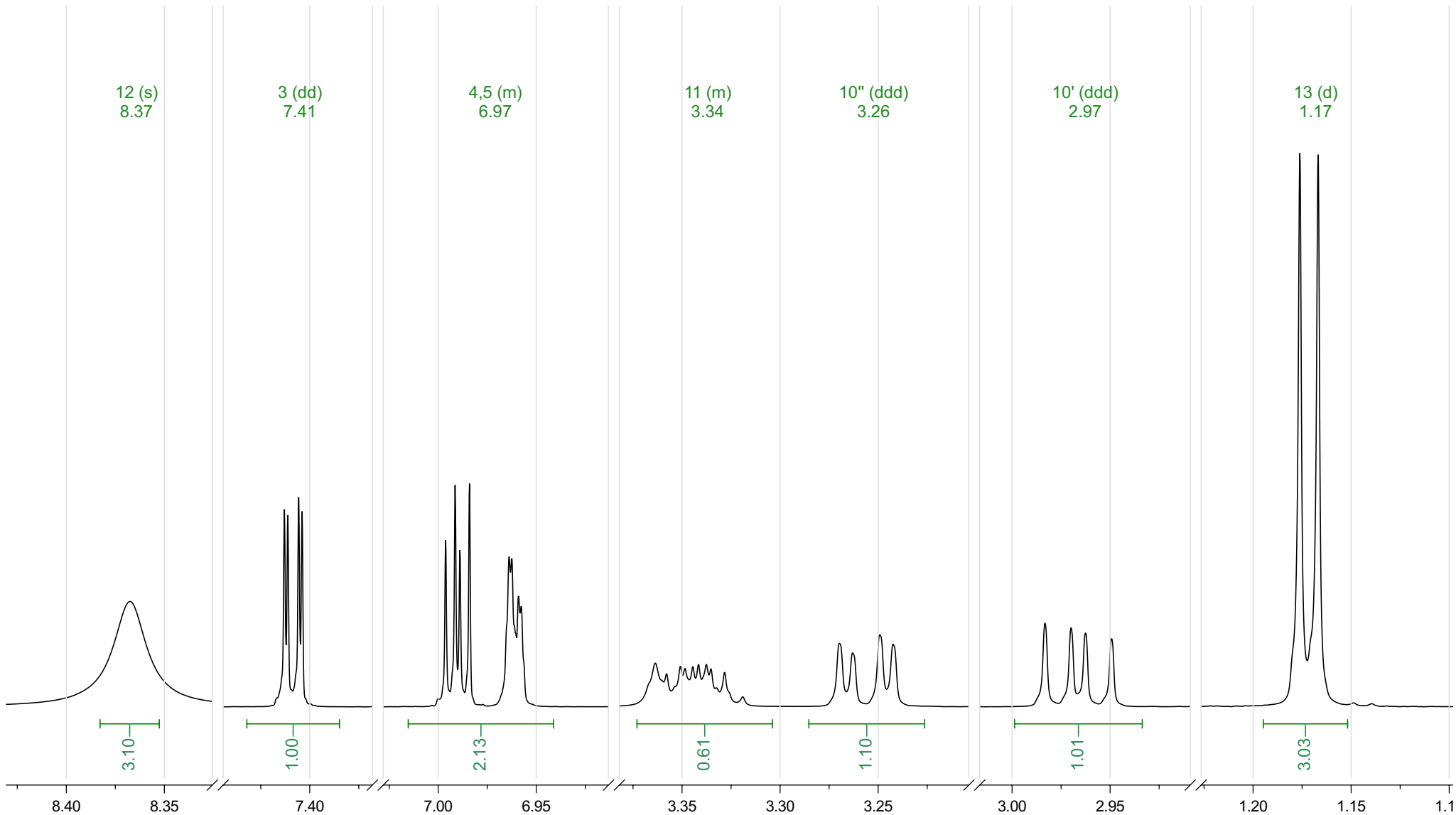
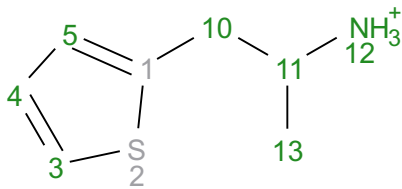
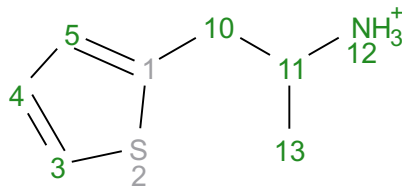


Analyte Thiopropamine H+
Acquisition Date 2016-06-28T16:42:12
Solvent dms0
Temperature 27
Number of Scans 4
Relaxation Delay 10
Spectrometer Frequency 699.81
Spectral Width 14044.9
Nucleus 1H
Acquired Size 131072

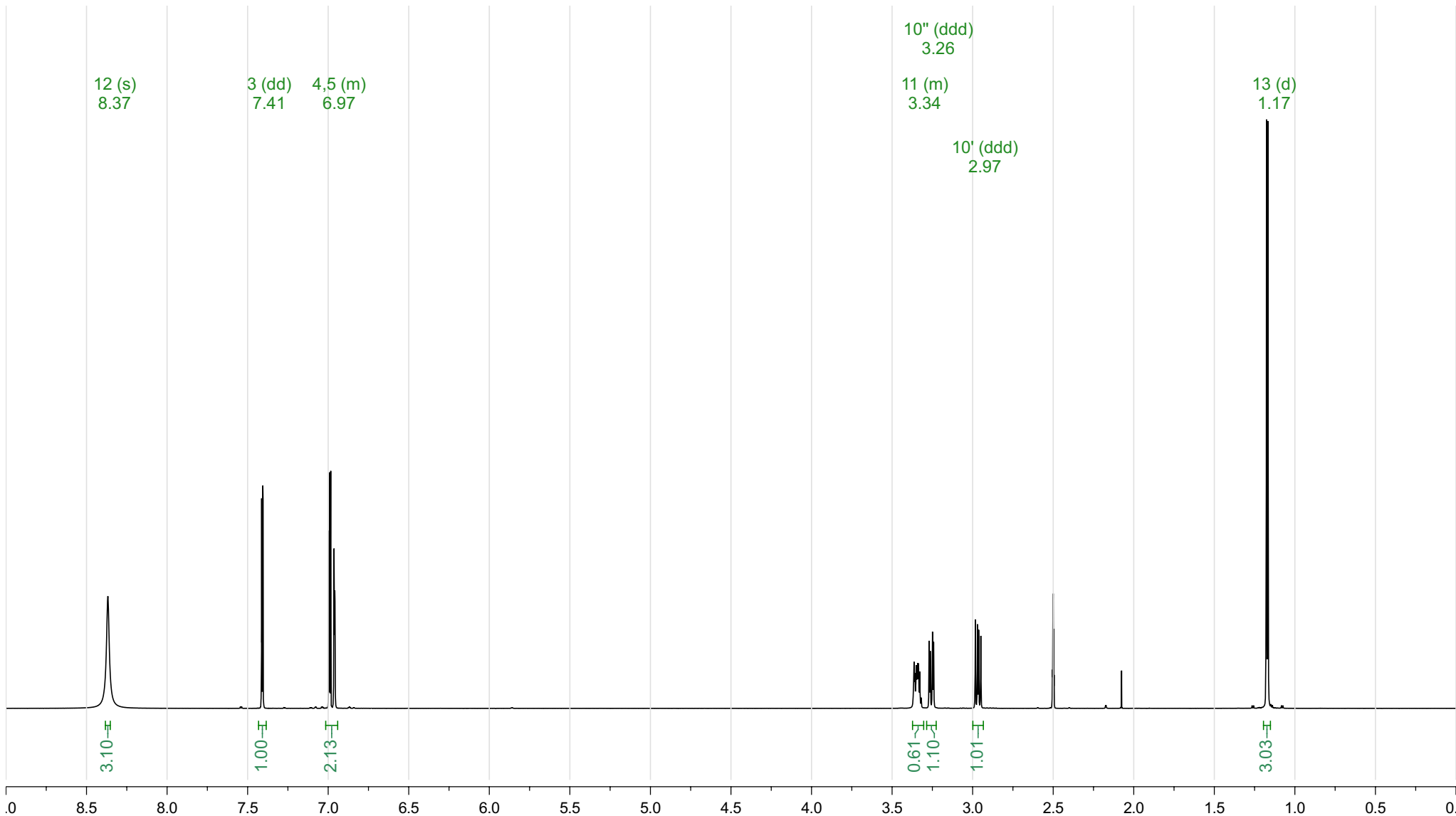
¹H NMR (700 MHz, DMSO-*d*₆) δ 8.37 (s, 3H), 7.41 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.02 – 6.94 (m, 2H), 3.37 – 3.30 (m, 1H), 3.26 (ddd, *J* = 14.4, 4.8, 1.0 Hz, 1H), 2.97 (ddd, *J* = 14.4, 9.3, 0.7 Hz, 1H), 1.17 (d, *J* = 6.5 Hz, 3H).



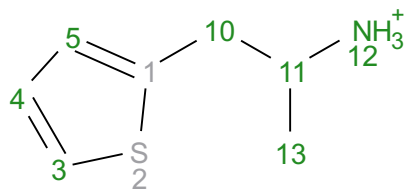
Analyte Thiopropamine H+
Acquisition Date 2016-06-28T16:42:12
Solvent dms0
Temperature 27
Number of Scans 4
Relaxation Delay 10
Spectrometer Frequency 699.81
Spectral Width 14044.9
Nucleus 1H
Acquired Size 131072



^1H NMR (700 MHz, $\text{DMSO-}d_6$) δ 8.37 (s, 3H), 7.41 (dd, $J = 5.1, 1.2$ Hz, 1H), 7.02 – 6.94 (m, 2H), 3.37 – 3.30 (m, 1H), 3.26 (ddd, $J = 14.4, 4.8, 1.0$ Hz, 1H), 2.97 (ddd, $J = 14.4, 9.3, 0.7$ Hz, 1H), 1.17 (d, $J = 6.5$ Hz, 3H).



Prediction Thiopropamine 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), 7.15 (dd, $J = 7.4, 1.5$ Hz, 1H), 6.91 (t, $J = 7.4$ Hz, 1H), 6.86 (dd, $J = 7.4, 1.5$ Hz, 1H), 4.09 – 4.03 (m, 1H), 3.63 (dd, $J = 12.3, 6.7$ Hz, 1H), 3.41 – 3.36 (m, 1H), 1.45 (d, $J = 5.9$ Hz, 3H).

