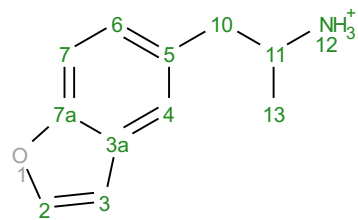
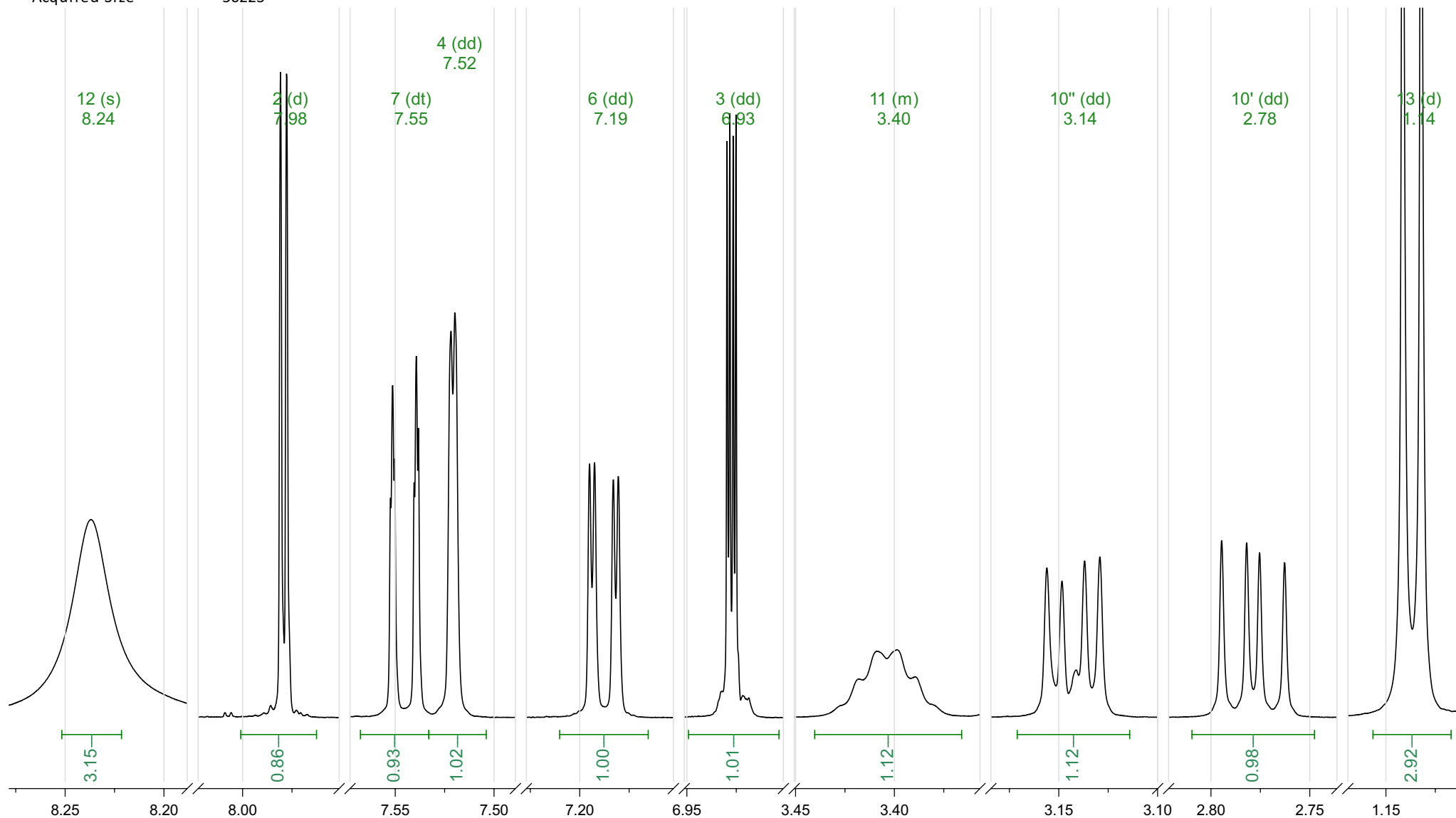


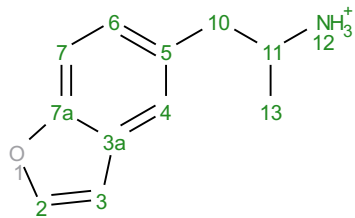
Analyte X51a: 5-APB H⁺
 Acquisition Date 2017-12-08T15:49:21
 Solvent dms0
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 50223



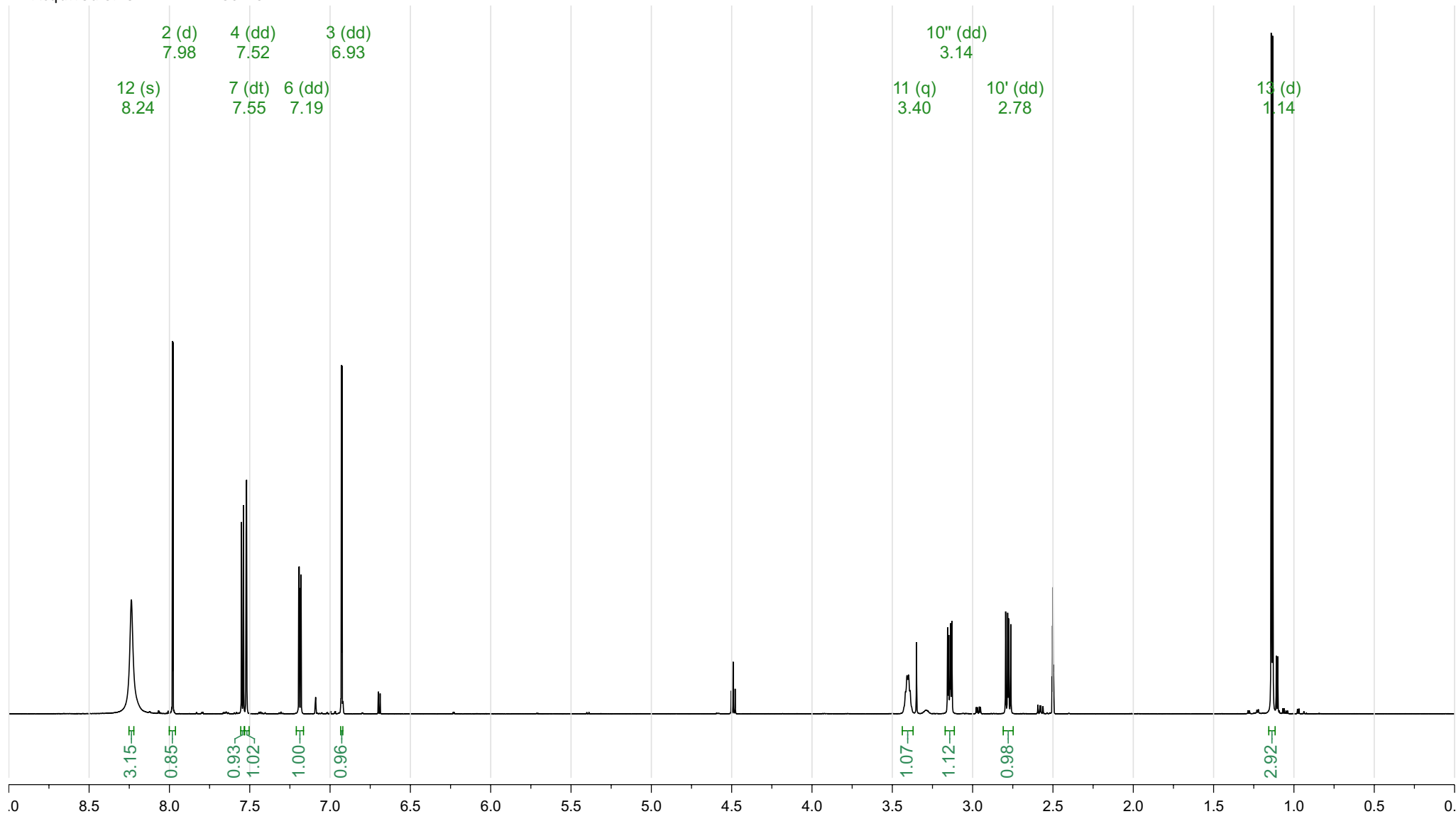
¹H NMR (700 MHz, DMSO-*d*₆) δ 8.24 (s, 3H), 7.98 (d, *J* = 2.2 Hz, 1H), 7.55 (dt, *J* = 8.4, 0.8 Hz, 1H), 7.52 (dd, *J* = 1.8, 0.7 Hz, 1H), 7.19 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.93 (dd, *J* = 2.2, 1.0 Hz, 1H), 3.42 – 3.37 (m, 1H), 3.14 (dd, *J* = 13.4, 5.3 Hz, 1H), 2.78 (dd, *J* = 13.4, 8.8 Hz, 1H), 1.14 (d, *J* = 6.5 Hz, 3H).



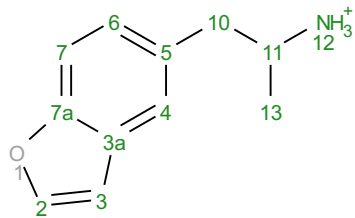
Analyte X51a: 5-APB H⁺
 Acquisition Date 2017-12-08T15:49:21
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 50223



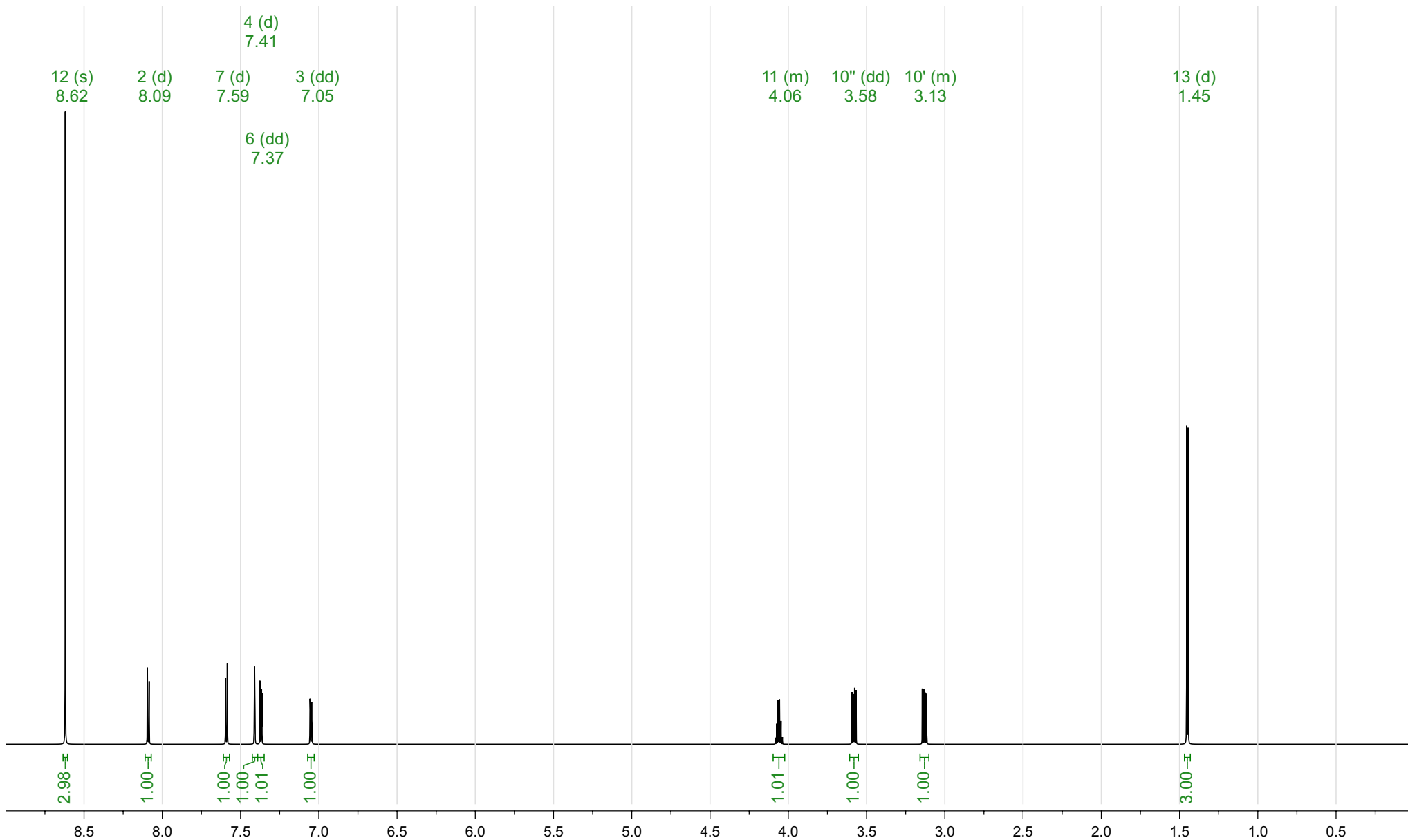
¹H NMR (700 MHz, DMSO-d₆) δ 8.24 (s, 3H), 7.98 (d, *J* = 2.2 Hz, 1H), 7.55 (dt, *J* = 8.4, 0.8 Hz, 1H), 7.52 (dd, *J* = 1.8, 0.7 Hz, 1H), 7.19 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.93 (dd, *J* = 2.2, 1.0 Hz, 1H), 3.42 – 3.37 (m, 1H), 3.14 (dd, *J* = 13.4, 5.3 Hz, 1H), 2.78 (dd, *J* = 13.4, 8.8 Hz, 1H), 1.14 (d, *J* = 6.5 Hz, 3H).



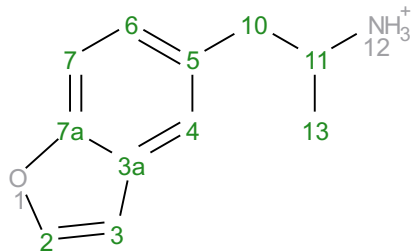
Prediction 5-APB H+
Origin Modgraph NMRPredict Desktop
Solvent DMSO-d6
Algorithm Best
GMMX Cycles 5
Version 15465
Frequency 700.00
Nucleus 1H



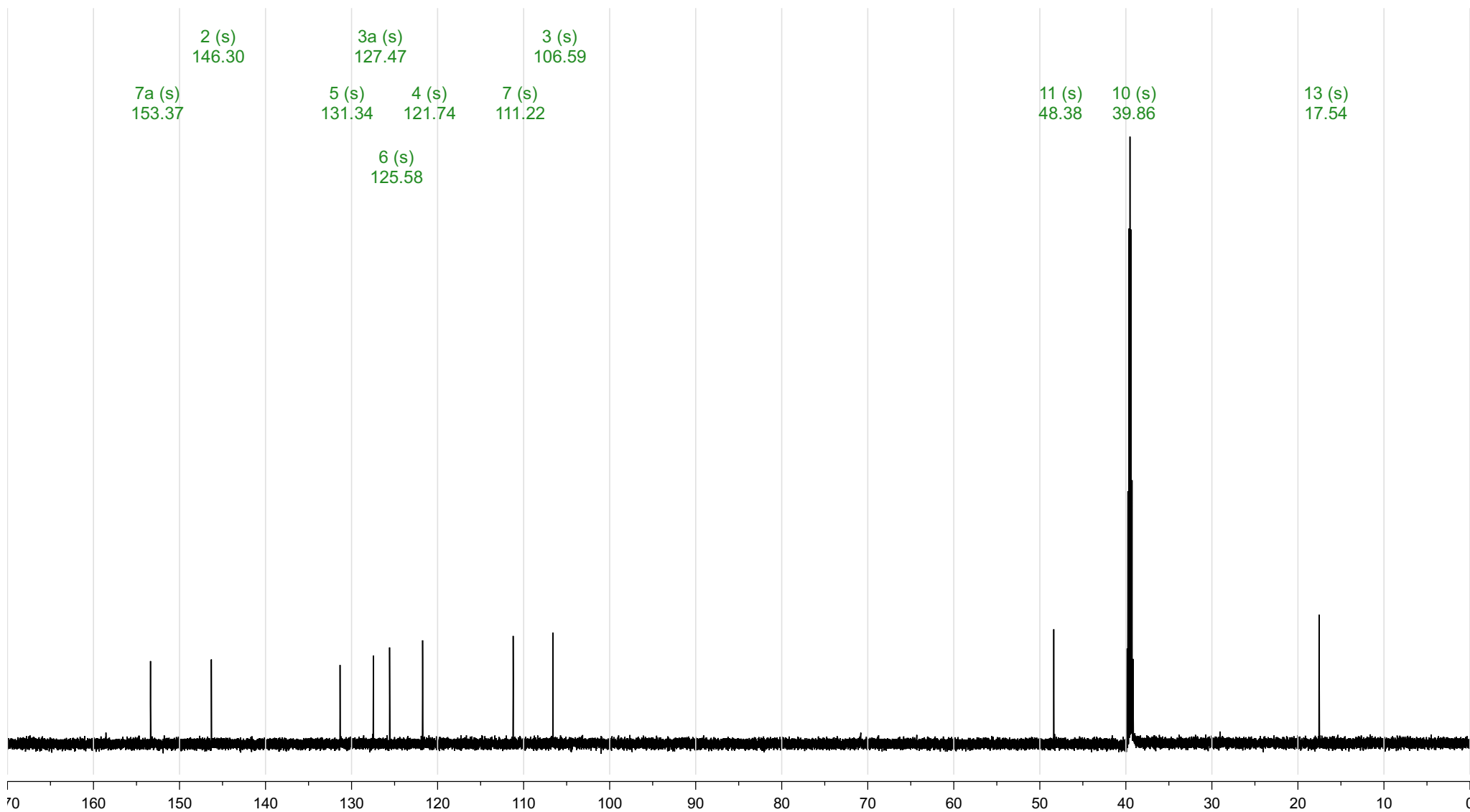
^1H NMR (700 MHz, DMSO- d_6) δ 8.62 (s, 3H), 8.09 (d, $J = 7.3$ Hz, 1H), 7.59 (d, $J = 7.3$ Hz, 1H), 7.41 (d, $J = 1.6$ Hz, 1H), 7.37 (dd, $J = 7.5, 1.4$ Hz, 1H), 7.05 (dd, $J = 7.4, 1.7$ Hz, 1H), 4.09 – 4.02 (m, 1H), 3.58 (dd, $J = 12.2, 6.9$ Hz, 1H), 3.16 – 3.11 (m, 1H), 1.45 (d, $J = 6.1$ Hz, 3H).



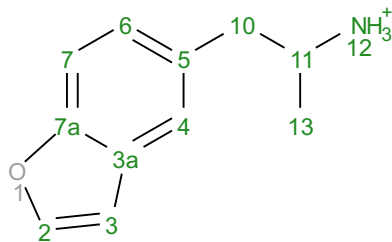
Analyte X51a: 5-APB H+
Acquisition Date 2017-12-08T15:51:26
Solvent dms0
Temperature 25
Number of Scans 512
Relaxation Delay 0
Spectrometer Frequency 175.98
Spectral Width 41666.7
Nucleus 13C
Acquired Size 125000



^{13}C NMR (176 MHz, $\text{DMSO-}d_6$) δ 153.37, 146.30, 131.34, 127.47, 125.58, 121.74, 111.22, 106.59, 48.38, 39.86, 17.54.



Prediction 5-APB H+
Origin Modgraph NMRPredict Desktop
Solvent Common NMR Solvents
Algorithm Neural Network
GMMX Cycles
Version 15465
Frequency 175.00
Nucleus 13C



^{13}C NMR (175 MHz, Common NMR Solvents) δ 157.31, 148.62, 134.94, 131.73, 124.68, 124.15, 112.20, 106.33, 48.51, 43.10, 23.27.

