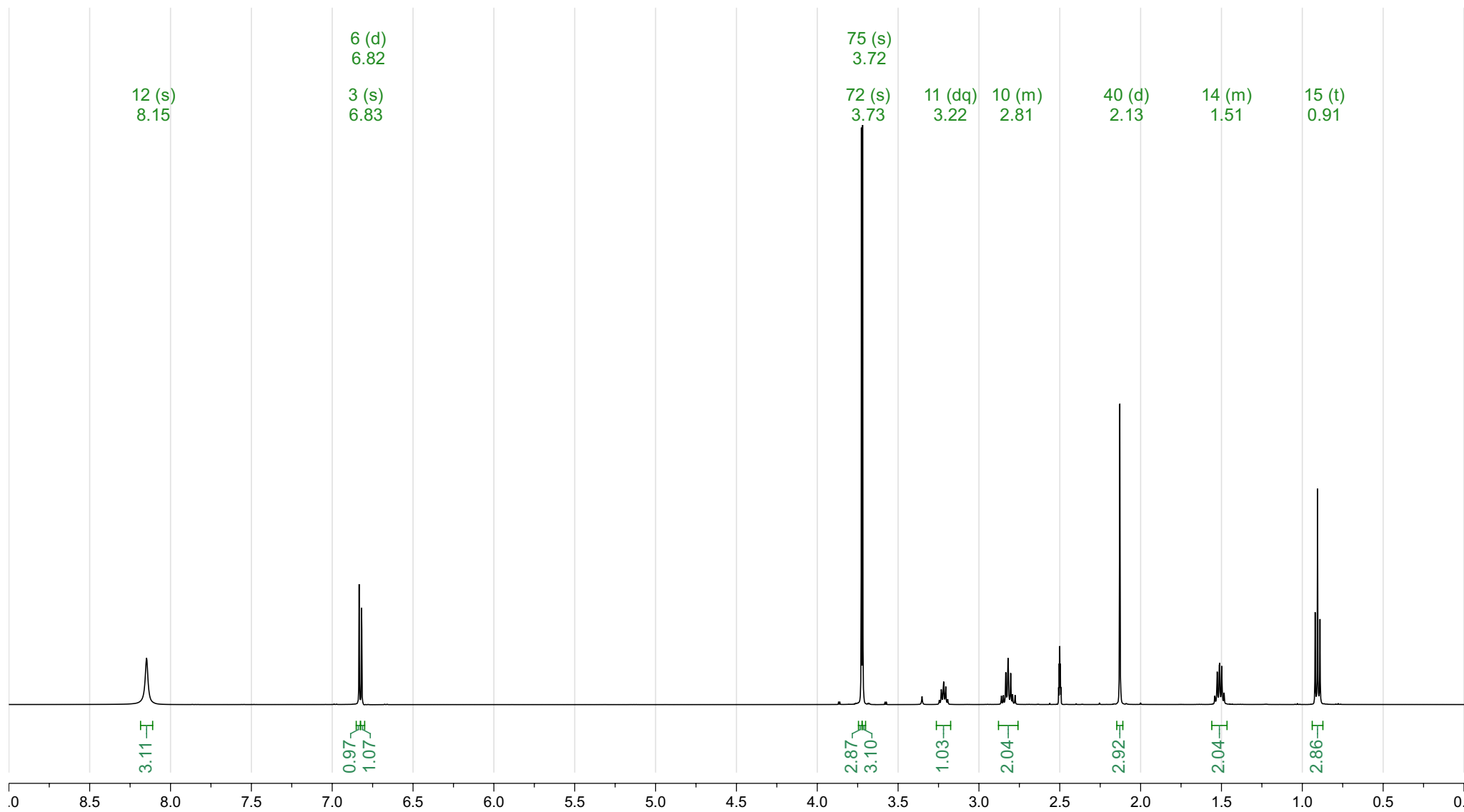
$^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  8.15 (s, 3H), 6.83 (s, 1H), 6.82 (d,  $J = 0.8$  Hz, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 3.22 (dq,  $J = 7.6, 6.1$  Hz, 1H), 2.88 – 2.76 (m, 2H), 2.13 (d,  $J = 0.7$  Hz, 3H), 1.56 – 1.47 (m, 2H), 0.91 (t,  $J = 7.5$  Hz, 3H).e



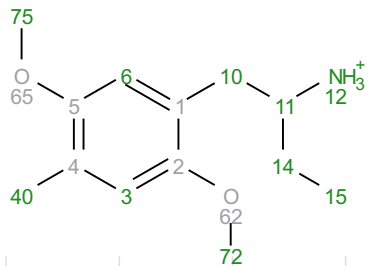
Analyte X60: 4C-D H+  
 Acquisition Date 2019-01-08T12:58:49  
 Solvent dmso  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 5  
 Experiment 1D  
 Spectrometer Frequency 499.67  
 Spectral Width 10000.0  
 Nucleus 1H  
 Acquired Size 65536



<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 8.15 (s, 3H), 6.83 (s, 1H), 6.82 (d, *J* = 0.8 Hz, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 3.22 (dq, *J* = 7.6, 6.1 Hz, 1H), 2.88 – 2.76 (m, 2H), 2.13 (d, *J* = 0.7 Hz, 3H), 1.56 – 1.47 (m, 2H), 0.91 (t, *J* = 7.5 Hz, 3H).e



Prediction 4C-D H+  
Origin Mnova Best  
Solvent DMSO-d6  
Version 1.0.0  
Frequency 500.00  
Nucleus 1H



$^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  7.33 (d,  $J$  = 8.5 Hz, 2H), 6.84 (t,  $J$  = 1.0 Hz, 1H), 6.70 (s, 1H), 3.81 (d,  $J$  = 3.6 Hz, 6H), 3.44 (qp,  $J$  = 8.5, 7.1 Hz, 1H), 3.15 (ddd,  $J$  = 12.6, 7.0, 1.0 Hz, 1H), 3.09 (ddd,  $J$  = 12.3, 7.1, 1.1 Hz, 1H), 2.20 (s, 3H), 1.85 – 1.66 (m, 2H), 1.07 (t,  $J$  = 8.0 Hz, 3H).

