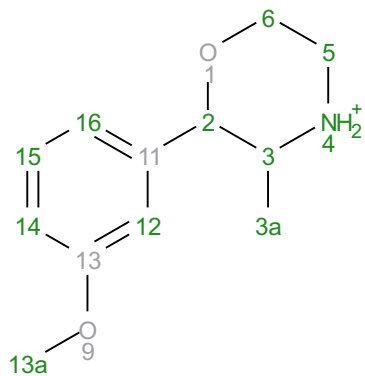
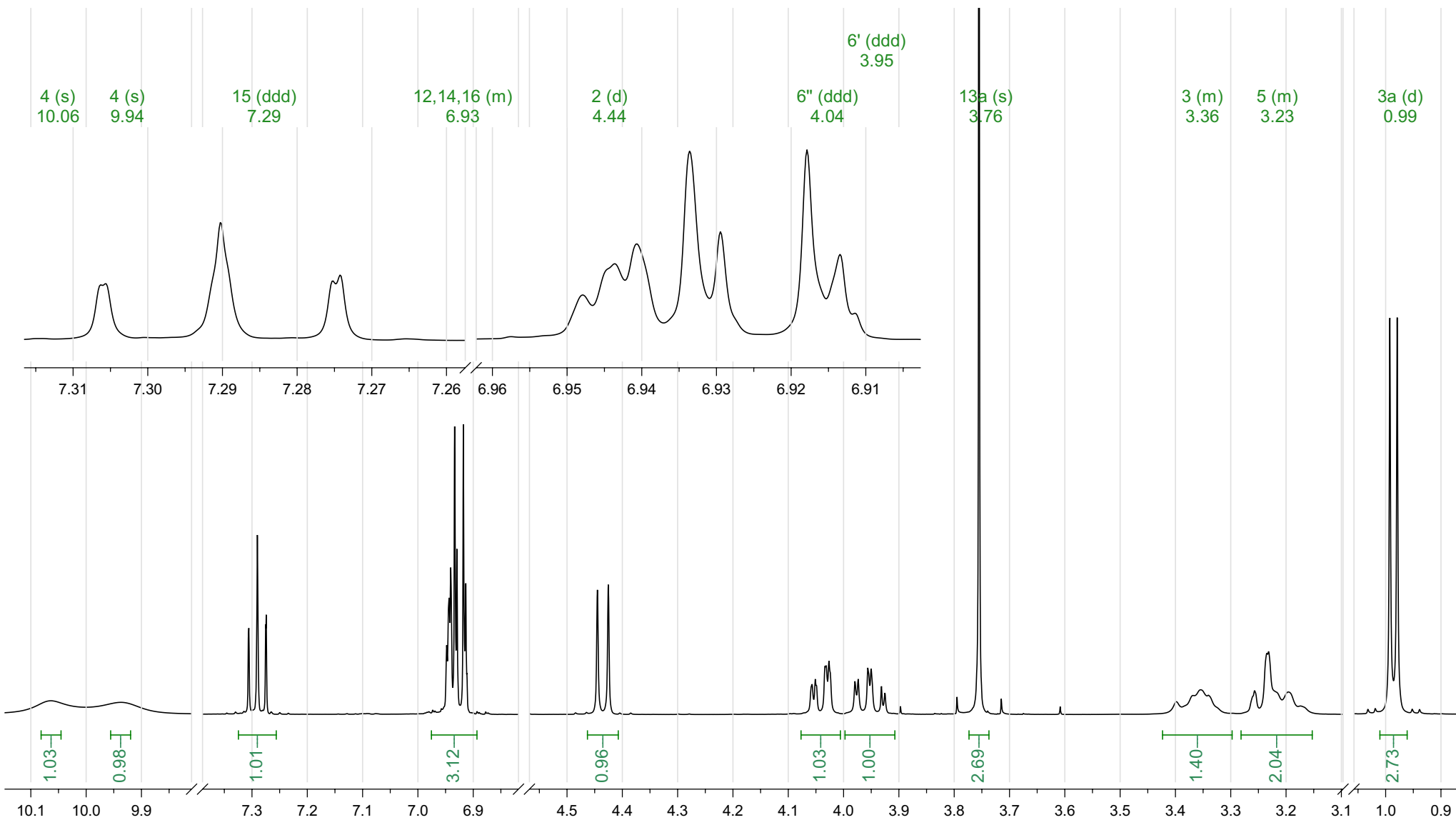


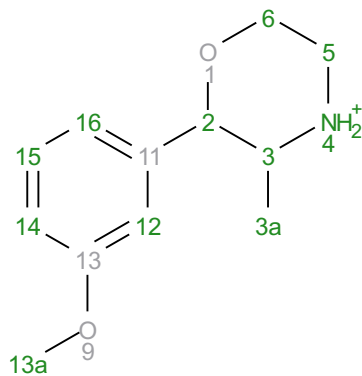
Analyte X48 3-MeO-PM H⁺
 Acquisition Date 2017-06-08T12:14:31
 Solvent dmsO
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



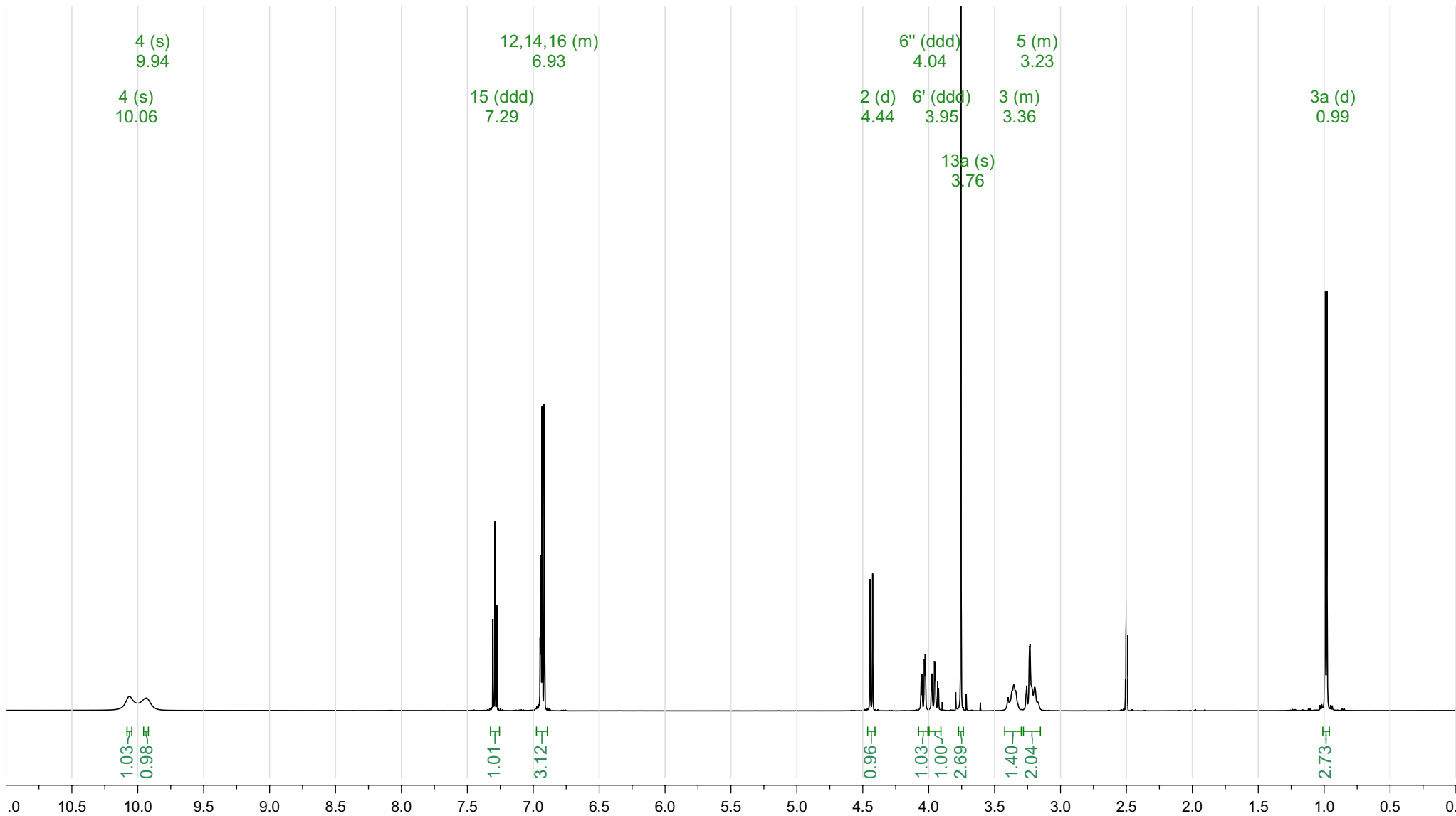
¹H NMR (500 MHz, DMSO-*d*₆) δ 10.06 (s, 1H), 9.94 (s, 1H), 7.29 (ddd, *J* = 8.1, 7.5, 0.6 Hz, 1H), 6.98 – 6.89 (m, 3H), 4.44 (d, *J* = 9.8 Hz, 1H), 4.04 (ddd, *J* = 12.5, 3.8, 1.2 Hz, 1H), 3.95 (ddd, *J* = 12.5, 11.4, 3.0 Hz, 1H), 3.76 (s, 3H), 3.42 – 3.30 (m, 1H), 3.28 – 3.15 (m, 2H), 0.99 (d, *J* = 6.6 Hz, 3H).



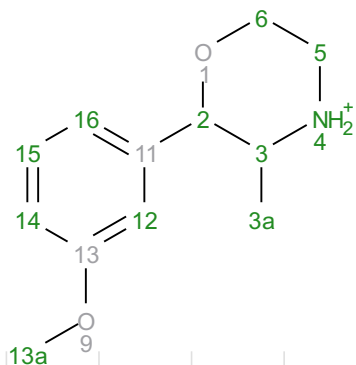
Analyte X48 3-MeO-PM H⁺
 Acquisition Date 2017-06-08T12:14:31
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



¹H NMR (500 MHz, DMSO-*d*₆) δ 10.06 (s, 1H), 9.94 (s, 1H), 7.29 (ddd, *J* = 8.1, 7.5, 0.6 Hz, 1H), 6.98 – 6.89 (m, 3H), 4.44 (d, *J* = 9.8 Hz, 1H), 4.04 (ddd, *J* = 12.5, 3.8, 1.2 Hz, 1H), 3.95 (ddd, *J* = 12.5, 11.4, 3.0 Hz, 1H), 3.76 (s, 3H), 3.42 – 3.30 (m, 1H), 3.28 – 3.15 (m, 2H), 0.99 (d, *J* = 6.6 Hz, 3H).



Prediction 3-MeO-PM H+
 Origin Modgraph NMRPredict Desktop
 Solvent DMSO-d6
 Algorithm Best
 GMMX Cycles 5
 Version 20560
 Frequency 500.00
 Nucleus 1H



¹H NMR (500 MHz, DMSO-*d*₆) δ 7.32 (t, *J* = 7.9 Hz, 1H), 7.20 (dt, *J* = 7.1, 5.7 Hz, 2H), 7.15 – 7.09 (m, 1H), 7.01 (dt, *J* = 2.0, 0.8 Hz, 1H), 6.82 (dt, *J* = 7.7, 1.1 Hz, 1H), 5.10 (dq, *J* = 3.8, 1.4 Hz, 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* = 13.4, 7.2, 6.2, 3.3 Hz, 1H), 3.81 (s, 3H), 3.55 (dq, *J* = 12.4, 5.6, 3.1 Hz, 1H), 3.50 – 3.40 (m, 1H), 1.27 (dd, *J* = 6.4, 1.5 Hz, 3H).

