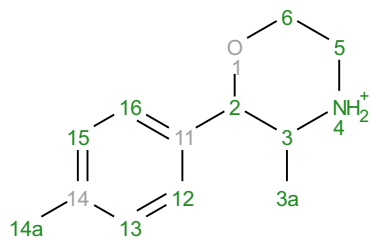
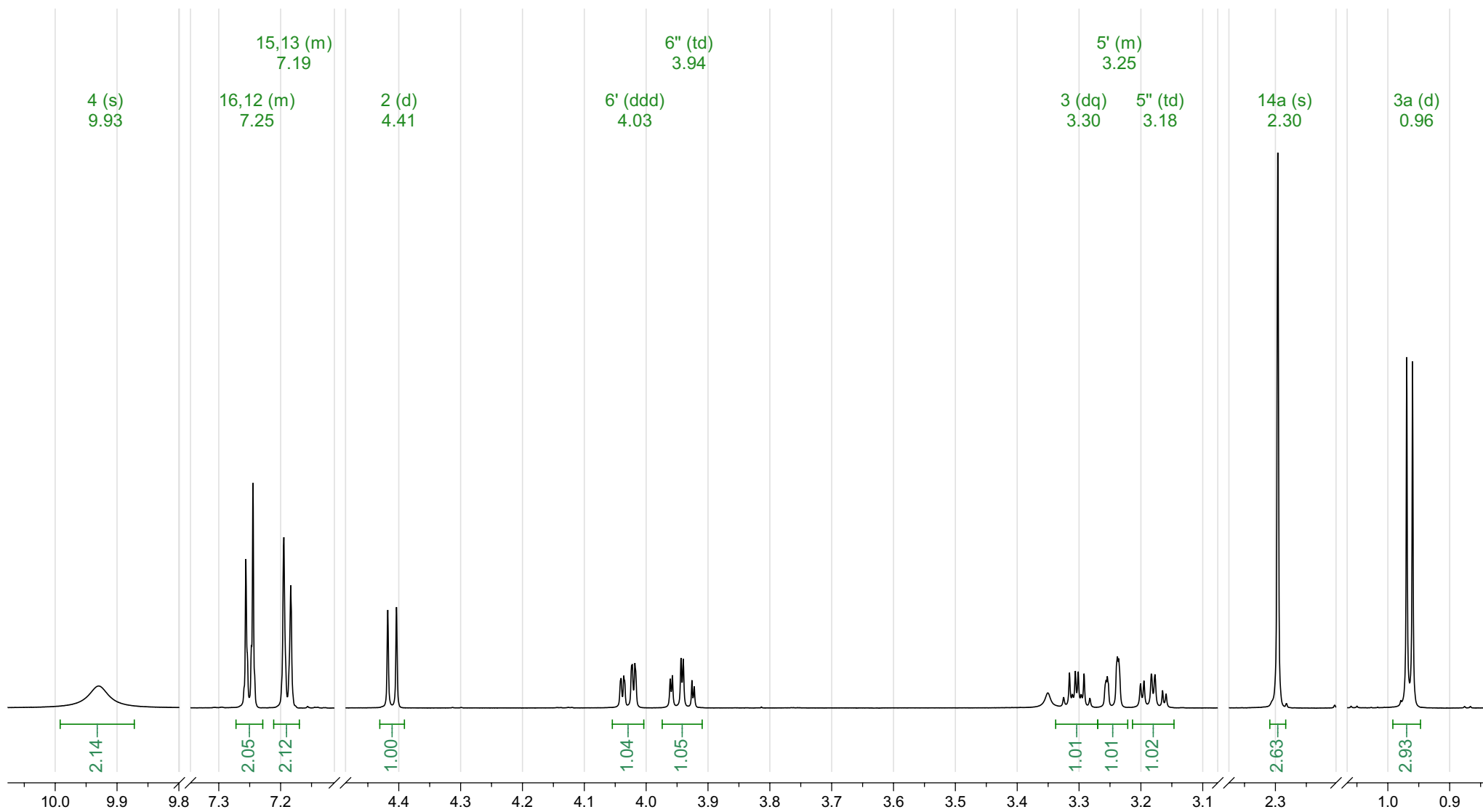


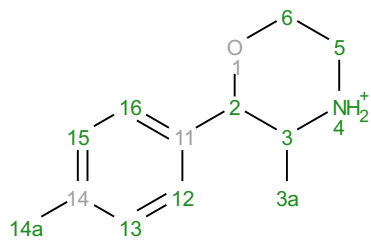
Analyte X58: 4-Me-PM H+
 Acquisition Date 2018-07-16T12:58:38
 Solvent dms0
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Experiment 1D
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 55804



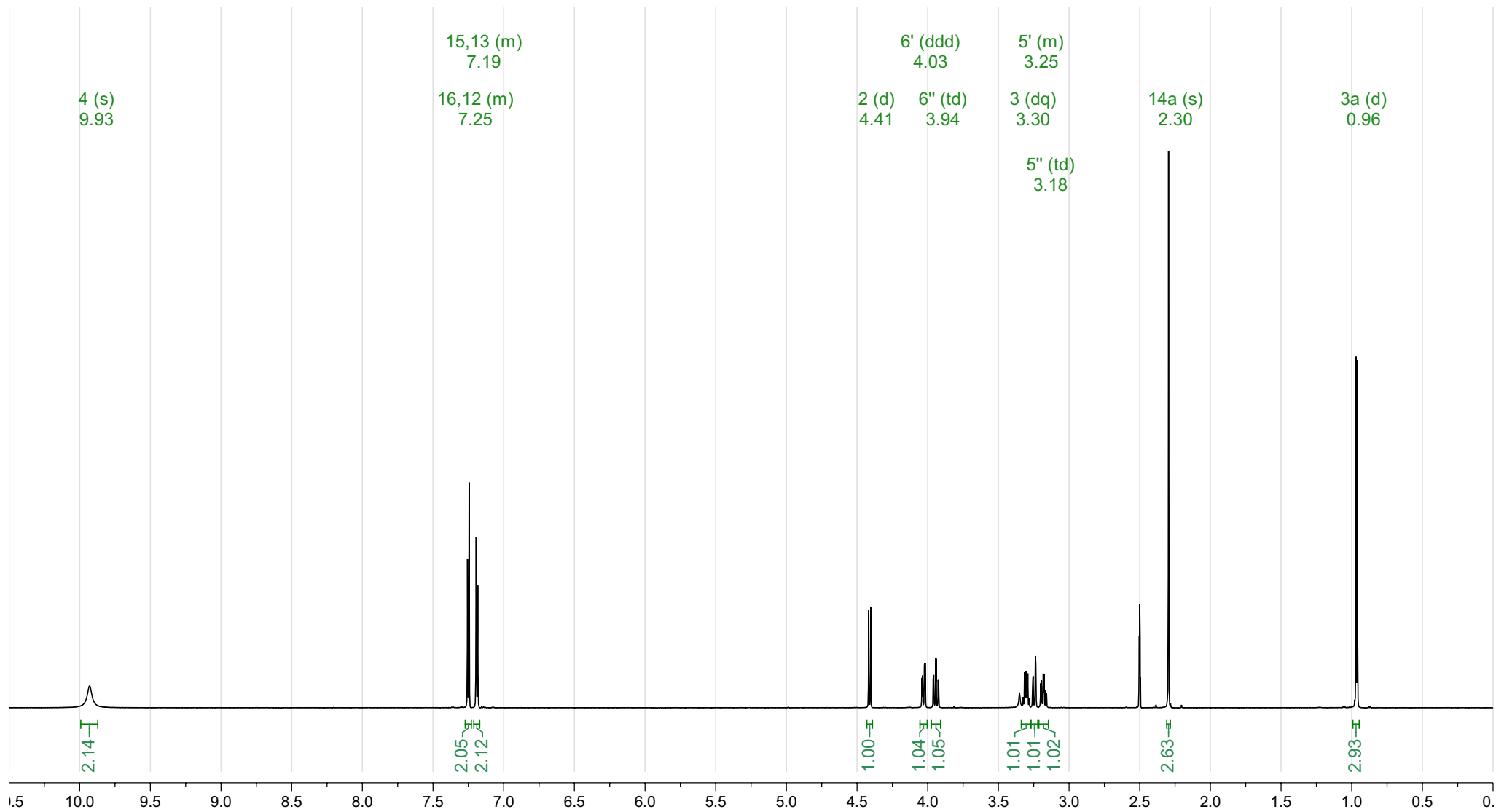
¹H NMR (700 MHz, DMSO-*d*₆) δ 9.93 (s, 2H), 7.27 – 7.23 (m, 2H), 7.21 – 7.17 (m, 2H), 4.41 (d, *J* = 9.9 Hz, 1H), 4.03 (ddd, *J* = 12.5, 3.9, 1.1 Hz, 1H), 3.94 (td, *J* = 12.3, 2.6 Hz, 1H), 3.30 (dq, *J* = 9.9, 6.6 Hz, 1H), 3.27 – 3.22 (m, 1H), 3.18 (td, *J* = 12.5, 4.0 Hz, 1H), 2.30 (s, 3H), 0.96 (d, *J* = 6.6 Hz, 3H).



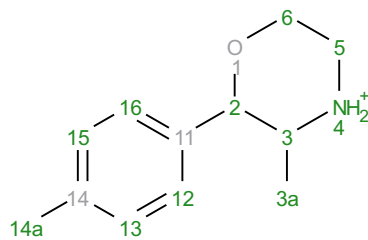
Analyte X58: 4-Me-PM H+
 Acquisition Date 2018-07-16T12:58:38
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Experiment 1D
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
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¹H NMR (700 MHz, DMSO-*d*₆) δ 9.93 (s, 2H), 7.27 – 7.23 (m, 2H), 7.21 – 7.17 (m, 2H), 4.41 (d, *J* = 9.9 Hz, 1H), 4.03 (ddd, *J* = 12.5, 3.9, 1.1 Hz, 1H), 3.94 (td, *J* = 12.3, 2.6 Hz, 1H), 3.30 (dq, *J* = 9.9, 6.6 Hz, 1H), 3.27 – 3.22 (m, 1H), 3.18 (td, *J* = 12.5, 4.0 Hz, 1H), 2.30 (s, 3H), 0.96 (d, *J* = 6.6 Hz, 3H).



Prediction 4-Me-PM H+
Origin Mnova Best
Solvent DMSO-d6
Version 1.0.0
Frequency 700.00
Nucleus 1H



^1H NMR (700 MHz, DMSO- d_6) δ 7.22 (d, $J = 7.3$ Hz, 2H), 7.20 – 7.16 (m, 2H), 6.38 (dt, $J = 6.9, 5.8$ Hz, 2H), 4.97 – 4.93 (m, 1H), 4.14 – 4.07 (m, 1H), 4.06 (td, $J = 7.0, 1.7$ Hz, 2H), 3.16 (tt, $J = 7.2, 5.7$ Hz, 2H), 2.34 (q, $J = 0.9$ Hz, 3H), 1.19 (dd, $J = 6.6, 1.5$ Hz, 3H).

