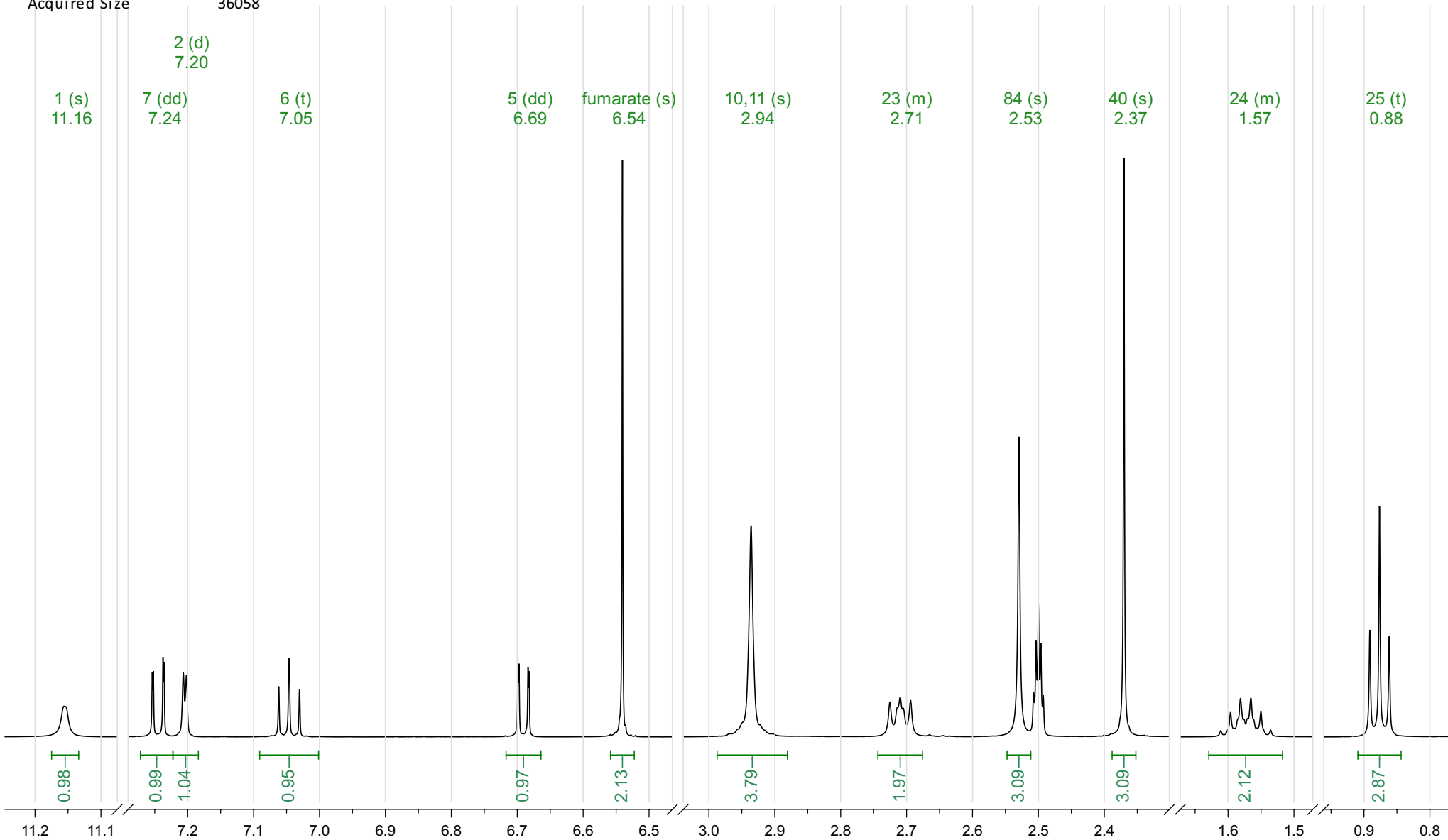
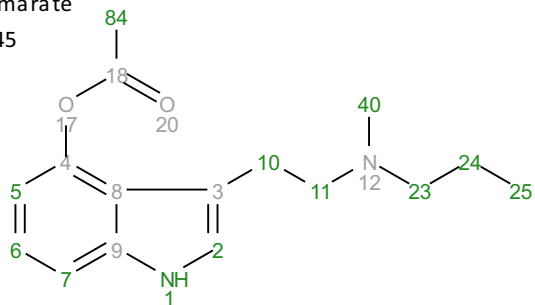


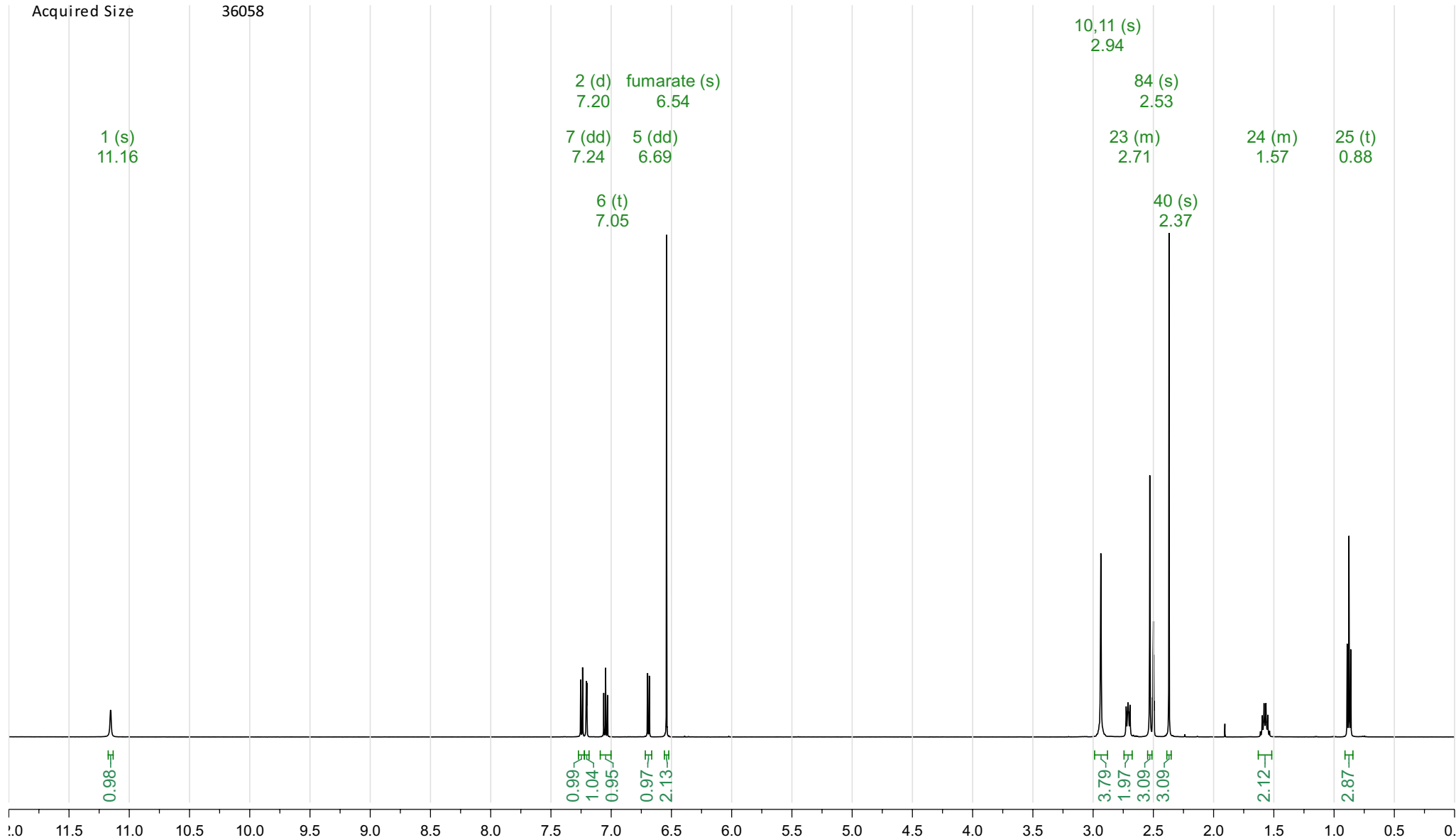
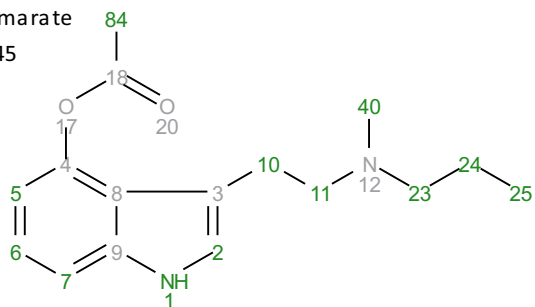
Analyte T43: 4-AcO-MPT fumarate  
 Acquisition Date 2018-02-21T13:23:45  
 Solvent dmsd  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 10  
 Spectrometer Frequency 499.88  
 Spectral Width 8012.8  
 Nucleus 1H  
 Acquired Size 36058

<sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ 11.16 (s, 1H), 7.24 (dd, J = 8.1, 0.8 Hz, 1H), 7.20 (d, J = 2.4 Hz, 1H), 7.05 (t, J = 7.9 Hz, 1H), 6.69 (dd, J = 7.6, 0.8 Hz, 1H), 6.54 (s, 2H), 2.94 (s, 4H), 2.74 – 2.68 (m, 2H), 2.53 (s, 3H), 2.37 (s, 3H), 1.63 – 1.52 (m, 2H), 0.88 (t, J = 7.4 Hz, 3H).



Analyte T43: 4-AcO-MPT fumarate 84  
 Acquisition Date 2018-02-21T13:23:45  
 Solvent dms0  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 10  
 Spectrometer Frequency 499.88  
 Spectral Width 8012.8  
 Nucleus 1H  
 Acquired Size 36058

<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 11.16 (s, 1H), 7.24 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.20 (d, *J* = 2.4 Hz, 1H), 7.05 (t, *J* = 7.9 Hz, 1H), 6.69 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.54 (s, 2H), 2.94 (s, 4H), 2.74 – 2.68 (m, 2H), 2.53 (s, 3H), 2.37 (s, 3H), 1.63 – 1.52 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H).



Prediction 4-AcO-MPT  
Origin Modgraph NMRPredict Desktop  
Solvent DMSO-d6  
Algorithm Best  
GMMX Cycles 5  
Version 20560  
Frequency 500.00  
Nucleus 1H

$^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  10.76 (d,  $J = 8.8$  Hz, 1H), 7.25 (dd,  $J = 7.8, 0.7$  Hz, 1H), 7.22 (d,  $J = 8.5$  Hz, 1H), 7.04 (t,  $J = 7.8$  Hz, 1H), 6.68 (dd,  $J = 7.7, 0.6$  Hz, 1H), 2.92 – 2.85 (m, 2H), 2.77 (t,  $J = 8.1$  Hz, 2H), 2.75 – 2.69 (m, 2H), 2.39 (s, 3H), 2.36 (s, 3H), 1.55 (tq,  $J = 8.1, 5.7$  Hz, 2H), 0.87 (t,  $J = 5.7$  Hz, 3H).

