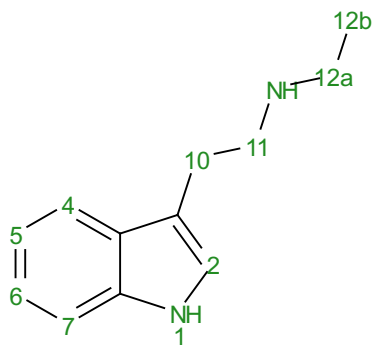
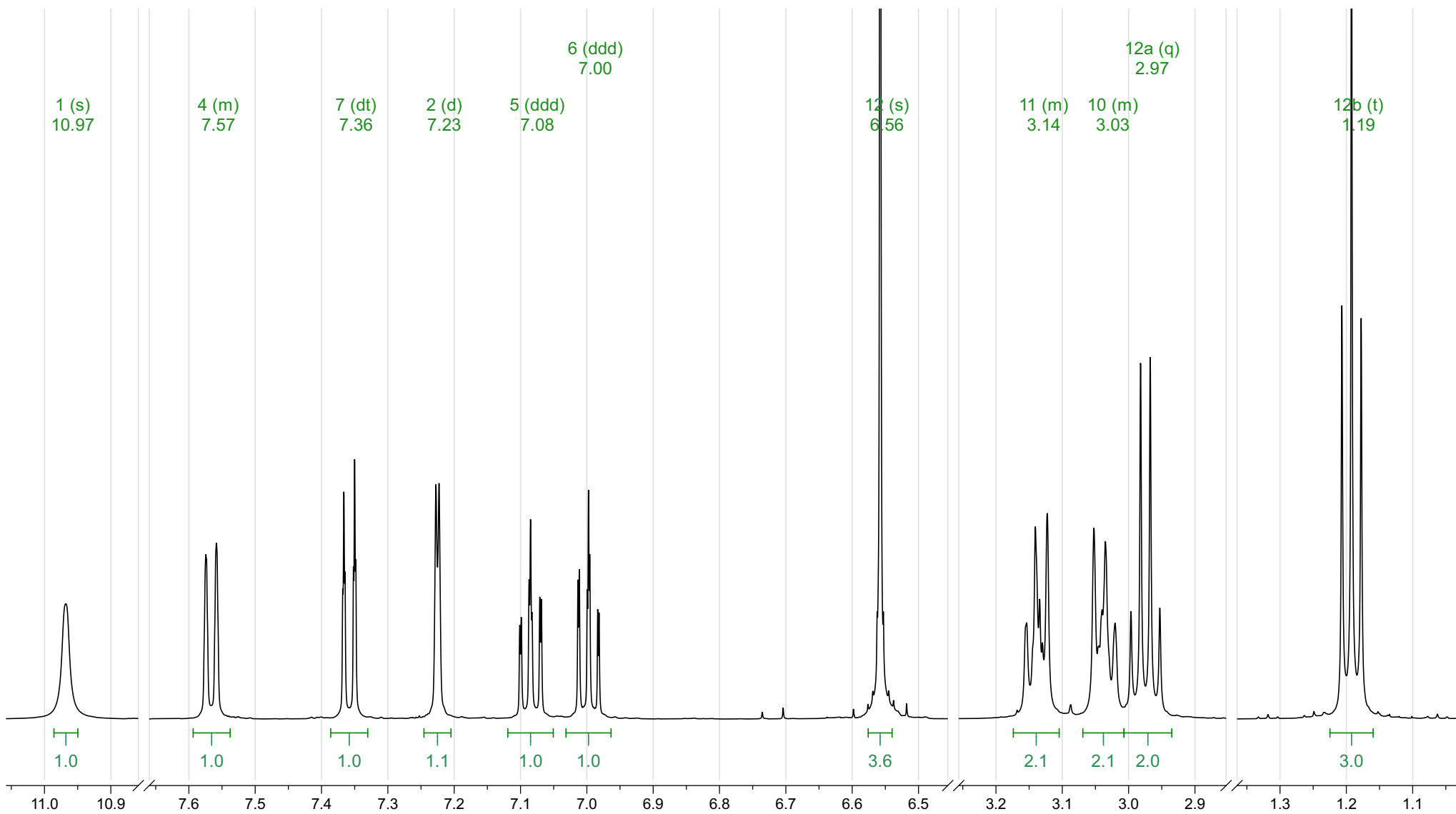


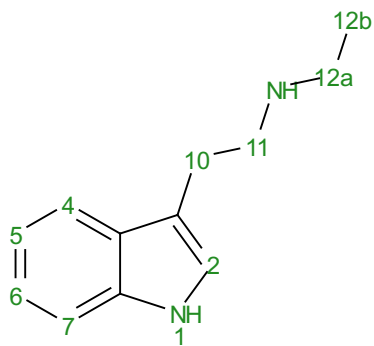
Analyte T47: NET fumarate  
 Acquisition Date 2019-09-25T18:43:25  
 Solvent dmso  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 1  
 Experiment 1D  
 Spectrometer 499.66  
 Frequency  
 Spectral Width 8012.8  
 Nucleus 1H  
 Acquired Size 48077



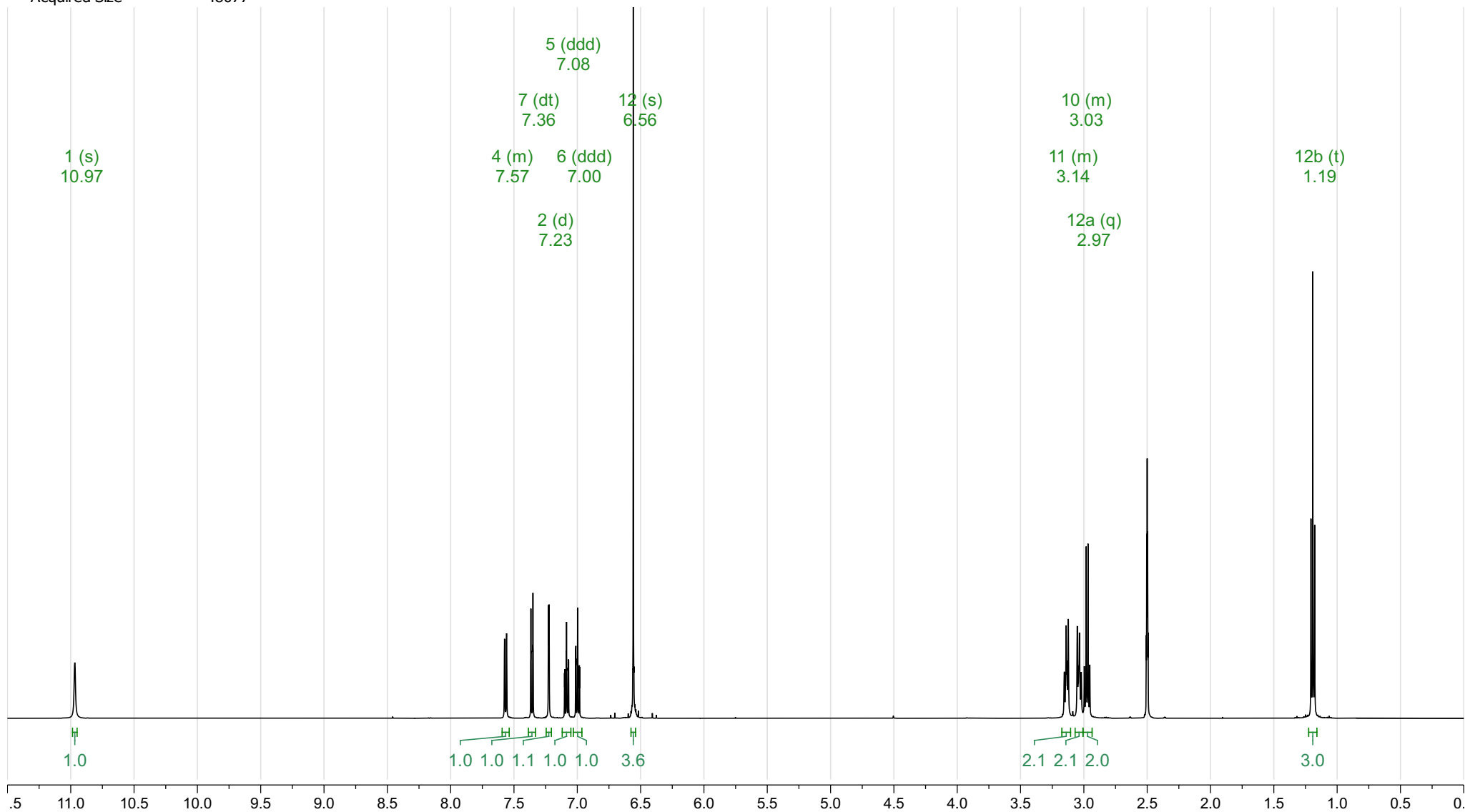
<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 10.97 (s, 1H), 7.59 – 7.54 (m, 1H), 7.36 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.23 (d, *J* = 2.4 Hz, 1H), 7.08 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 7.00 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 6.56 (s, 4H), 3.17 – 3.10 (m, 2H), 3.07 – 3.01 (m, 2H), 2.97 (q, *J* = 7.2 Hz, 2H), 1.19 (t, *J* = 7.3 Hz, 3H).



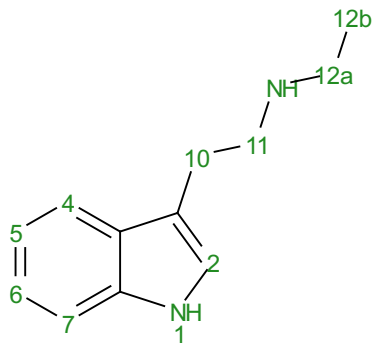
Analyte T47: NET fumarate  
Acquisition Date 2019-09-25T18:43:25  
Solvent dmso  
Temperature 25  
Number of Scans 16  
Relaxation Delay 1  
Experiment 1D  
Spectrometer 499.66  
Frequency  
Spectral Width 8012.8  
Nucleus  $^1\text{H}$   
Acquired Size 48077



$^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ )  $\delta$  10.97 (s, 1H), 7.59 – 7.54 (m, 1H), 7.36 (dt,  $J = 8.1, 0.9$  Hz, 1H), 7.23 (d,  $J = 2.4$  Hz, 1H), 7.08 (ddd,  $J = 8.1, 7.0, 1.2$  Hz, 1H), 7.00 (ddd,  $J = 8.0, 7.0, 1.0$  Hz, 1H), 6.56 (s, 4H), 3.17 – 3.10 (m, 2H), 3.07 – 3.01 (m, 2H), 2.97 (q,  $J = 7.2$  Hz, 2H), 1.19 (t,  $J = 7.3$  Hz, 3H).



Prediction 4-ProO-DMT  
Origin Modgraph NMRPredict Desktop  
Solvent DMSO-d6  
Algorithm Best  
GMMX Cycles 10  
Version 1.15 (5.076)  
Frequency 500.00  
Nucleus 1H



$^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  10.84 (d,  $J = 7.1$  Hz, 1H), 7.54 – 7.46 (m, 1H), 7.41 – 7.33 (m, 1H), 7.23 (d,  $J = 6.9$  Hz, 1H), 7.15 – 7.05 (m, 2H), 2.92 – 2.80 (m, 7H), 1.32 (t,  $J = 6.0$  Hz, 3H).

