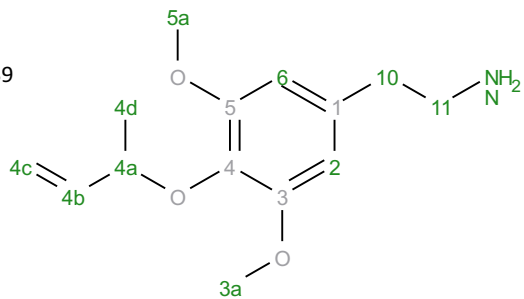
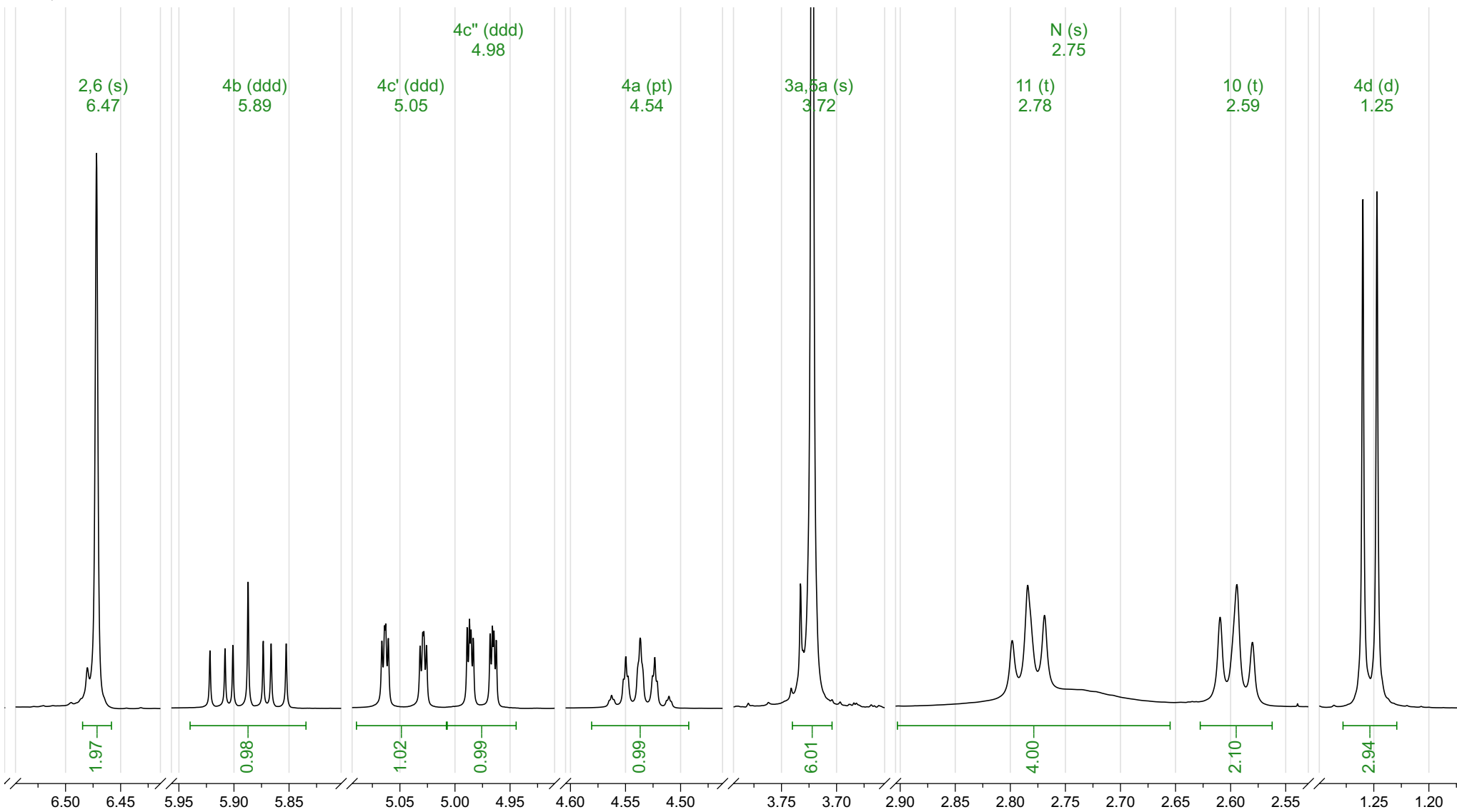


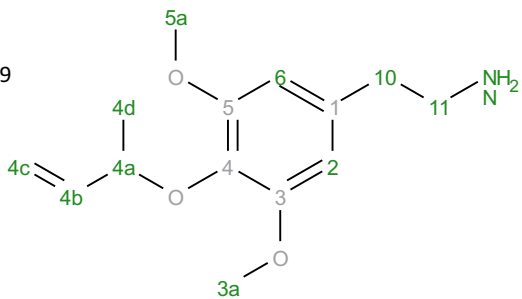
Analyte P26: MAL-2 fb  
 Acquisition Date 2019-03-08T15:24:39  
 Solvent dms0  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 1  
 Experiment 1D  
 Spectrometer Frequency 499.66  
 Spectral Width 8012.8  
 Nucleus 1H  
 Acquired Size 48077



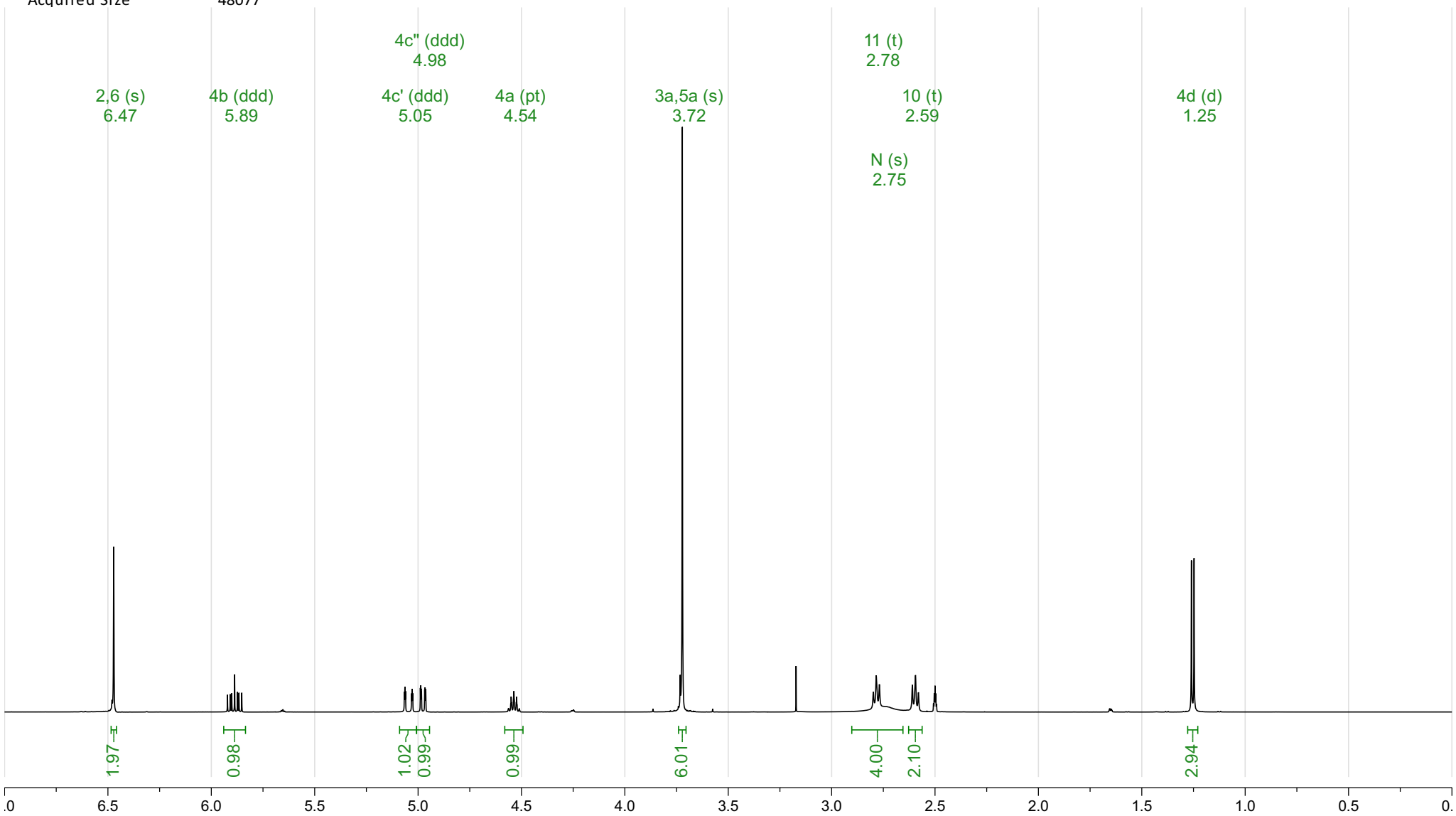
<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 6.47 (s, 2H), 5.89 (ddd, *J* = 17.3, 10.4, 6.8 Hz, 1H), 5.05 (ddd, *J* = 17.4, 1.8, 1.2 Hz, 1H), 4.98 (ddd, *J* = 10.4, 1.8, 1.1 Hz, 1H), 4.54 (pt, *J* = 6.5, 1.2 Hz, 1H), 3.72 (s, 6H), 2.78 (t, *J* = 7.4 Hz, 2H), 2.75 (s, 2H), 2.59 (t, *J* = 7.3 Hz, 2H), 1.25 (d, *J* = 6.4 Hz, 3H).



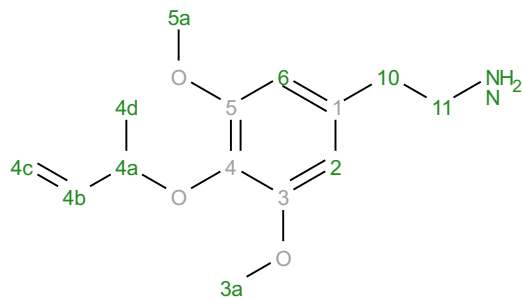
Analyte P26: MAL-2 fb  
 Acquisition Date 2019-03-08T15:24:39  
 Solvent dms0  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 1  
 Experiment 1D  
 Spectrometer Frequency 499.66  
 Spectral Width 8012.8  
 Nucleus 1H  
 Acquired Size 48077



<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 6.47 (s, 2H), 5.89 (ddd, *J* = 17.3, 10.4, 6.8 Hz, 1H), 5.05 (ddd, *J* = 17.4, 1.8, 1.2 Hz, 1H), 4.98 (ddd, *J* = 10.4, 1.8, 1.1 Hz, 1H), 4.54 (pt, *J* = 6.5, 1.2 Hz, 1H), 3.72 (s, 6H), 2.78 (t, *J* = 7.4 Hz, 2H), 2.75 (s, 2H), 2.59 (t, *J* = 7.3 Hz, 2H), 1.25 (d, *J* = 6.4 Hz, 3H).



Prediction MAL-2 fb  
Origin Mnova Best  
Solvent DMSO-d6  
Version 1.0.0  
Frequency 500.00  
Nucleus 1H



<sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ 6.48 (t, *J* = 1.0 Hz, 2H), 5.85 – 5.75 (m, 1H), 5.35 – 5.25 (m, 2H), 4.74 (dtd, *J* = 7.9, 6.9, 5.8 Hz, 1H), 3.82 (s, 4H), 3.35 – 3.29 (m, 2H), 3.22 – 3.12 (m, 2H), 2.90 (tt, *J* = 7.3, 1.1 Hz, 2H), 1.33 (dd, *J* = 6.8, 1.0 Hz, 3H).

