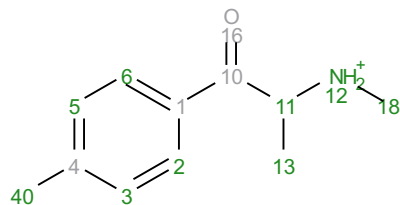
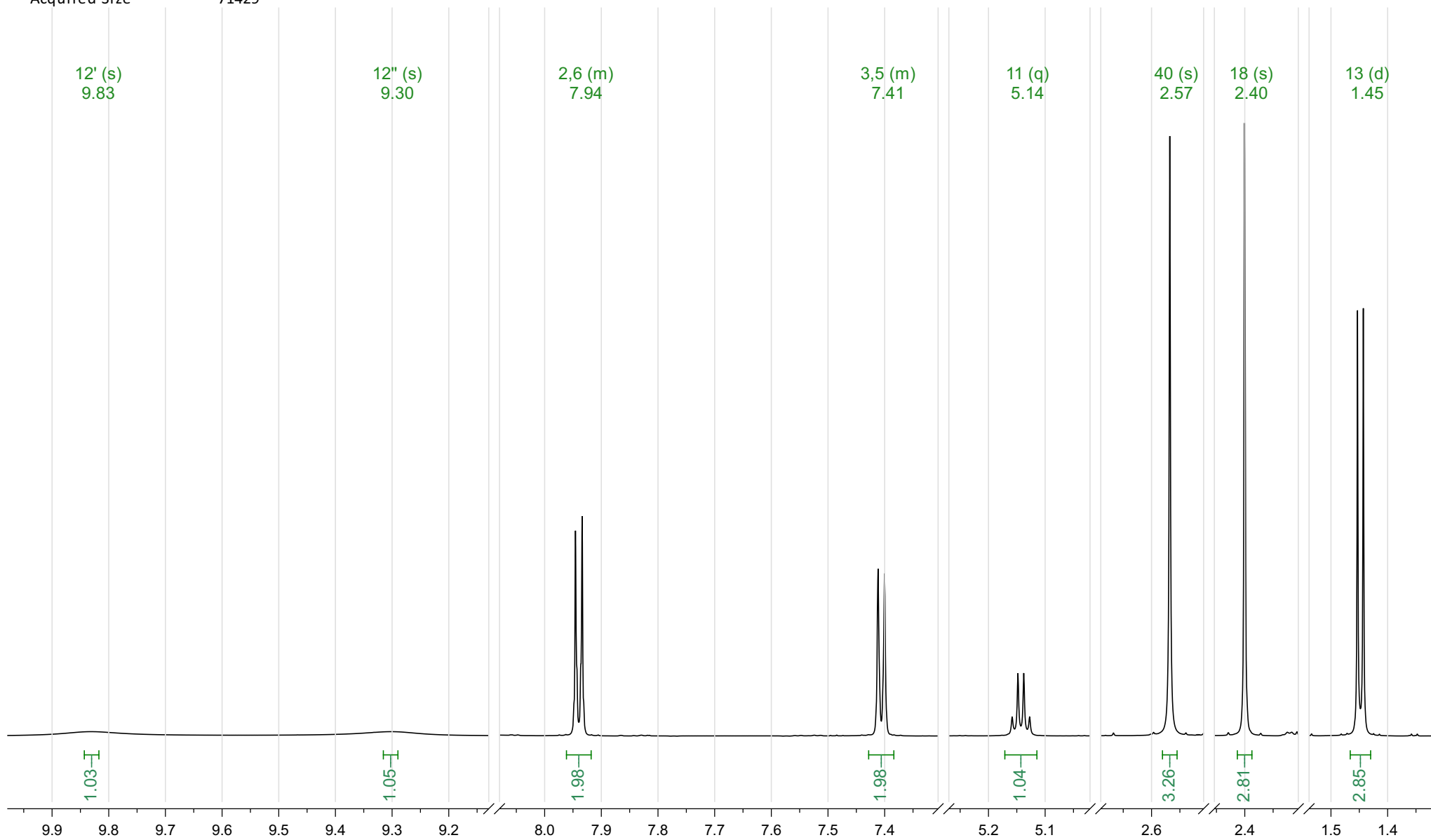


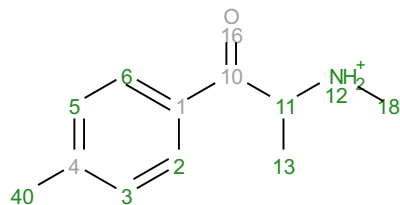
Analyte X56: Mephedrone H+  
Acquisition Date 2018-03-21T15:59:20  
Solvent dmso  
Temperature 25  
Number of Scans 64  
Relaxation Delay 1  
Spectrometer Frequency 699.81  
Spectral Width 11160.7  
Nucleus 1H  
Acquired Size 71429



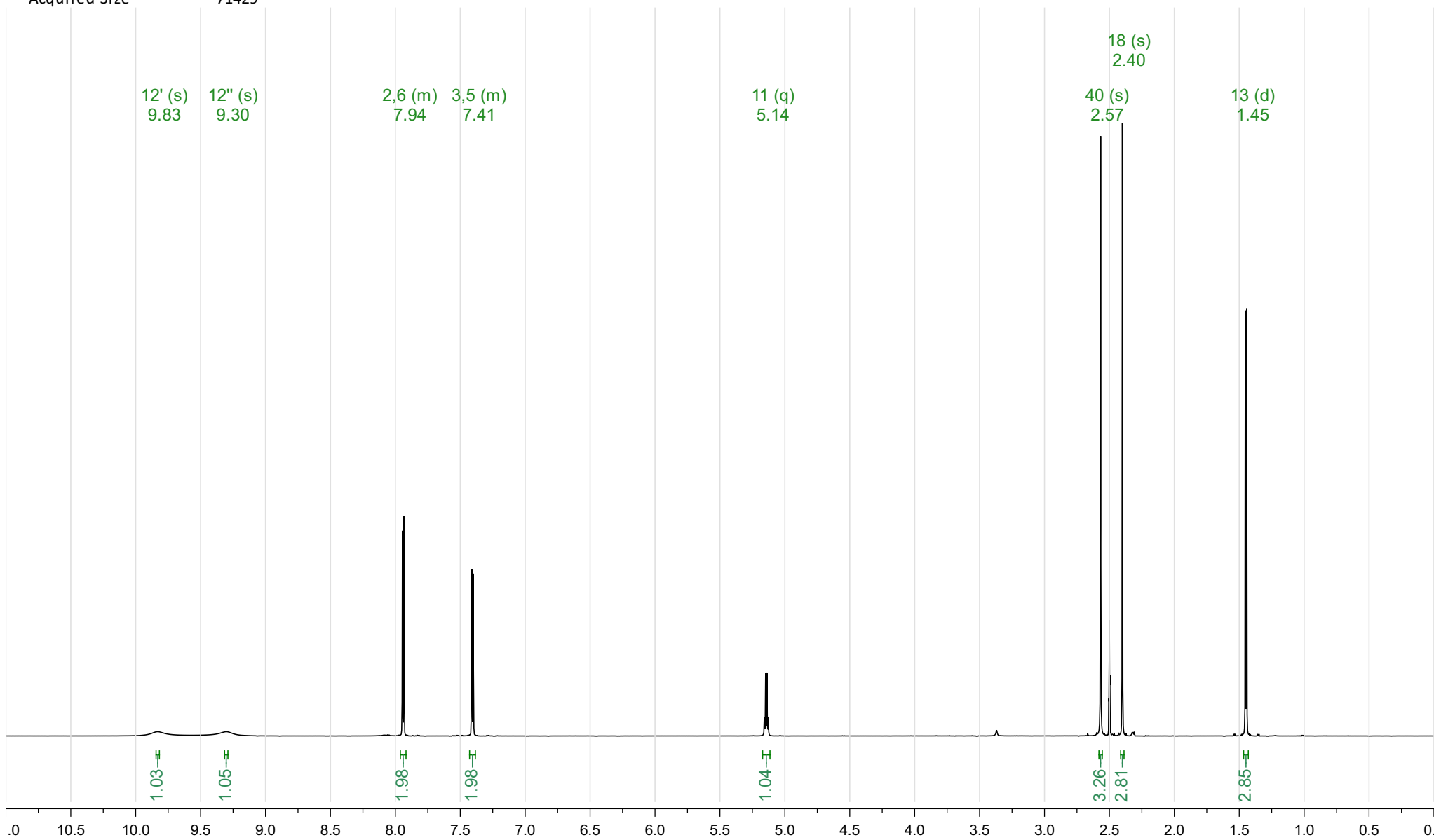
<sup>1</sup>H NMR (700 MHz, DMSO-*d*<sub>6</sub>) δ 9.83 (s, 1H), 9.30 (s, 1H), 7.96 – 7.92 (m, 2H), 7.43 – 7.38 (m, 2H), 5.14 (q, *J* = 7.2 Hz, 1H), 2.57 (s, 3H), 2.40 (s, 3H), 1.45 (d, *J* = 7.2 Hz, 3H).



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Acquisition Date 2018-03-21T15:59:20  
Solvent dmso  
Temperature 25  
Number of Scans 64  
Relaxation Delay 1  
Spectrometer Frequency 699.81  
Spectral Width 11160.7  
Nucleus 1H  
Acquired Size 71429



$^1\text{H}$  NMR (700 MHz, DMSO- $d_6$ )  $\delta$  9.83 (s, 1H), 9.30 (s, 1H), 7.96 – 7.92 (m, 2H), 7.43 – 7.38 (m, 2H), 5.14 (q,  $J = 7.2$  Hz, 1H), 2.57 (s, 3H), 2.40 (s, 3H), 1.45 (d,  $J = 7.2$  Hz, 3H).



Prediction Mephedrone H+

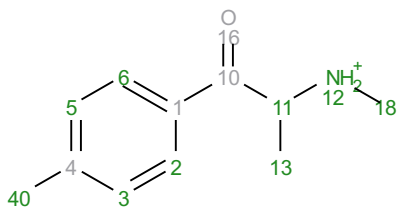
Origin Mnova Best

Solvent DMSO-d6

Version 1.0.0

Frequency 500.00

Nucleus 1H



$^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$  7.90 – 7.84 (m, 2H), 7.73 (ddt,  $J = 11.6, 8.1, 3.6$  Hz, 1H), 7.31 (ddt,  $J = 11.6, 8.1, 3.6$  Hz, 1H), 7.25 (d,  $J = 7.3$  Hz, 2H), 5.12 – 5.01 (m, 1H), 2.47 – 2.39 (m, 6H), 1.41 (d,  $J = 6.8$  Hz, 3H).

