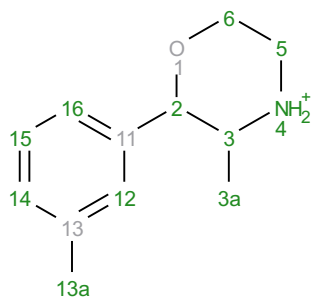
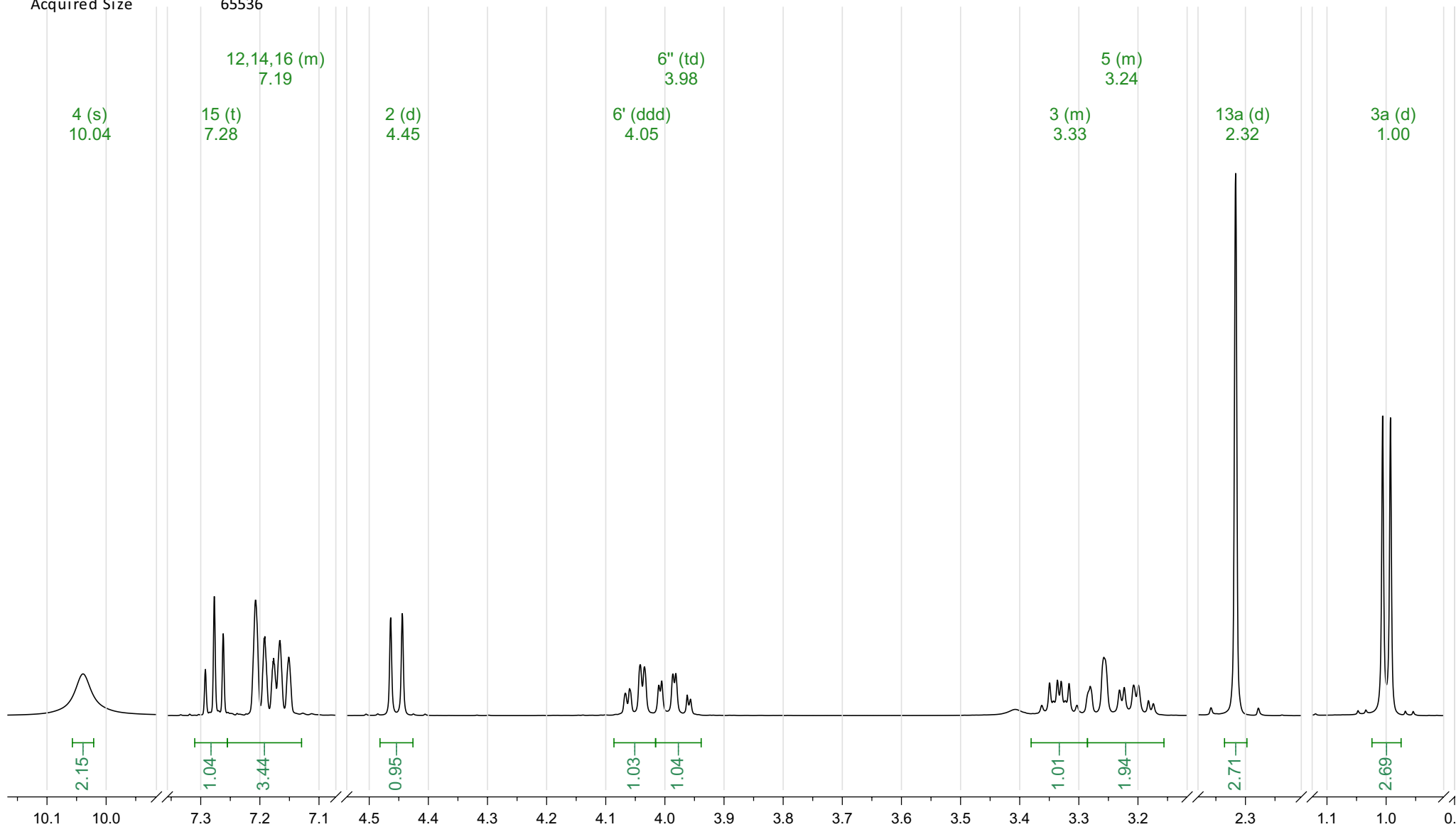


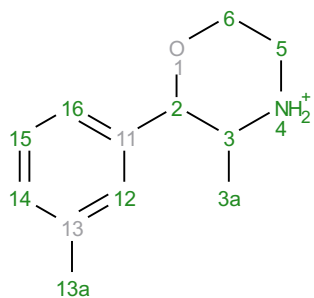
Analyte X49 3-Me-PM H⁺
 Acquisition Date 2017-06-08T12:24:04
 Solvent dms0
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



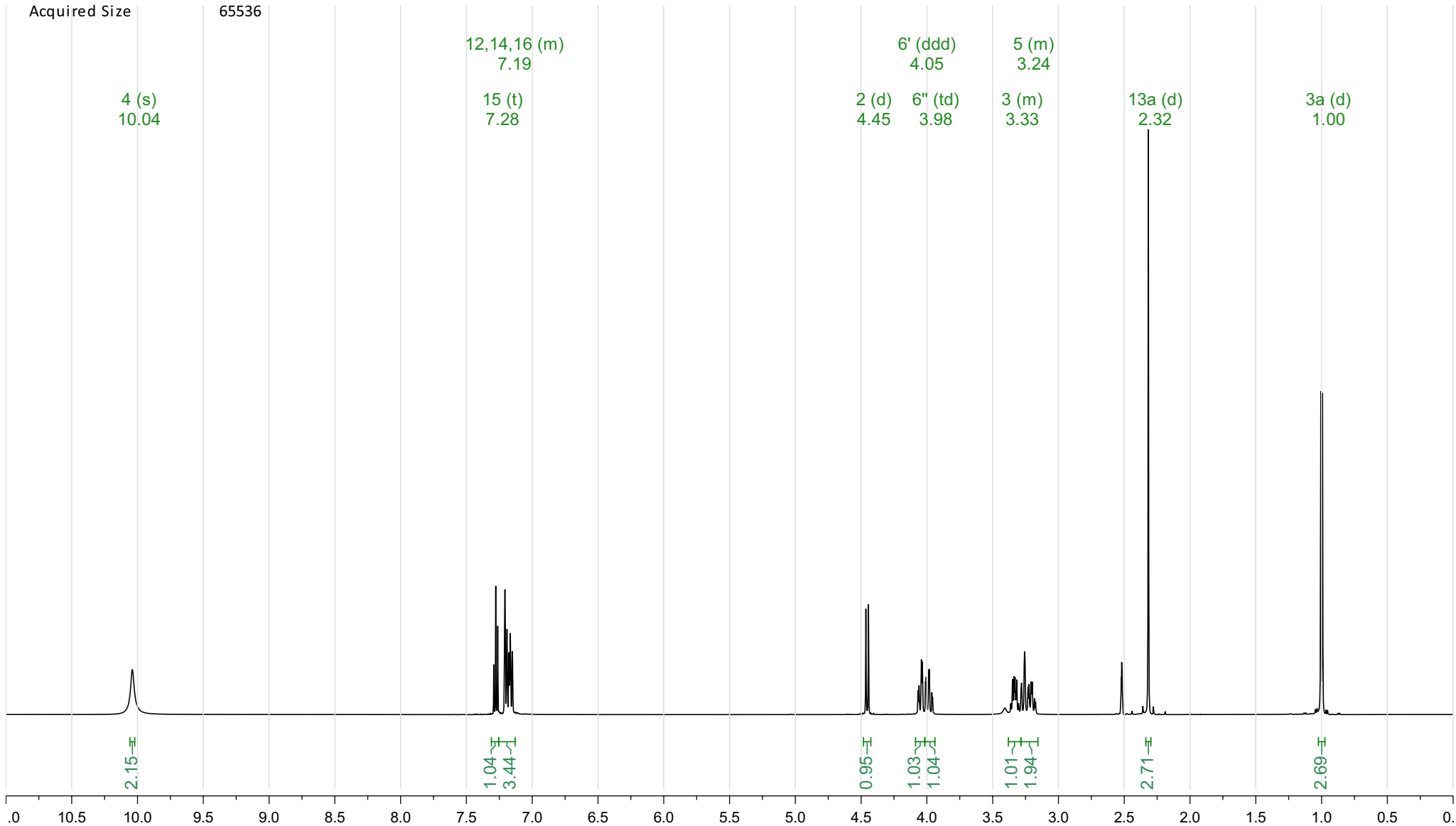
¹H NMR (500 MHz, DMSO-*d*₆) δ 10.04 (s, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.26 – 7.13 (m, 3H), 4.45 (d, *J* = 9.8 Hz, 1H), 4.05 (ddd, *J* = 12.5, 4.0, 1.1 Hz, 1H), 3.98 (td, *J* = 12.1, 2.7 Hz, 1H), 3.38 – 3.29 (m, 1H), 3.29 – 3.16 (m, 2H), 2.32 (d, *J* = 0.9 Hz, 3H), 1.00 (d, *J* = 6.6 Hz, 3H).



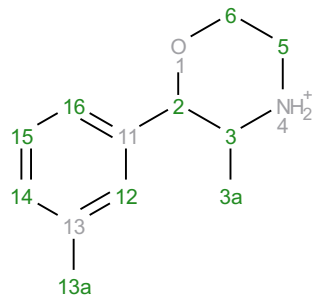
Analyte X49 3-Me-PM H+
 Acquisition Date 2017-06-08T12:24:04
 Solvent dms0
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



¹H NMR (500 MHz, DMSO-*d*₆) δ 10.04 (s, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.26 – 7.13 (m, 3H), 4.45 (d, *J* = 9.8 Hz, 1H), 4.05 (ddd, *J* = 12.5, 4.0, 1.1 Hz, 1H), 3.98 (td, *J* = 12.1, 2.7 Hz, 1H), 3.38 – 3.29 (m, 1H), 3.29 – 3.16 (m, 2H), 2.32 (d, *J* = 0.9 Hz, 3H), 1.00 (d, *J* = 6.6 Hz, 3H).



Prediction 3-Me-PM H+
Origin Modgraph NMRPredict Desktop
Solvent DMSO-d6
Algorithm Best
GMMX Cycles 10
Version 20560
Frequency 500.00
Nucleus 1H



^1H NMR (500 MHz, DMSO- d_6) δ 7.38 – 7.30 (m, 2H), 7.20 (dt, $J = 7.1, 5.7$ Hz, 3H), 7.07 (dqdd, $J = 5.0, 3.9, 2.0, 1.0$ Hz, 1H), 5.13 – 5.07 (m, 1H), 5.03 (ddd, $J = 12.4, 5.8, 3.2$ Hz, 1H), 4.93 (ddd, $J = 12.4, 5.8, 3.3$ Hz, 1H), 4.26 (ddtd, $J = 13.5, 7.3, 6.2, 3.3$ Hz, 1H), 3.60 – 3.50 (m, 1H), 3.45 (dq, $J = 12.4, 5.8, 3.2$ Hz, 1H), 2.33 (t, $J = 1.0$ Hz, 3H), 1.27 (dd, $J = 6.4, 1.5$ Hz, 3H).

