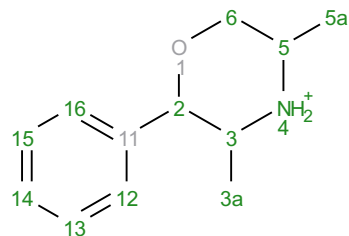
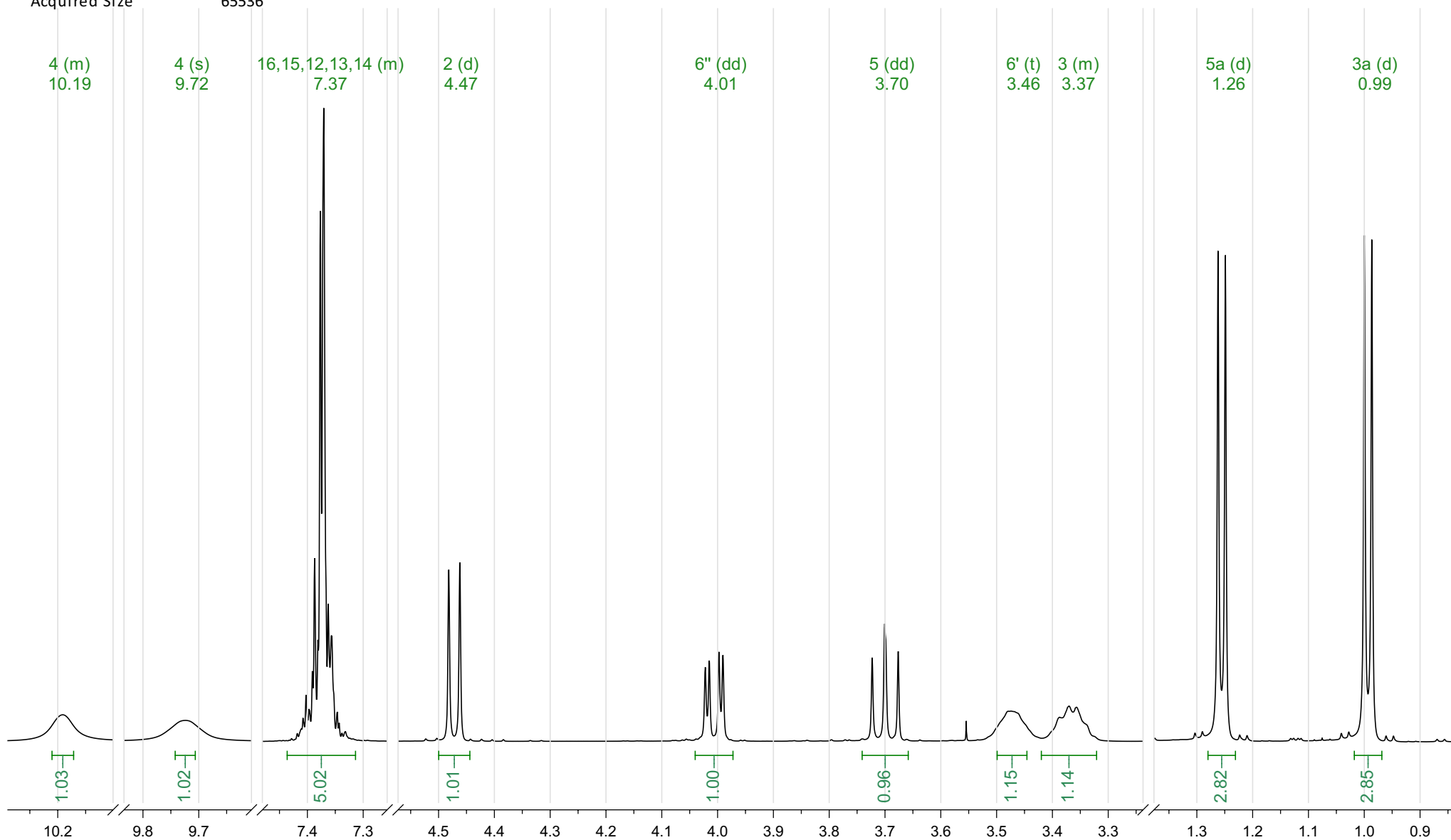


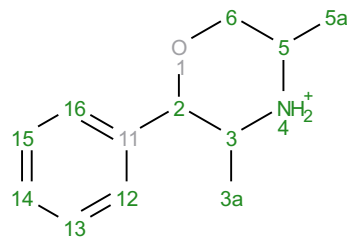
Analyte X46 PDM-35 H+  
Acquisition Date 2017-06-08T11:55:14  
Solvent dms  
Temperature 25  
Number of Scans 16  
Relaxation Delay 5  
Spectrometer Frequency 499.67  
Spectral Width 10000.0  
Nucleus 1H  
Acquired Size 65536



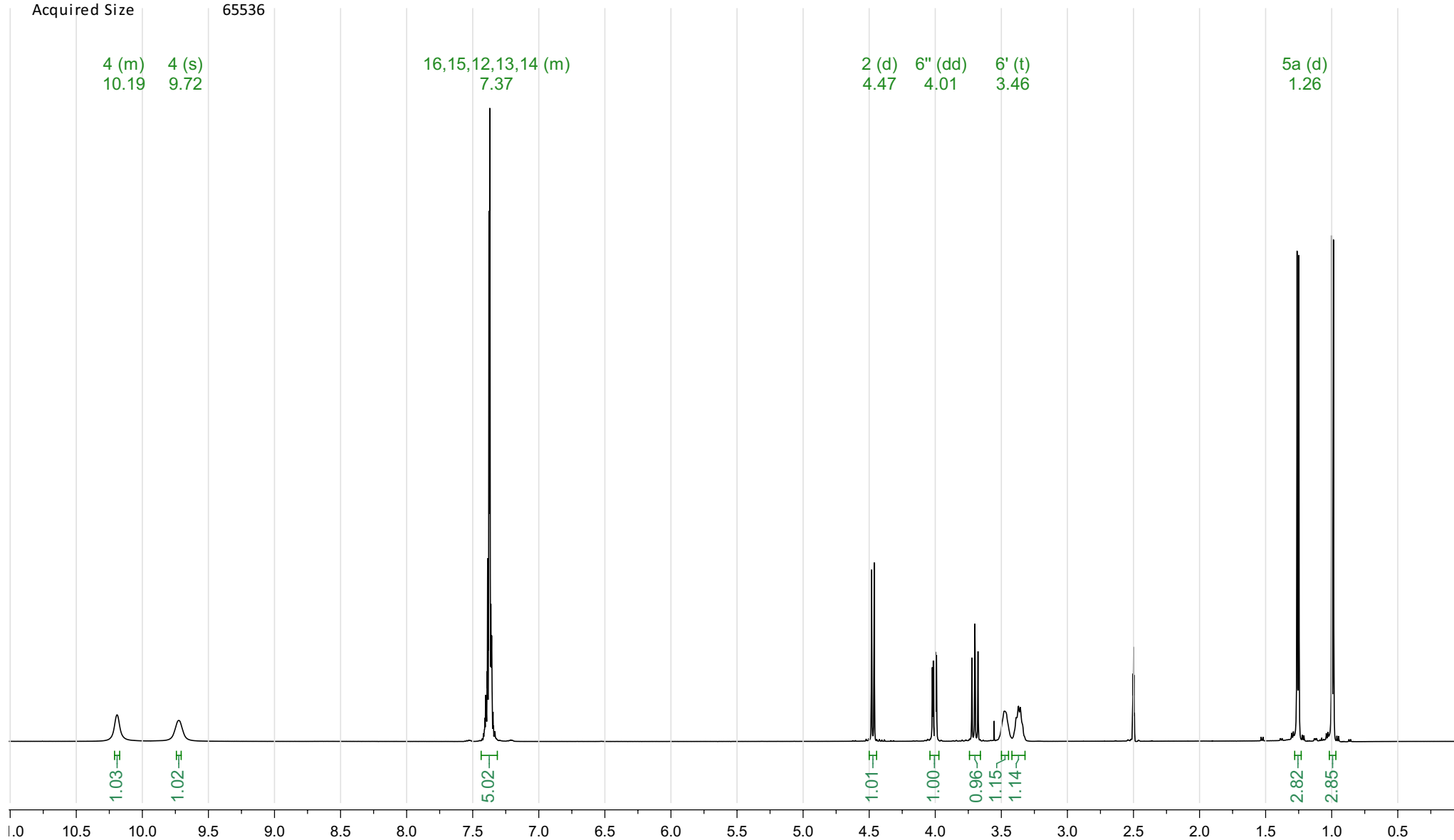
<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 10.21 – 10.17 (m, 1H), 9.72 (s, 1H), 7.44 – 7.31 (m, 5H), 4.47 (d, *J* = 9.9 Hz, 1H), 4.01 (dd, *J* = 12.2, 3.6 Hz, 1H), 3.70 (dd, *J* = 12.3, 11.0 Hz, 1H), 3.46 (t, *J* = 8.5 Hz, 1H), 3.42 – 3.32 (m, 1H), 1.26 (d, *J* = 6.6 Hz, 3H), 0.99 (d, *J* = 6.7 Hz, 3H).



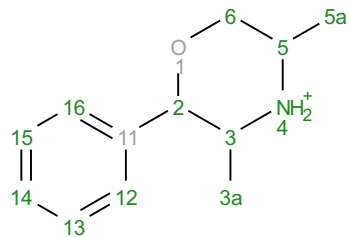
Analyte X46 PDM-35 H+  
Acquisition Date 2017-06-08T11:55:14  
Solvent dms0  
Temperature 25  
Number of Scans 16  
Relaxation Delay 5  
Spectrometer Frequency 499.67  
Spectral Width 10000.0  
Nucleus 1H  
Acquired Size 65536



<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 10.21 – 10.17 (m, 1H), 9.72 (s, 1H), 7.44 – 7.31 (m, 5H), 4.47 (d, *J* = 9.9 Hz, 1H), 4.01 (dd, *J* = 12.2, 3.6 Hz, 1H), 3.70 (dd, *J* = 12.3, 11.0 Hz, 1H), 3.46 (t, *J* = 8.5 Hz, 1H), 3.42 – 3.32 (m, 1H), 1.26 (d, *J* = 6.6 Hz, 3H), 0.99 (d, *J* = 6.7 Hz, 3H).



Prediction PDM-35 H+  
Origin Modgraph NMRPredict Desktop  
Solvent DMSO-d6  
Algorithm Best  
GMMX Cycles 10  
Version 20560  
Frequency 500.00  
Nucleus 1H



<sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 7.48 – 7.36 (m, 5H), 7.20 (t, *J* = 7.6 Hz, 2H), 5.10 (dt, *J* = 4.0, 1.5 Hz, 1H), 4.31 – 4.21 (m, 1H), 4.21 – 4.13 (m, 1H), 3.96 – 3.82 (m, 2H), 1.30 – 1.24 (m, 6H).

