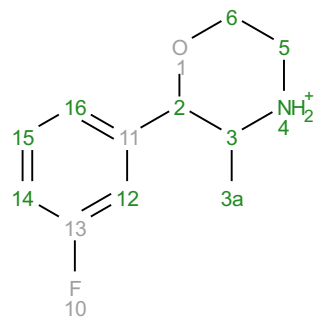
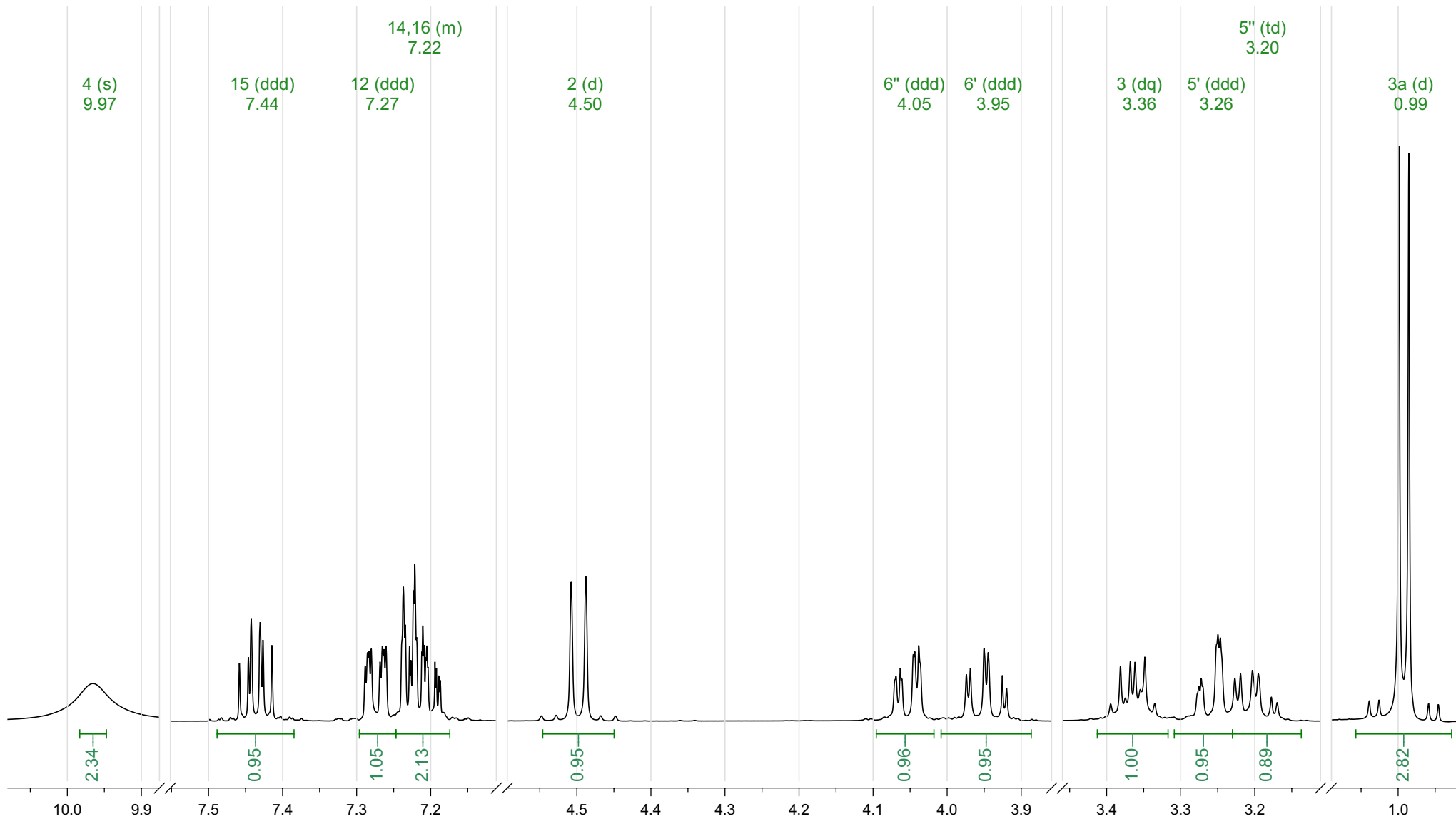


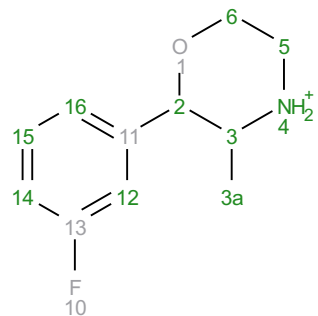
Analyte X27: 3-FPM H+
 Acquisition Date 2016-10-13T16:57:03
 Solvent dms0
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



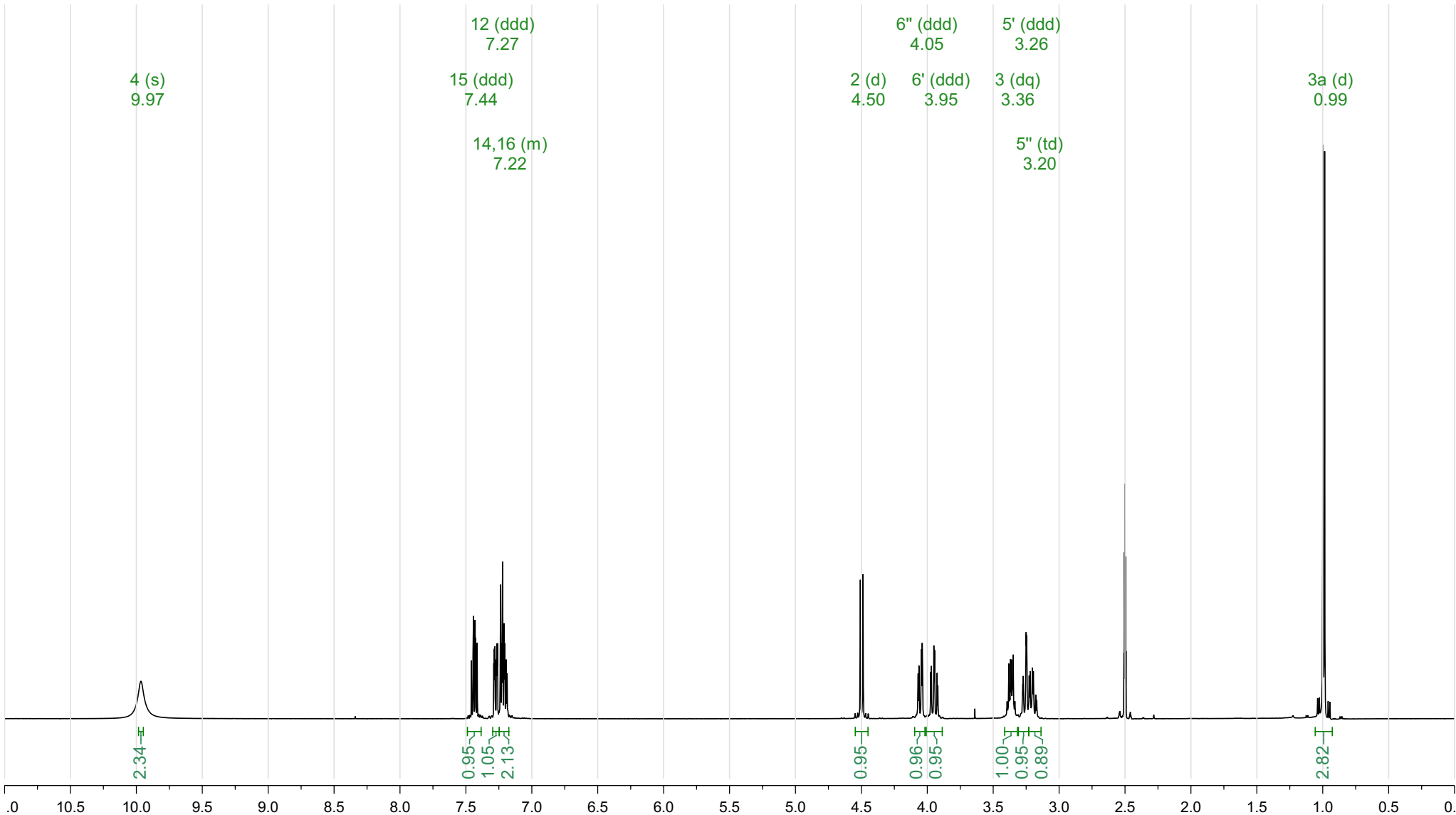
¹H NMR (500 MHz, DMSO-*d*₆) δ 9.97 (s, 2H), 7.44 (ddd, *J* = 8.4, 7.7, 6.0 Hz, 1H), 7.27 (ddd, *J* = 10.0, 2.7, 1.5 Hz, 1H), 7.25 – 7.17 (m, 2H), 4.50 (d, *J* = 9.8 Hz, 1H), 4.05 (ddd, *J* = 12.5, 3.9, 1.2 Hz, 1H), 3.95 (ddd, *J* = 12.6, 11.8, 2.8 Hz, 1H), 3.36 (dq, *J* = 9.8, 6.6 Hz, 1H), 3.26 (ddd, *J* = 12.8, 2.8, 1.2 Hz, 1H), 3.20 (td, *J* = 12.2, 3.9 Hz, 1H), 0.99 (d, *J* = 6.6 Hz, 3H).



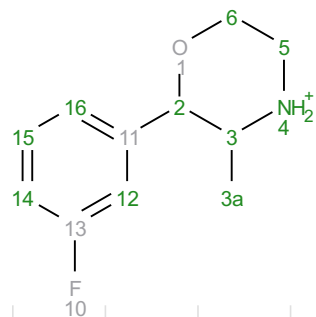
Analyte X27: 3-FPM H+
 Acquisition Date 2016-10-13T16:57:03
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



¹H NMR (500 MHz, DMSO-*d*₆) δ 9.97 (s, 2H), 7.44 (ddd, *J* = 8.4, 7.7, 6.0 Hz, 1H), 7.27 (ddd, *J* = 10.0, 2.7, 1.5 Hz, 1H), 7.25 – 7.17 (m, 2H), 4.50 (d, *J* = 9.8 Hz, 1H), 4.05 (ddd, *J* = 12.5, 3.9, 1.2 Hz, 1H), 3.95 (ddd, *J* = 12.6, 11.8, 2.8 Hz, 1H), 3.36 (dq, *J* = 9.8, 6.6 Hz, 1H), 3.26 (ddd, *J* = 12.8, 2.8, 1.2 Hz, 1H), 3.20 (td, *J* = 12.2, 3.9 Hz, 1H), 0.99 (d, *J* = 6.6 Hz, 3H).



Prediction 3-FPM 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-d₆) δ 7.47 (td, *J* = 7.9, 5.0 Hz, 1H), 7.26 (dt, *J* = 7.9, 2.0 Hz, 1H), 7.24 – 7.16 (m, 4H), 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), 1.27 (dd, *J* = 6.4, 1.5 Hz, 3H).

