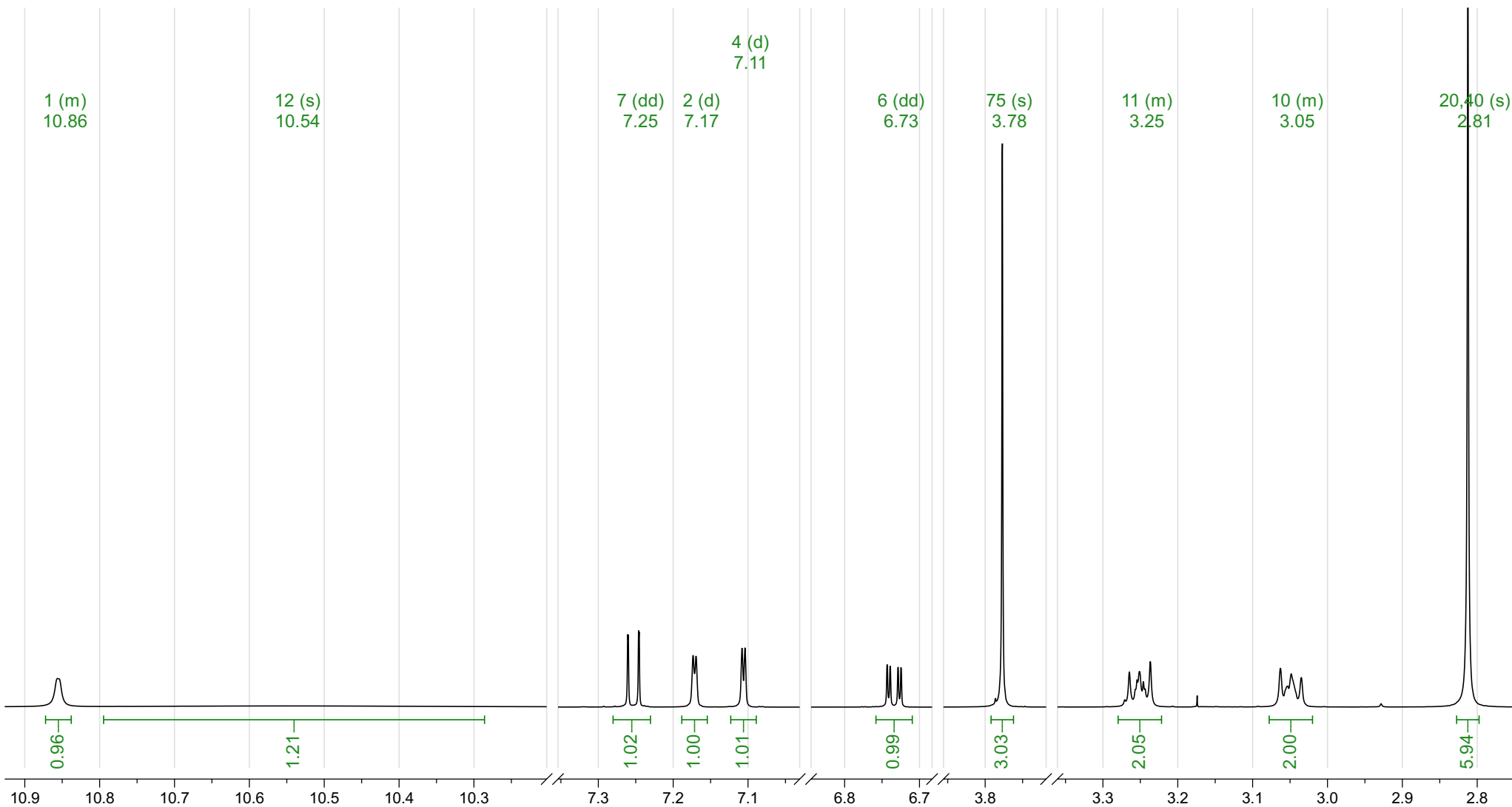
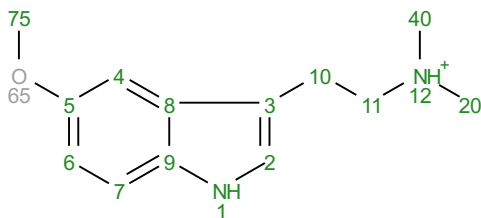


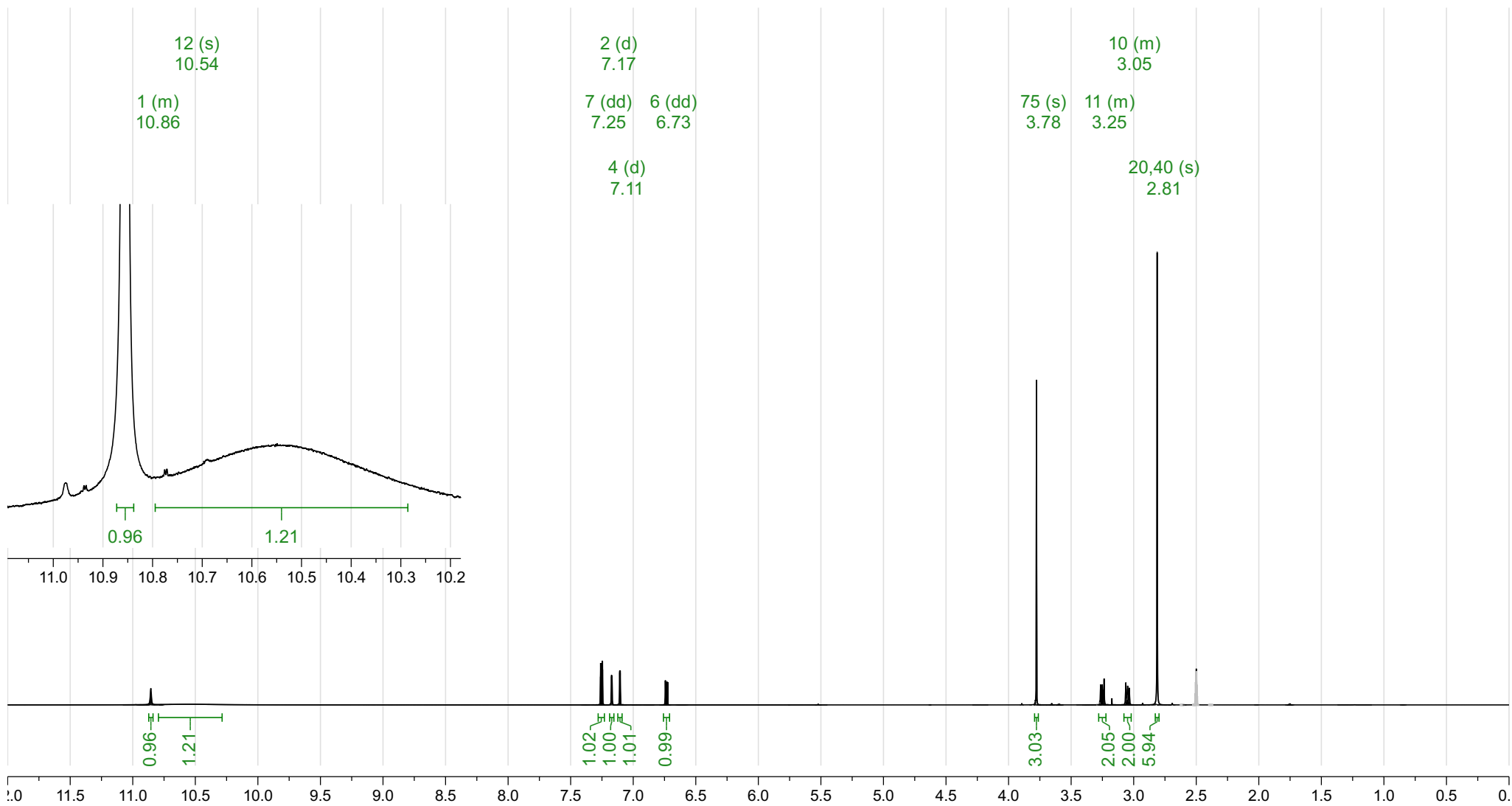
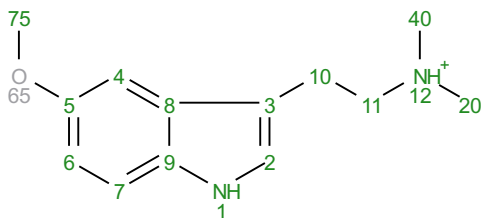
Analyte T44: 5-MeO-DMT oxalate  
 Acquisition Date 2018-11-02T09:27:47  
 Solvent dmsO  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 1  
 Experiment 1D  
 Spectrometer Frequency 599.82  
 Spectral Width 9615.4  
 Nucleus 1H  
 Acquired Size 43269

$^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ )  $\delta$  10.87 – 10.84 (m, 1H), 10.54 (s, 1H), 7.25 (dd,  $J$  = 8.8, 0.5 Hz, 1H), 7.17 (d,  $J$  = 2.4 Hz, 1H), 7.11 (d,  $J$  = 2.4 Hz, 1H), 6.73 (dd,  $J$  = 8.7, 2.4 Hz, 1H), 3.78 (s, 3H), 3.28 – 3.22 (m, 2H), 3.08 – 3.02 (m, 2H), 2.81 (s, 6H).



Analyte T44: 5-MeO-DMT oxalate  
 Acquisition Date 2018-11-02T09:27:47  
 Solvent dmso  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 1  
 Experiment 1D  
 Spectrometer Frequency 599.82  
 Spectral Width 9615.4  
 Nucleus 1H  
 Acquired Size 43269

<sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) δ 10.87 – 10.84 (m, 1H), 10.54 (s, 1H), 7.25 (dd, *J* = 8.8, 0.5 Hz, 1H), 7.17 (d, *J* = 2.4 Hz, 1H), 7.11 (d, *J* = 2.4 Hz, 1H), 6.73 (dd, *J* = 8.7, 2.4 Hz, 1H), 3.78 (s, 3H), 3.28 – 3.22 (m, 2H), 3.08 – 3.02 (m, 2H), 2.81 (s, 6H).



Prediction 5-MeO-DMT H<sup>+</sup>

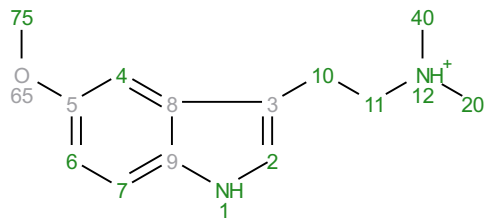
Origin Mnova Best

Solvent DMSO-d<sub>6</sub>

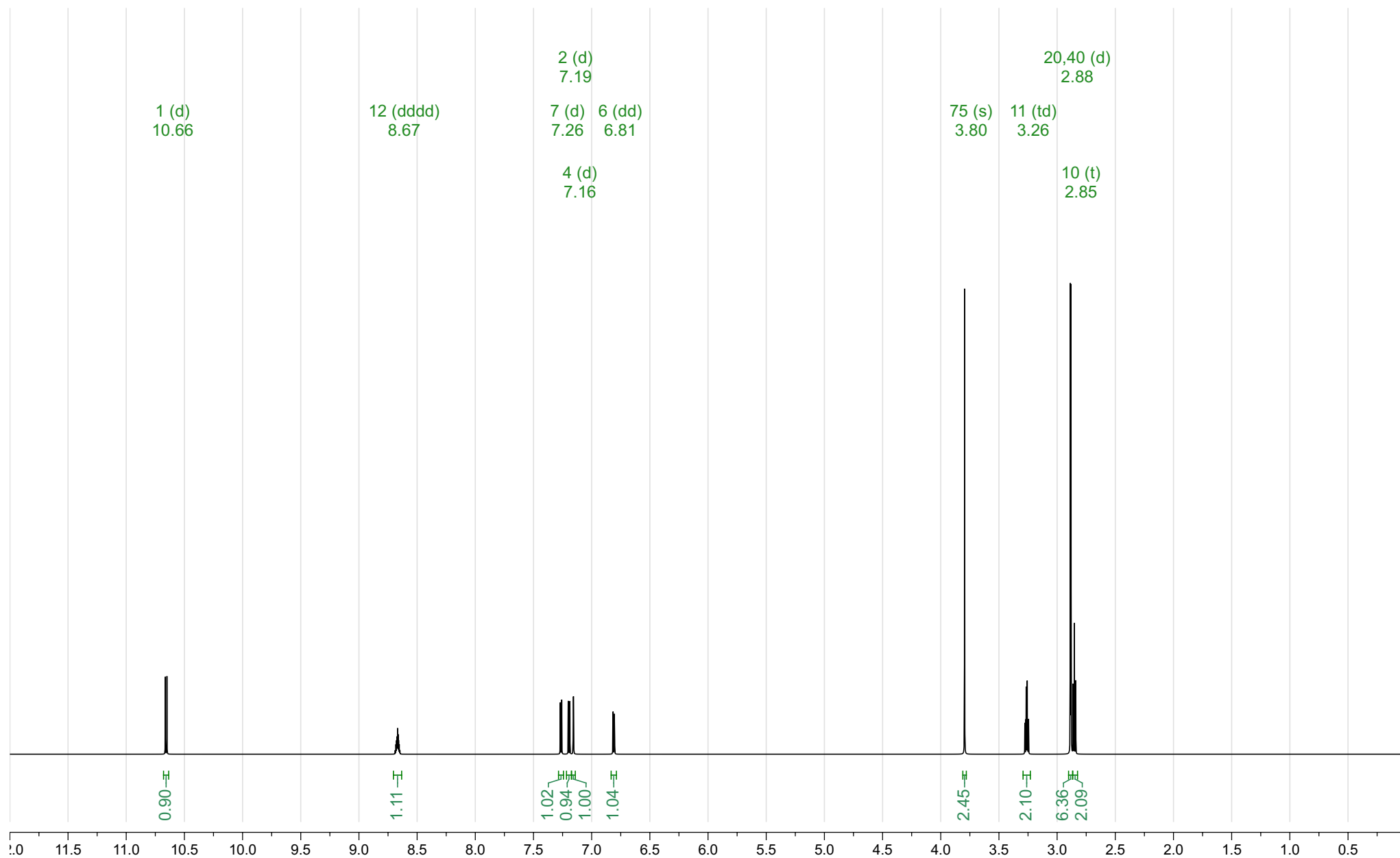
Version 1.0.0

Frequency 600.00

Nucleus <sup>1</sup>H

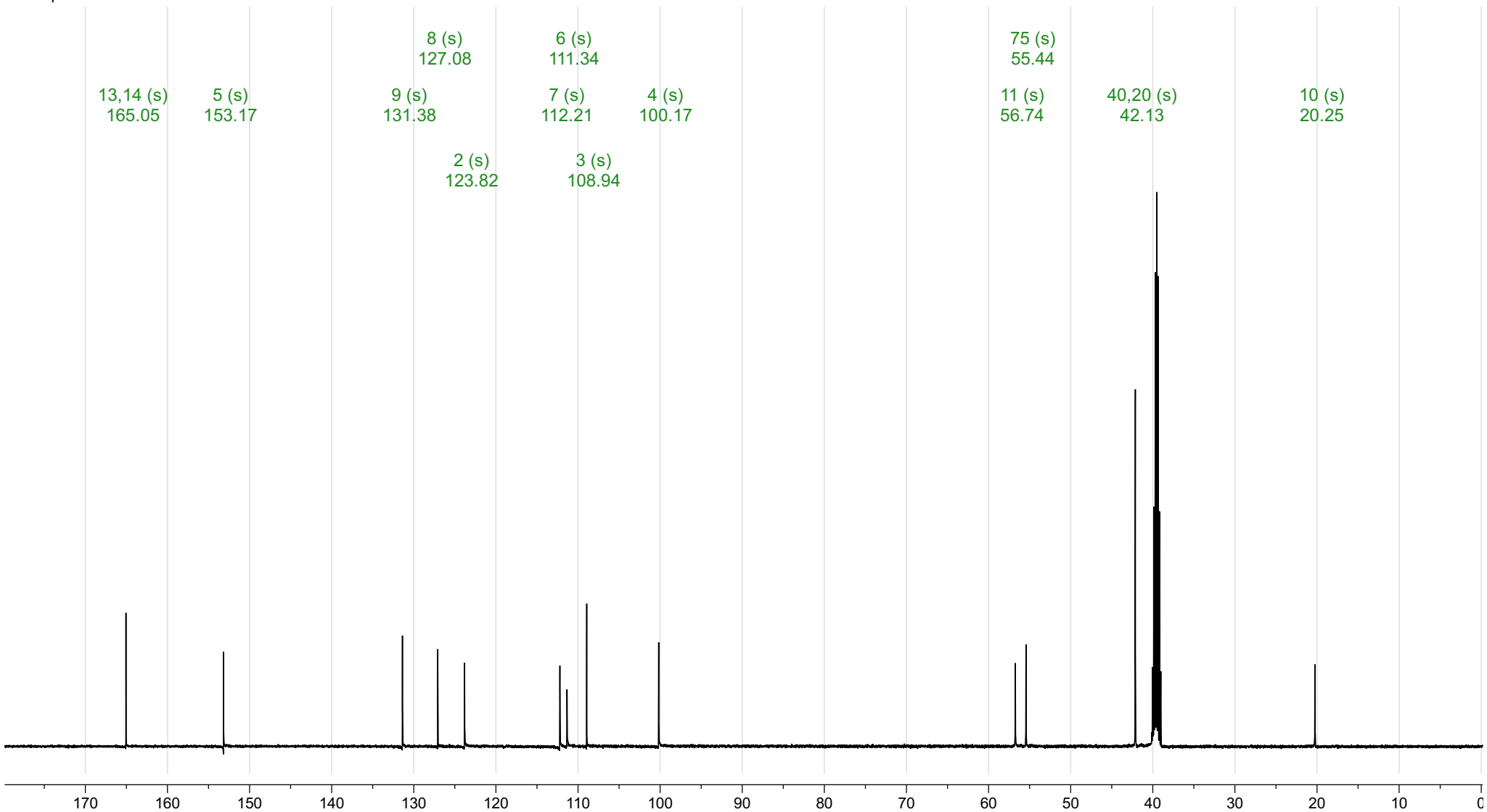
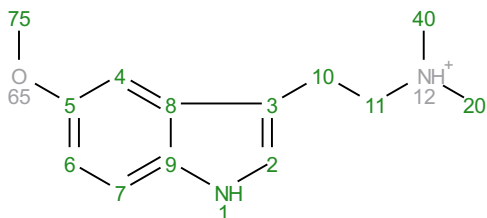


<sup>1</sup>H NMR (600 MHz, DMSO-d<sub>6</sub>) δ 10.66 (d, *J* = 8.4 Hz, 1H), 8.67 (dddd, *J* = 8.7, 6.7, 5.4, 3.5 Hz, 1H), 7.26 (d, *J* = 7.4 Hz, 1H), 7.19 (d, *J* = 8.2 Hz, 1H), 7.16 (d, *J* = 1.5 Hz, 1H), 6.81 (dd, *J* = 7.4, 1.5 Hz, 1H), 3.80 (s, 2H), 3.26 (td, *J* = 7.1, 5.3 Hz, 2H), 2.88 (d, *J* = 3.6 Hz, 6H), 2.85 (t, *J* = 7.1 Hz, 2H).



Analyte T44: 5-MeO-DMT oxalate  
Acquisition Date 2018-11-02T10:25:00  
Solvent dmso  
Temperature 25  
Number of Scans 256  
Relaxation Delay 0  
Experiment 1D  
Spectrometer Frequency 125.65  
Spectral Width 30487.8  
Nucleus 13C  
Acquired Size 60976

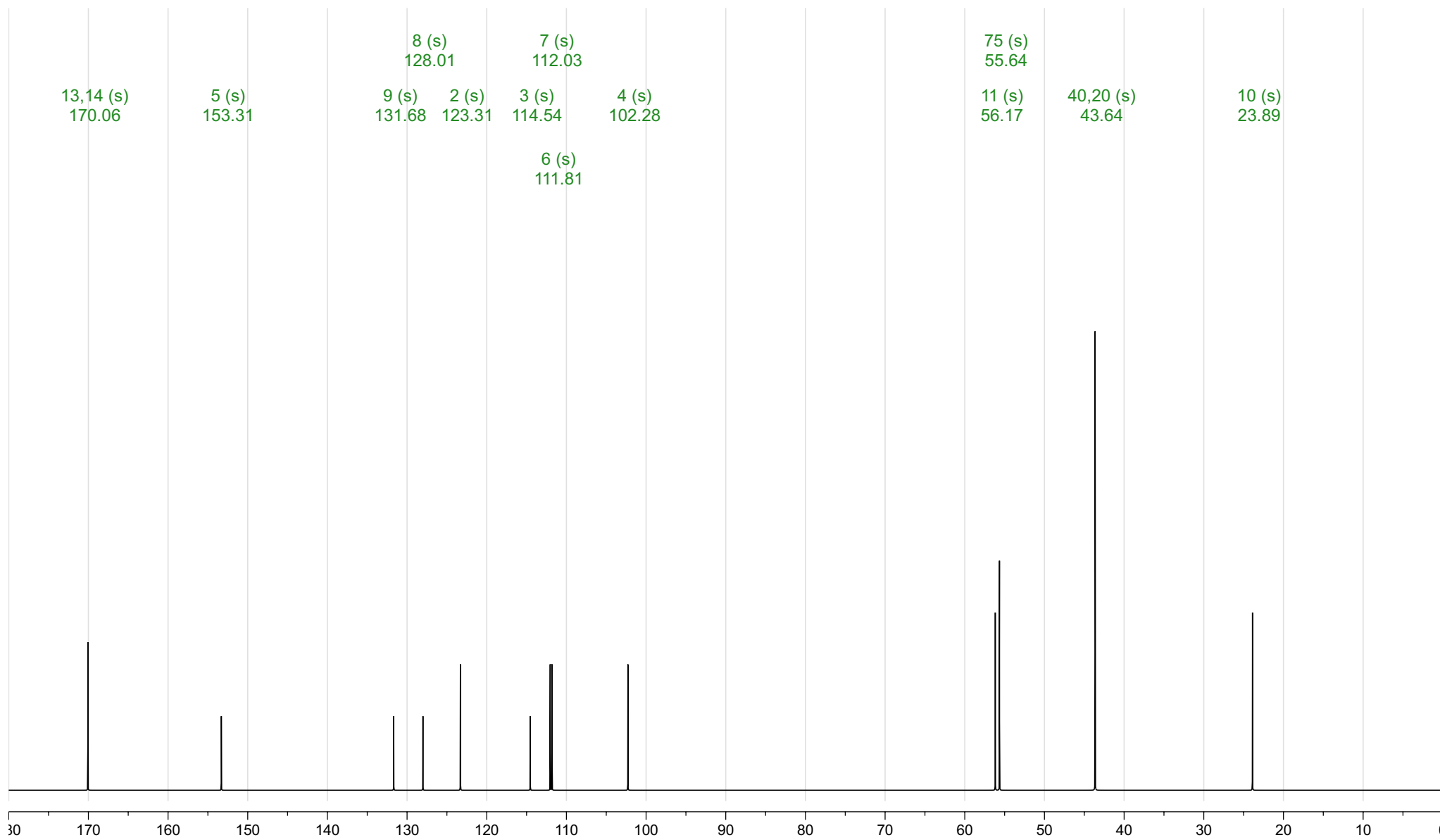
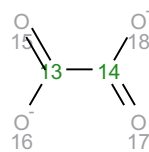
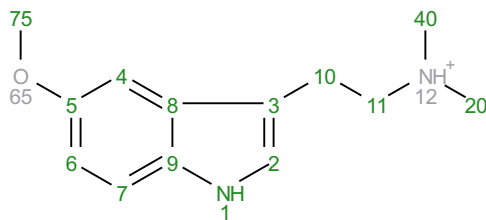
<sup>13</sup>C NMR (126 MHz, DMSO-d<sub>6</sub>) δ 165.05, 153.17, 131.38, 127.08, 123.82, 112.21, 111.34, 108.94, 100.17, 56.74, 55.44, 42.13, 20.25.



Prediction 5-MeO-DMT oxalate

Origin Mnova Best  
Solvent DMSO-d6  
Version 1.0.0  
Frequency 150.00  
Nucleus 13C

$^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ )  $\delta$  170.06, 153.31, 131.68, 128.01, 123.31, 114.54, 112.03, 111.81, 102.28, 56.17, 55.64, 43.64, 23.89.



Analyte T44: 5-MeO-DMT oxalate  
Acquisition Date 2018-11-02T09:29:58  
Solvent dmso  
Temperature 25  
Number of Scans 2  
Relaxation Delay 1  
Experiment HSQC-EDITED  
Spectrometer Frequency (599.82, 150.83)  
Spectral Width (9615.4, 25641.0)  
Nucleus (1H, 13C)  
Acquired Size (1024, 200)

