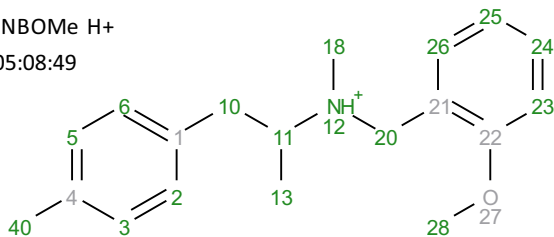
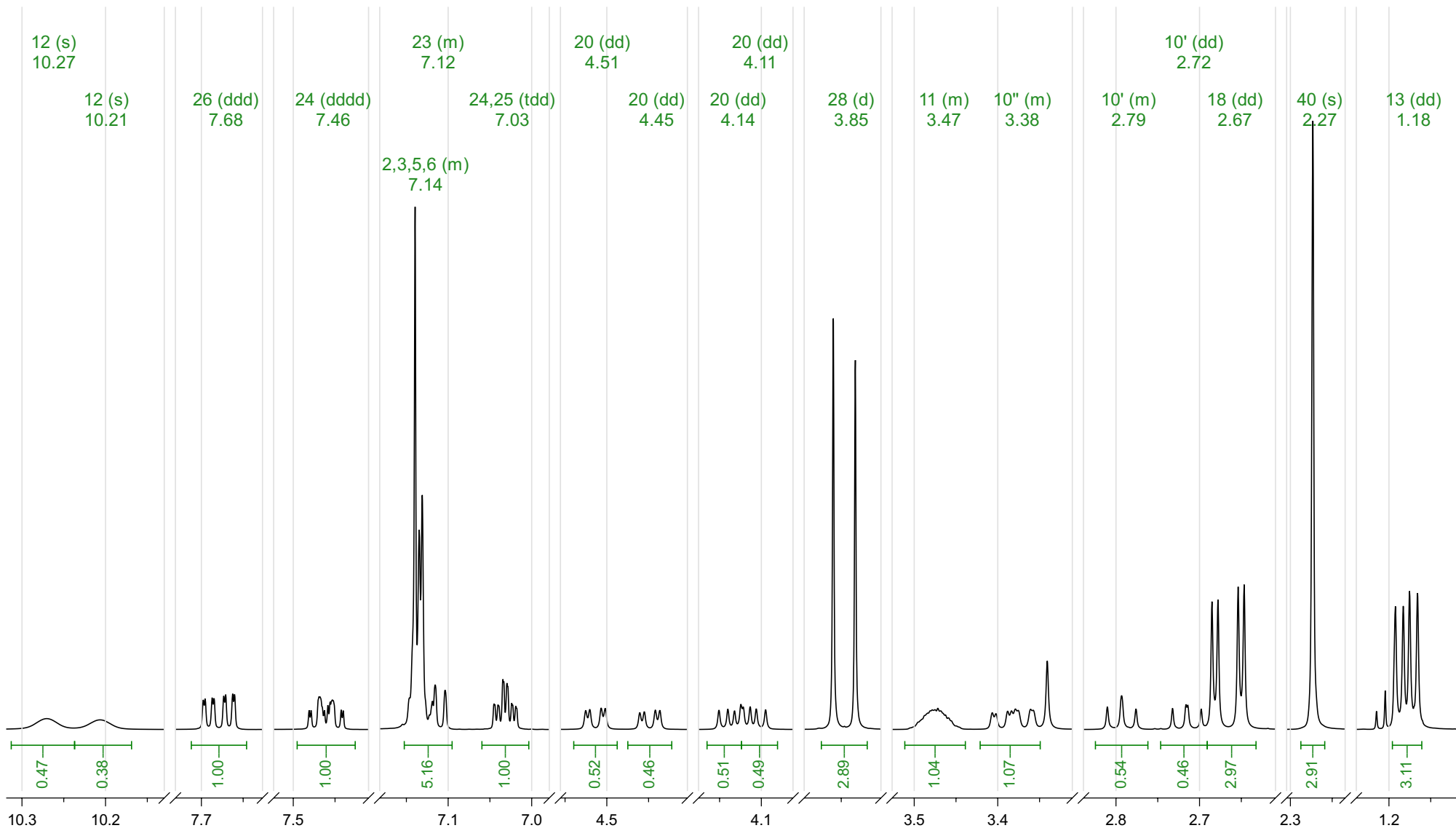


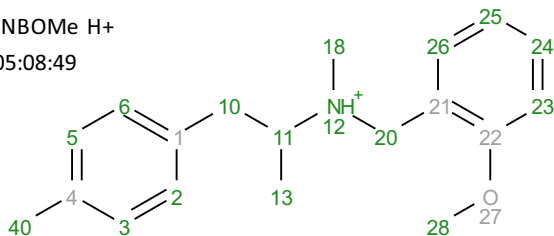
Analyte B11: 4-MMA-NBOMe H+
 Acquisition Date 2014-08-19T05:08:49
 Solvent dms0
 Temperature 27
 Number of Scans 64
 Relaxation Delay 5
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 50223



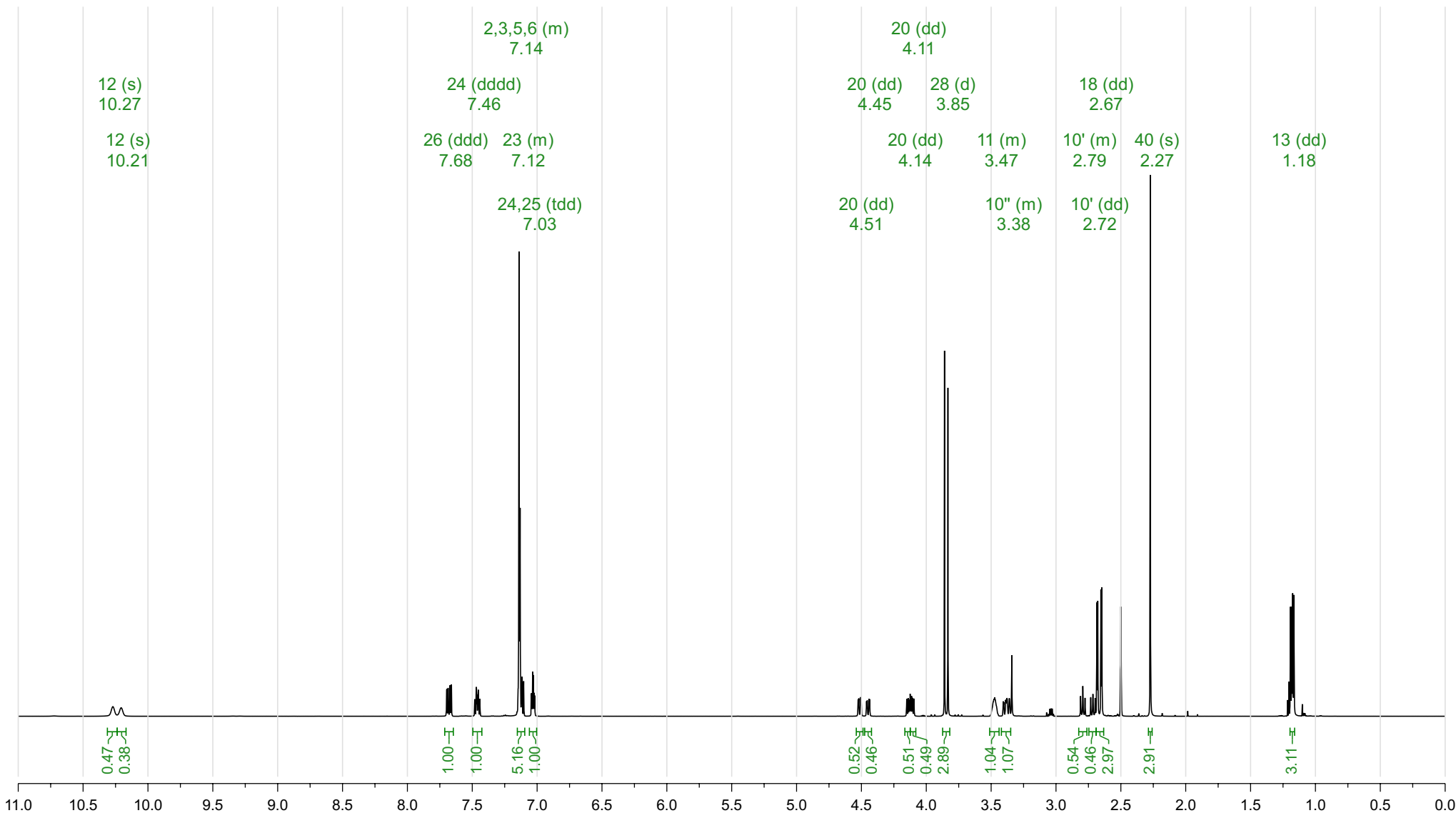
¹H NMR (700 MHz, DMSO-*d*₆) δ 10.27 (s, OH), 10.21 (s, OH), 7.68 (ddd, *J* = 17.2, 7.4, 1.7 Hz, 1H), 7.46 (dddd, *J* = 11.1, 8.2, 7.4, 1.7 Hz, 1H), 7.14 – 7.13 (m, 4H), 7.16 – 7.09 (m, 1H), 7.03 (tdd, *J* = 7.5, 3.3, 1.0 Hz, 1H), 4.51 (dd, *J* = 13.0, 3.4 Hz, 1H), 4.45 (dd, *J* = 13.0, 3.8 Hz, OH), 4.14 (dd, *J* = 13.0, 7.5 Hz, OH), 4.11 (dd, *J* = 12.9, 7.8 Hz, 1H), 3.85 (d, *J* = 18.4 Hz, 3H), 3.52 – 3.43 (m, 1H), 3.42 – 3.33 (m, 1H), 2.82 – 2.76 (m, 1H), 2.72 (dd, *J* = 12.9, 11.1 Hz, OH), 2.67 (dd, *J* = 21.9, 5.0 Hz, 3H), 2.27 (s, 3H), 1.18 (dd, *J* = 11.9, 6.6 Hz, 3H).



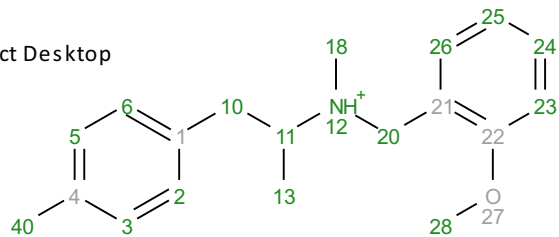
Analyte B11: 4-MMA-NBOMe H⁺
 Acquisition Date 2014-08-19T05:08:49
 Solvent dms0
 Temperature 27
 Number of Scans 64
 Relaxation Delay 5
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 50223



¹H NMR (700 MHz, DMSO-*d*₆) δ 10.27 (s, OH), 10.21 (s, OH), 7.68 (ddd, *J* = 17.2, 7.4, 1.7 Hz, 1H), 7.46 (dddd, *J* = 11.1, 8.2, 7.4, 1.7 Hz, 1H), 7.14 – 7.13 (m, 4H), 7.16 – 7.09 (m, 1H), 7.03 (tdd, *J* = 7.5, 3.3, 1.0 Hz, 1H), 4.51 (dd, *J* = 13.0, 3.4 Hz, 1H), 4.45 (dd, *J* = 13.0, 3.8 Hz, 0H), 4.14 (dd, *J* = 13.0, 7.5 Hz, 0H), 4.11 (dd, *J* = 12.9, 7.8 Hz, 1H), 3.85 (d, *J* = 18.4 Hz, 3H), 3.52 – 3.43 (m, 1H), 3.42 – 3.33 (m, 1H), 2.82 – 2.76 (m, 1H), 2.72 (dd, *J* = 12.9, 11.1 Hz, 0H), 2.67 (dd, *J* = 21.9, 5.0 Hz, 3H), 2.27 (s, 3H), 1.18 (dd, *J* = 11.9, 6.6 Hz, 3H).



Prediction 4-MMA-NBOMe H+
 Origin Modgraph NMRPredict Desktop
 Solvent DMSO-d6
 Algorithm Best
 GMMX Cycles 50
 Version 12489
 Frequency 700.00
 Nucleus 1H



¹H NMR (700 MHz, DMSO-*d*₆) δ 7.20 (s, 1H), 7.19 – 7.14 (m, 1H), 7.07 (dt, *J* = 7.2, 1.6 Hz, 2H), 7.03 – 6.99 (m, 2H), 6.94 – 6.88 (m, 2H), 6.86 (td, *J* = 7.4, 2.0 Hz, 1H), 4.83 (d, *J* = 1.2 Hz, 2H), 4.06 (h, *J* = 6.2 Hz, 1H), 3.74 (s, 3H), 3.36 – 3.30 (m, 1H), 2.91 – 2.85 (m, 1H), 2.69 (s, 3H), 2.21 (d, *J* = 1.4 Hz, 3H), 1.40 (d, *J* = 6.0 Hz, 3H).

