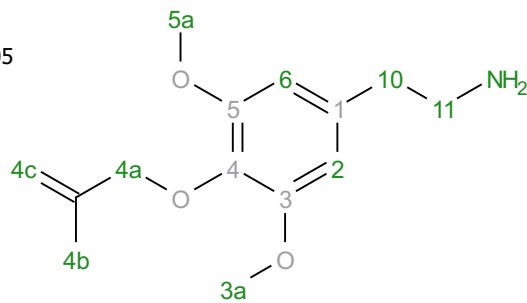
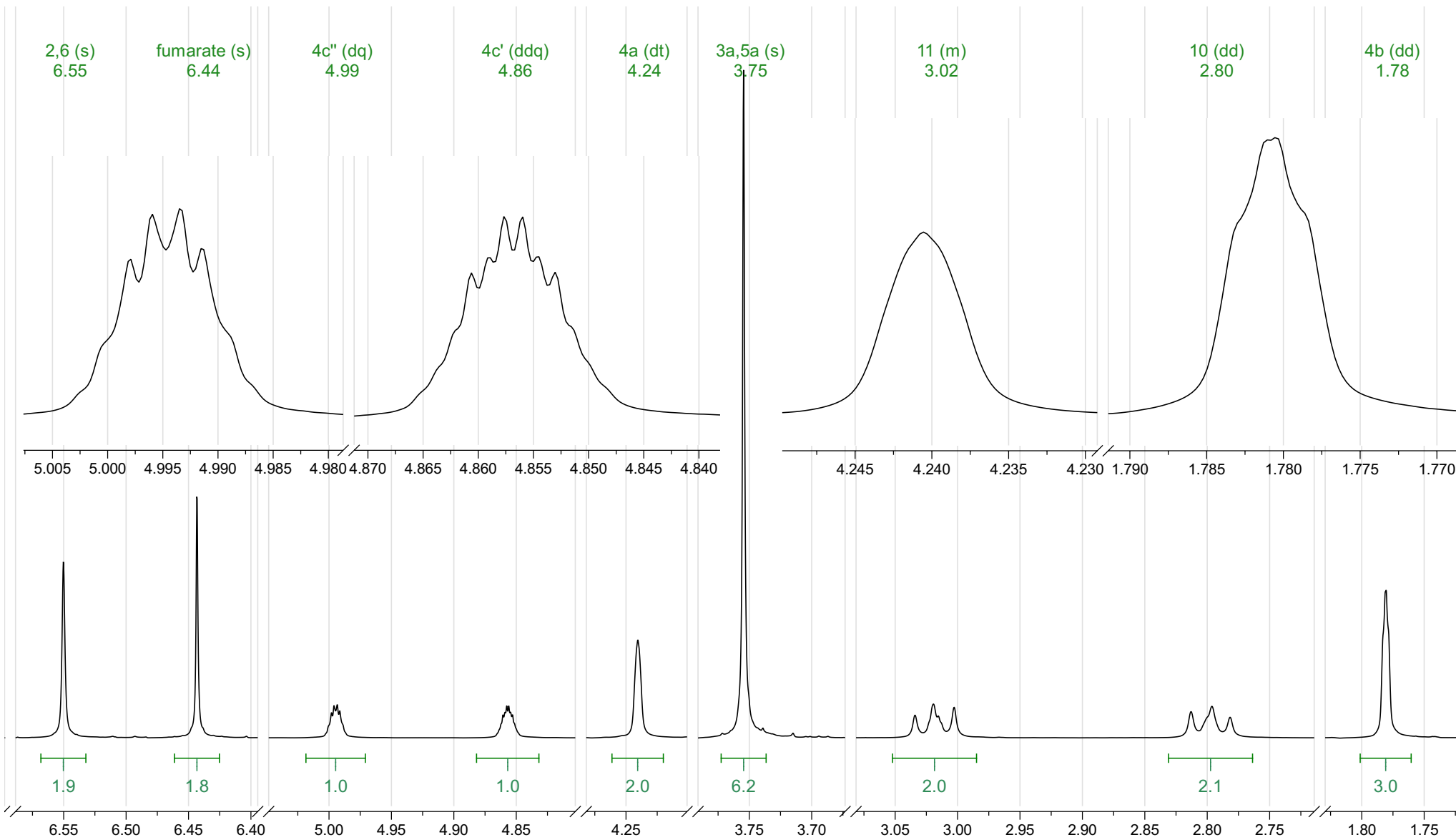


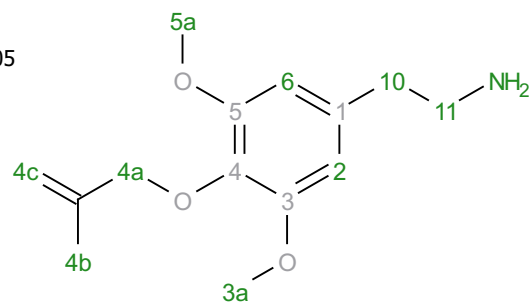
Analyte P32: MAL fumarate  
 Acquisition Date 2019-09-25T17:50:05  
 Solvent dmsd  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 1  
 Spectrometer Frequency 499.66  
 Spectral Width 8012.8  
 Nucleus 1H  
 Acquired Size 48077



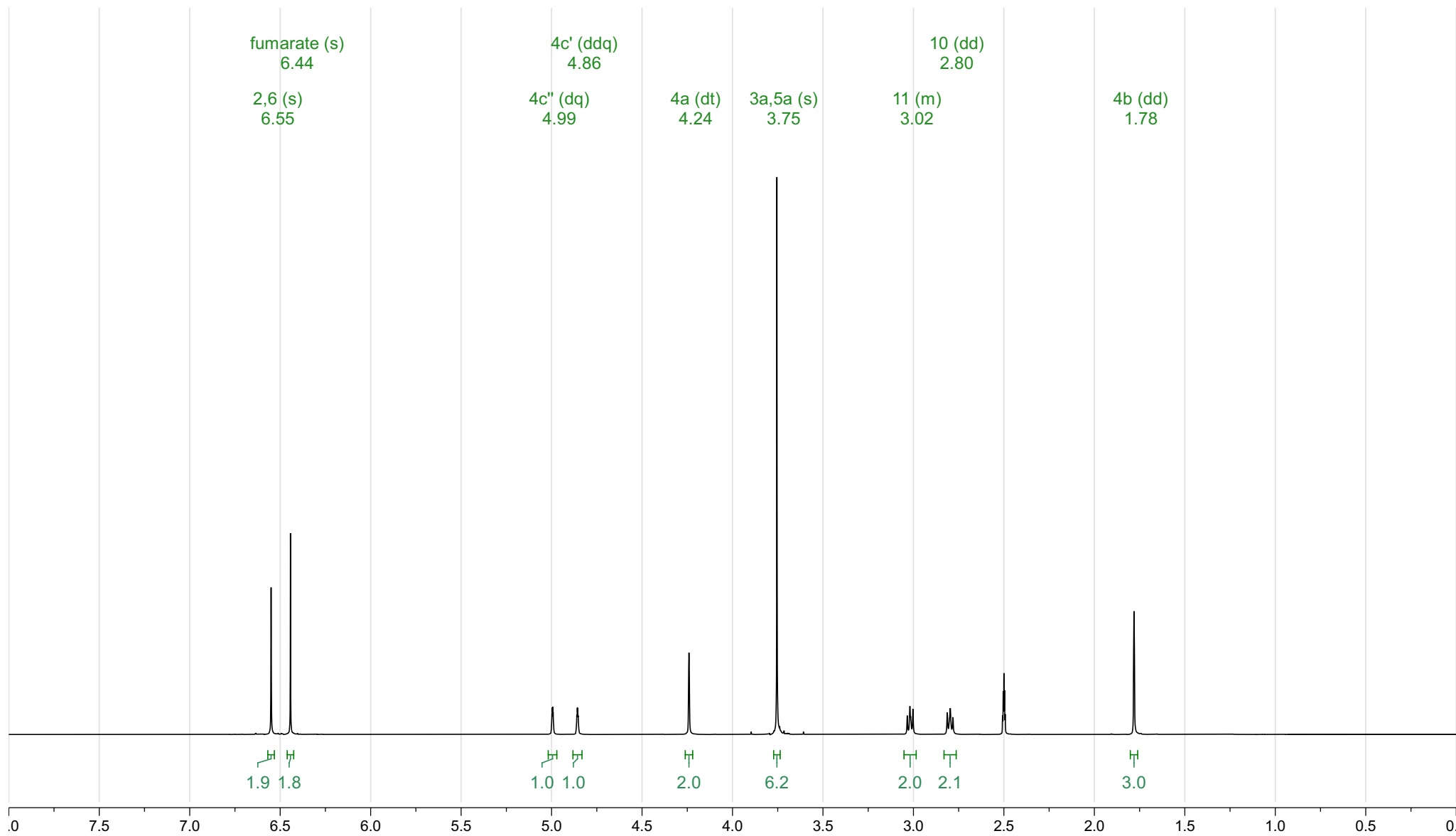
<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 6.55 (s, 2H), 6.44 (s, 2H), 4.99 (dq, *J* = 2.3, 1.2 Hz, 1H), 4.86 (ddq, *J* = 2.3, 1.6, 0.8 Hz, 1H), 4.24 (dt, *J* = 1.2, 0.6 Hz, 2H), 3.75 (s, 6H), 3.05 – 2.98 (m, 2H), 2.80 (dd, *J* = 8.9, 6.7 Hz, 2H), 1.78 (dd, *J* = 1.5, 0.9 Hz, 3H).



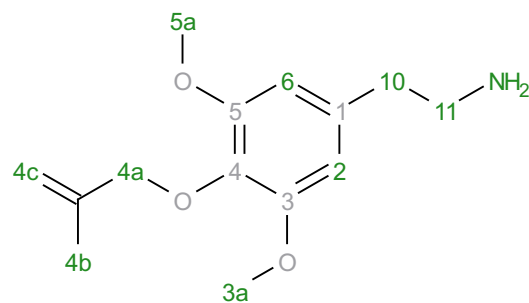
Analyte P32: MAL fumarate  
Acquisition Date 2019-09-25T17:50:05  
Solvent dmso  
Temperature 25  
Number of Scans 16  
Relaxation Delay 1  
Spectrometer Frequency 499.66  
Spectral Width 8012.8  
Nucleus 1H  
Acquired Size 48077



$^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )  $\delta$  6.55 (s, 2H), 6.44 (s, 2H), 4.99 (dq,  $J = 2.3, 1.2$  Hz, 1H), 4.86 (ddq,  $J = 2.3, 1.6, 0.8$  Hz, 1H), 4.24 (dt,  $J = 1.2, 0.6$  Hz, 2H), 3.75 (s, 6H), 3.05 – 2.98 (m, 2H), 2.80 (dd,  $J = 8.9, 6.7$  Hz, 2H), 1.78 (dd,  $J = 1.5, 0.9$  Hz, 3H).



Prediction MAL  
 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- $d_6$ )  $\delta$  6.53 (t,  $J$  = 1.0 Hz, 2H), 5.29 (p,  $J$  = 1.5 Hz, 1H), 4.79 (p,  $J$  = 1.5 Hz, 1H), 4.58 (d,  $J$  = 13.2 Hz, 1H), 4.58 (s, 3H), 3.84 (s, 6H), 3.33 – 3.25 (m, 2H), 2.97 (tt,  $J$  = 4.9, 1.0 Hz, 2H), 1.80 (t,  $J$  = 1.5 Hz, 3H).

