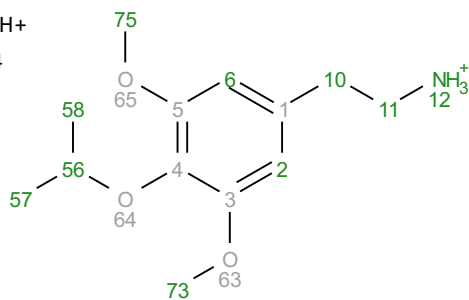
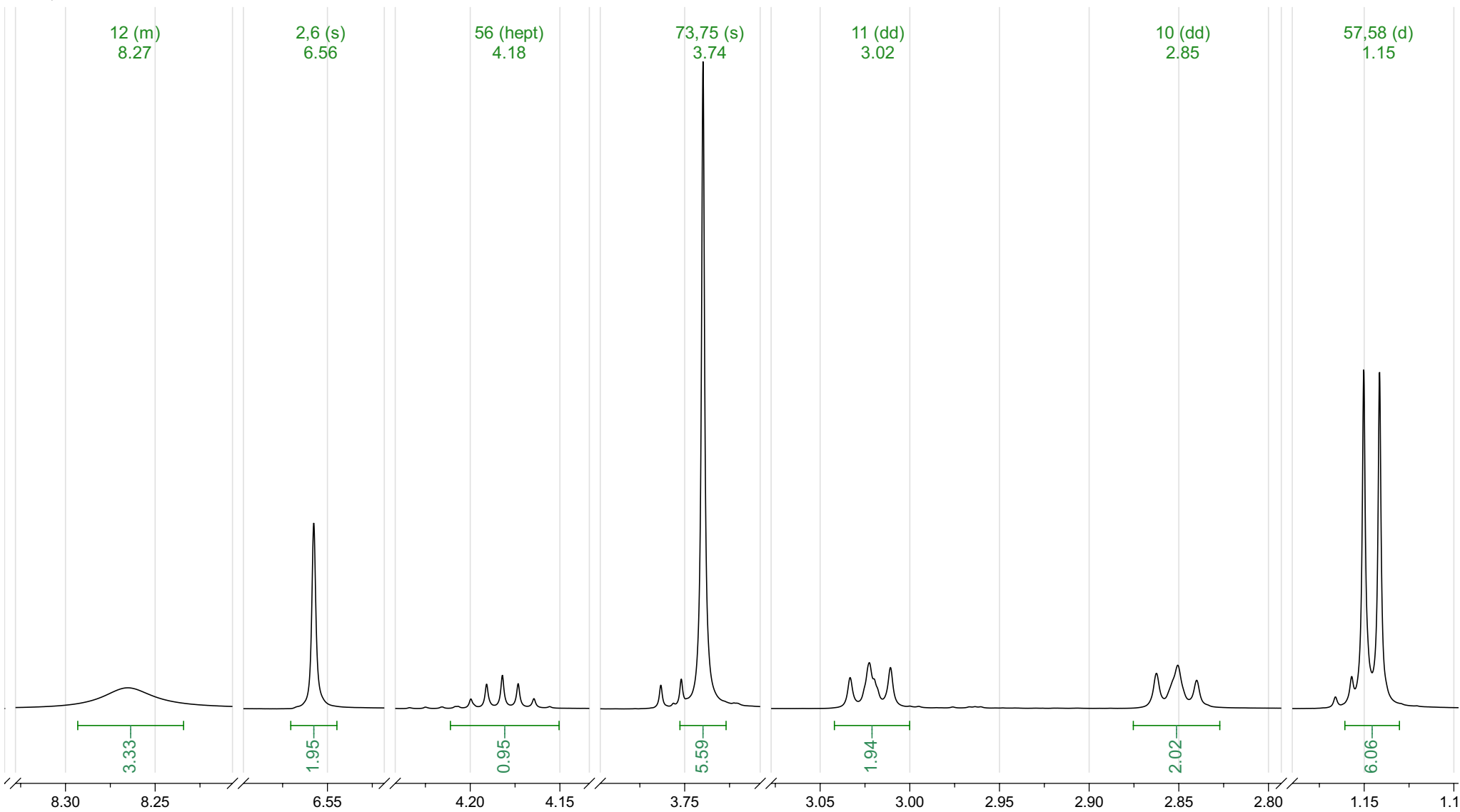


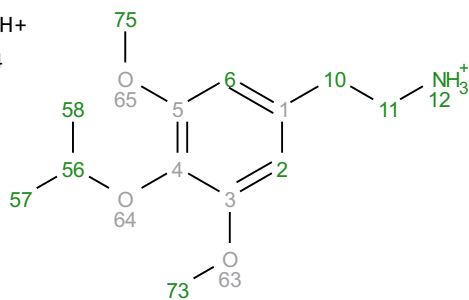
Analyte P22: Isoprosaline H+  
Acquisition Date 2018-07-16T11:57:54  
Solvent dmso  
Temperature 25  
Number of Scans 16  
Relaxation Delay 5  
Experiment 1D  
Spectrometer Frequency 699.81  
Spectral Width 11160.7  
Nucleus 1H  
Acquired Size 55804



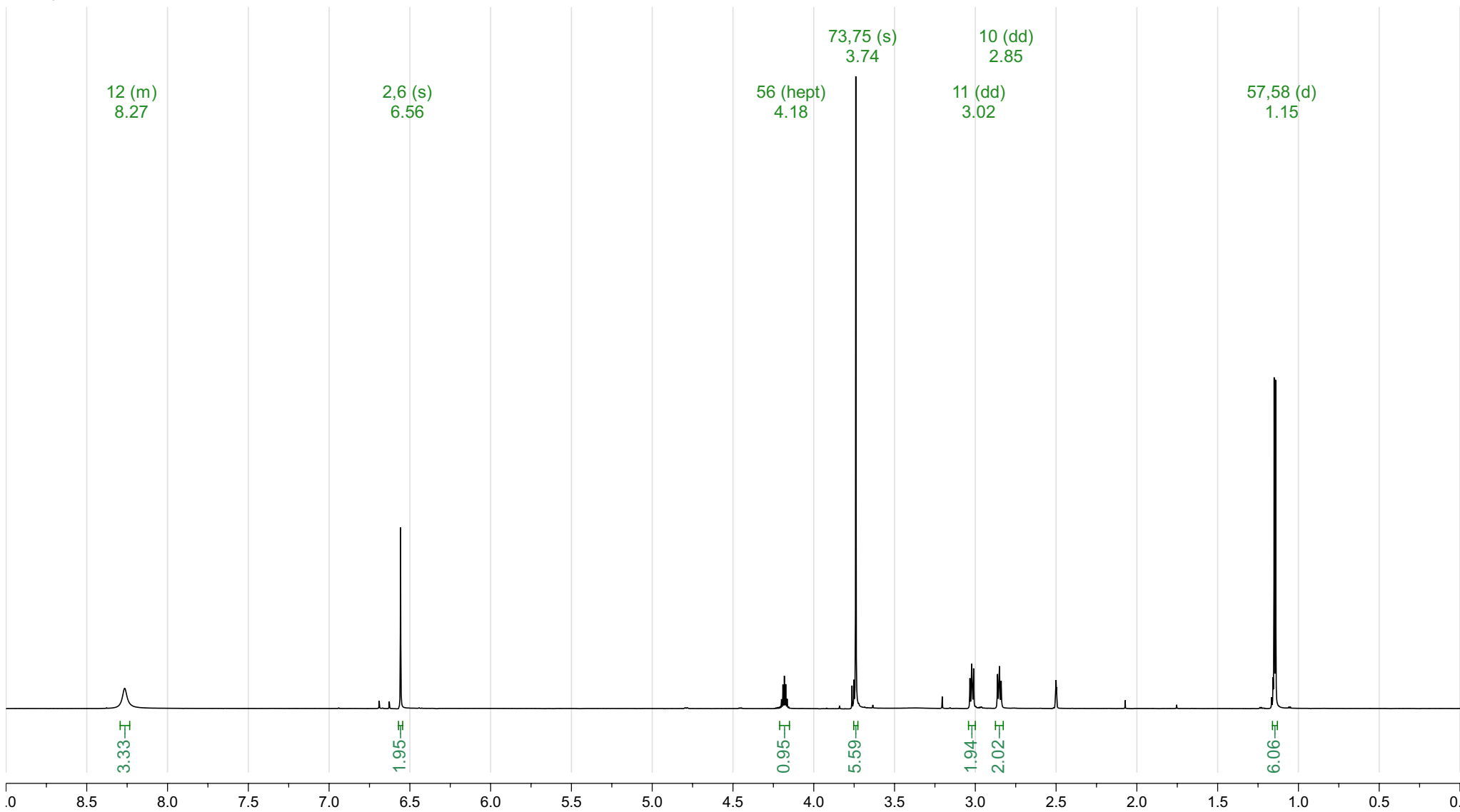
<sup>1</sup>H NMR (700 MHz, DMSO-*d*<sub>6</sub>) δ 8.29 – 8.23 (m, 3H), 6.56 (s, 2H), 4.18 (hept, *J* = 6.2 Hz, 1H), 3.74 (s, 6H), 3.02 (dd, *J* = 9.0, 6.8 Hz, 2H), 2.85 (dd, *J* = 9.0, 6.8 Hz, 2H), 1.15 (d, *J* = 6.2 Hz, 6H).



Analyte P22: Isoprosaline H+  
 Acquisition Date 2018-07-16T11:57:54  
 Solvent dms0  
 Temperature 25  
 Number of Scans 16  
 Relaxation Delay 5  
 Experiment 1D  
 Spectrometer Frequency 699.81  
 Spectral Width 11160.7  
 Nucleus 1H  
 Acquired Size 55804



$^1\text{H}$  NMR (700 MHz, DMSO- $d_6$ )  $\delta$  8.29 – 8.23 (m, 3H), 6.56 (s, 2H), 4.18 (hept,  $J = 6.2$  Hz, 1H), 3.74 (s, 6H), 3.02 (dd,  $J = 9.0, 6.8$  Hz, 2H), 2.85 (dd,  $J = 9.0, 6.8$  Hz, 2H), 1.15 (d,  $J = 6.2$  Hz, 6H).



Prediction Isoprosaline H+

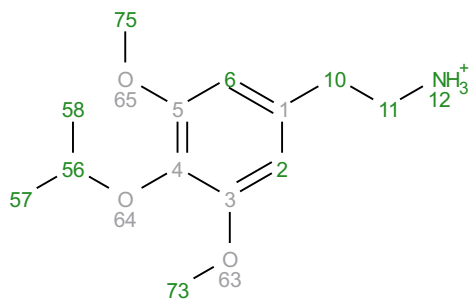
Origin Mnova Best

Solvent DMSO-d6

Version 1.0.0

Frequency 700.00

Nucleus 1H



$^1\text{H}$  NMR (700 MHz, DMSO- $d_6$ )  $\delta$  8.33 (t,  $J = 7.2$  Hz, 3H), 6.55 (t,  $J = 1.1$  Hz, 2H), 4.61 (hept,  $J = 6.9$  Hz, 1H), 3.82 (s, 4H), 3.33 (h,  $J = 7.1$  Hz, 2H), 2.95 (dt,  $J = 14.3, 1.0$  Hz, 1H), 1.29 (d,  $J = 6.9$  Hz, 6H).

