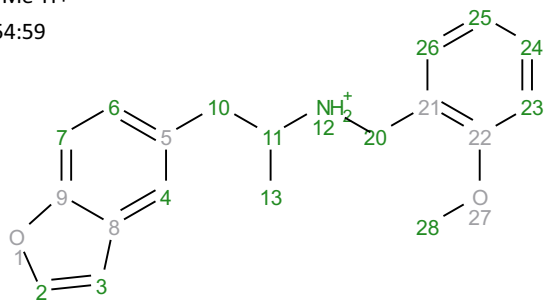
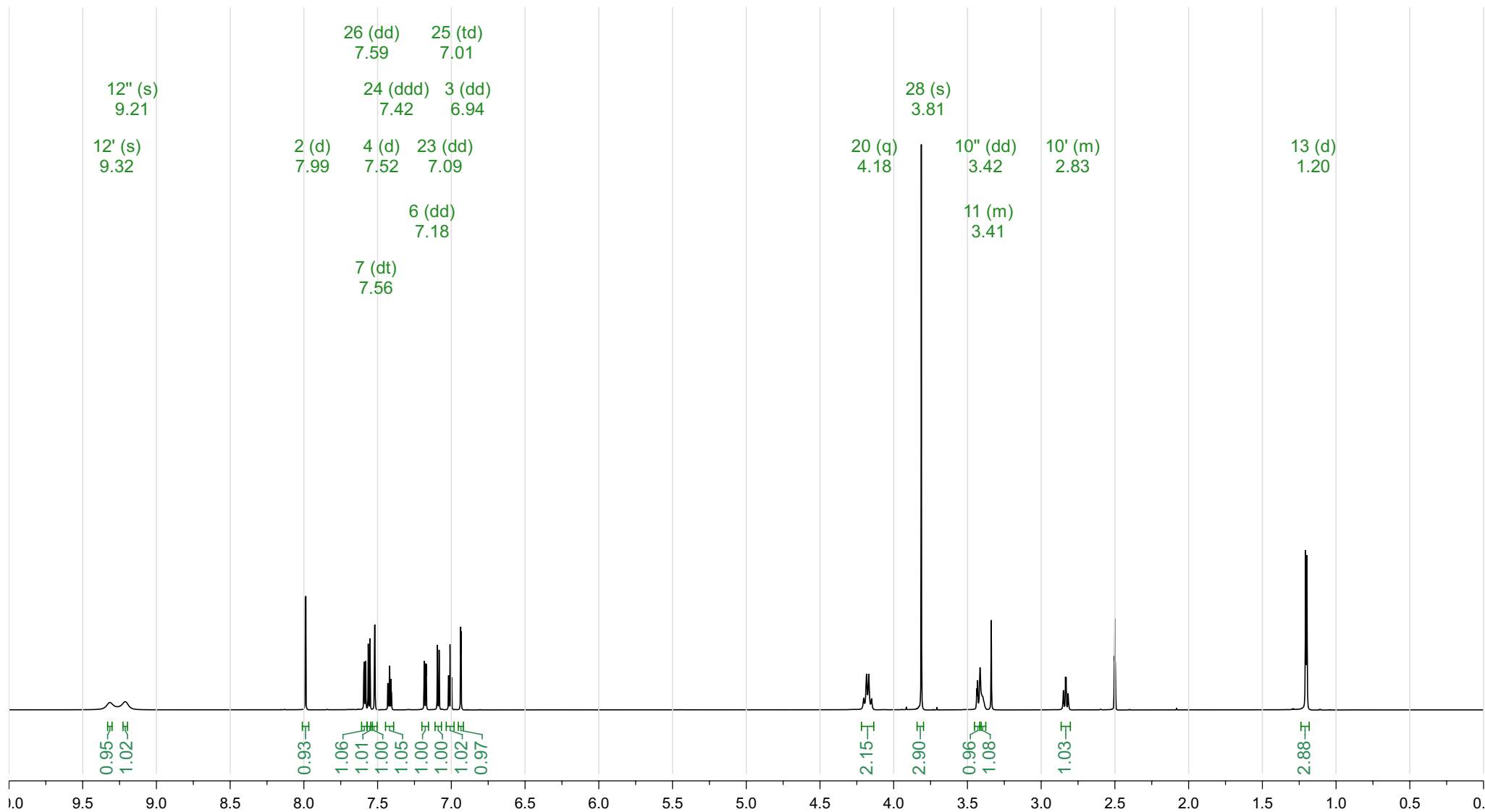


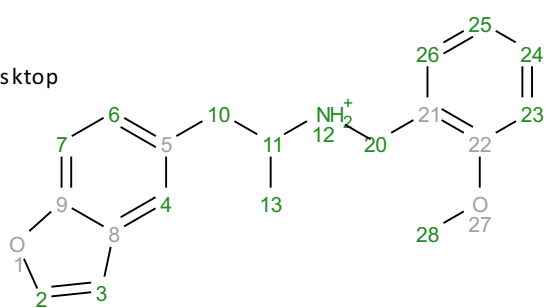
Analyte B12: 5-APB-NBOMe H⁺
 Acquisition Date 2014-08-19T05:54:59
 Solvent dmso
 Temperature 27
 Number of Scans 64
 Relaxation Delay 5
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 50223



¹H NMR (700 MHz, DMSO-*d*₆) δ 9.32 (s, 1H), 9.21 (s, 1H), 7.99 (d, *J* = 2.2 Hz, 1H), 7.59 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.56 (dt, *J* = 8.4, 0.8 Hz, 1H), 7.52 (d, *J* = 1.7 Hz, 1H), 7.42 (ddd, *J* = 8.3, 7.4, 1.7 Hz, 1H), 7.18 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.09 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.01 (td, *J* = 7.4, 1.0 Hz, 1H), 6.94 (dd, *J* = 2.2, 1.0 Hz, 1H), 4.18 (q, *J* = 13.2 Hz, 2H), 3.81 (s, 3H), 3.42 (dd, *J* = 13.3, 4.0 Hz, 1H), 3.42–3.38 (m, 1H), 2.86–2.80 (m, 1H), 1.20 (d, *J* = 6.6 Hz, 3H).



Prediction 5-APB-NBOMe H+
 Origin Modgraph NMRPredict Desktop
 Solvent DMSO-d6
 Algorithm Best
 GMMX Cycles 50
 Version 14011
 Frequency 700.00
 Nucleus 1H



¹H NMR (700 MHz, DMSO-d₆) δ 8.09 (d, *J* = 7.5 Hz, 1H), 7.59 (d, *J* = 7.5 Hz, 1H), 7.41 (t, *J* = 1.5 Hz, 1H), 7.37 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.20 (s, 2H), 7.15 (dq, *J* = 7.9, 1.4 Hz, 1H), 7.05 (dd, *J* = 7.5, 1.5 Hz, 1H), 6.98 (td, *J* = 7.5, 2.1 Hz, 1H), 6.90 (ddq, *J* = 7.7, 3.9, 2.1 Hz, 2H), 4.65 (d, *J* = 0.9 Hz, 1H), 4.53 (d, *J* = 1.2 Hz, 1H), 4.06 (q, *J* = 7.0 Hz, 1H), 3.74 (s, 2H), 3.58 (dd, *J* = 12.4, 7.0 Hz, 1H), 3.13 (dd, *J* = 12.6, 6.9 Hz, 1H), 1.45 (d, *J* = 6.8 Hz, 3H).

