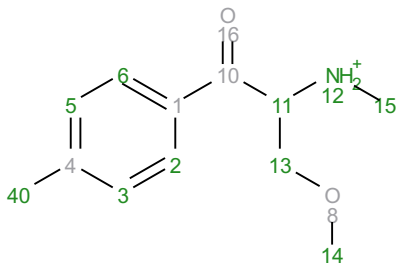
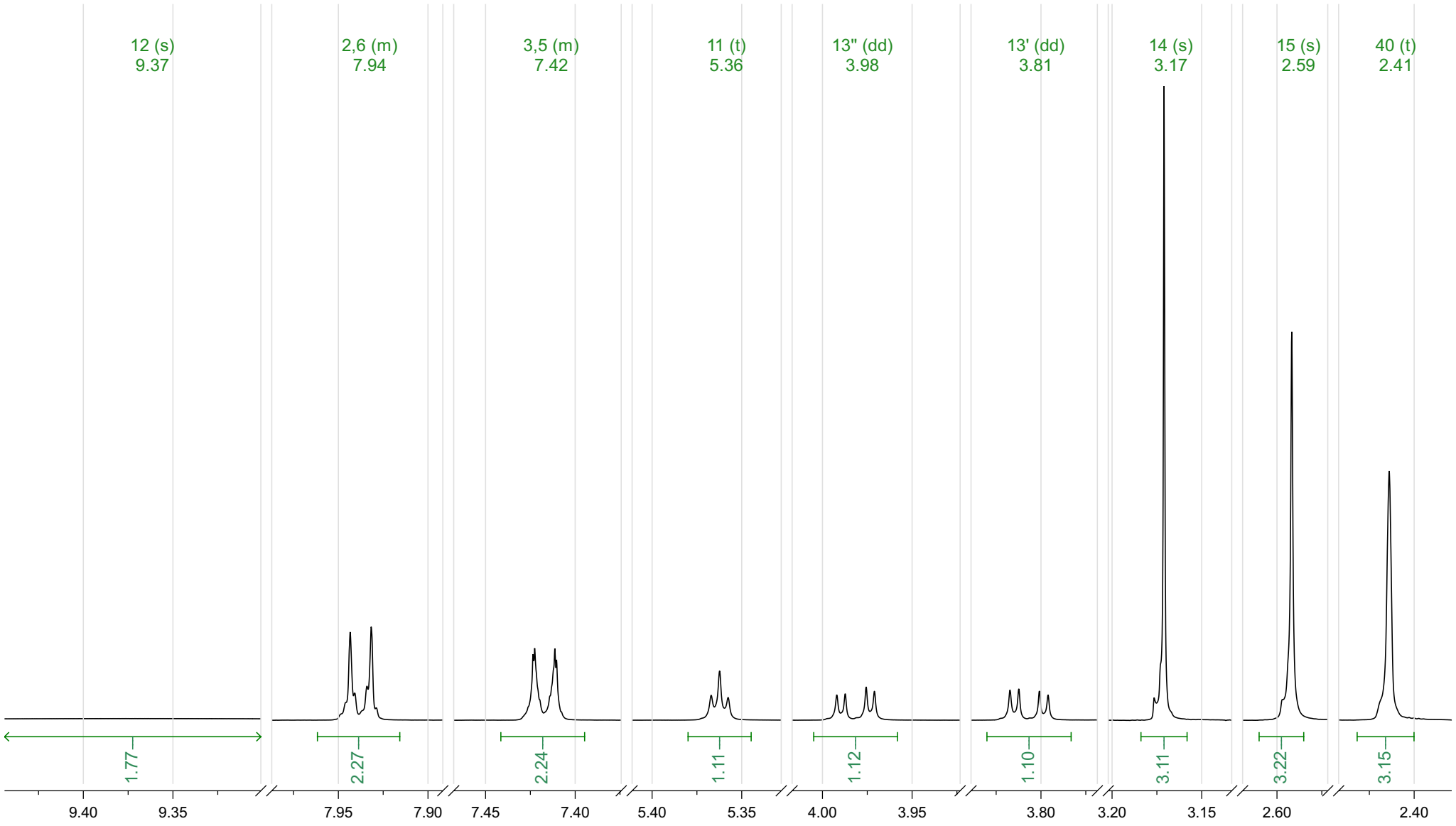
Analyte	X16: Mexedrone H+
Acquisition Date	2016-06-28T16:15:17
Solvent	dmso
Temperature	27
Number of Scans	4
Relaxation Delay	10
Spectrometer Frequency	699.81
Spectral Width	14044.9
Nucleus	1H
Acquired Size	131072



^{1}H NMR (700 MHz, DMSO-d_6) δ 9.37 (s, 2H), 7.96 – 7.92 (m, 2H), 7.44 – 7.39 (m, 2H), 5.36 (t, *J* = 3.3 Hz, 1H), 3.98 (dd, *J* = 11.4, 3.2 Hz, 1H), 3.81 (dd, *J* = 11.5, 3.4 Hz, 1H), 3.17 (s, 3H), 2.59 (s, 3H), 2.41 (t, *J* = 0.7 Hz, 3H).



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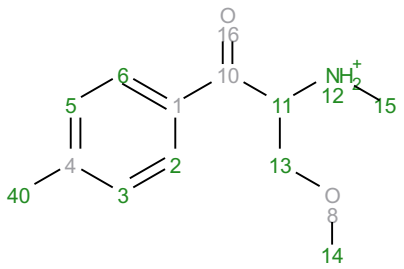
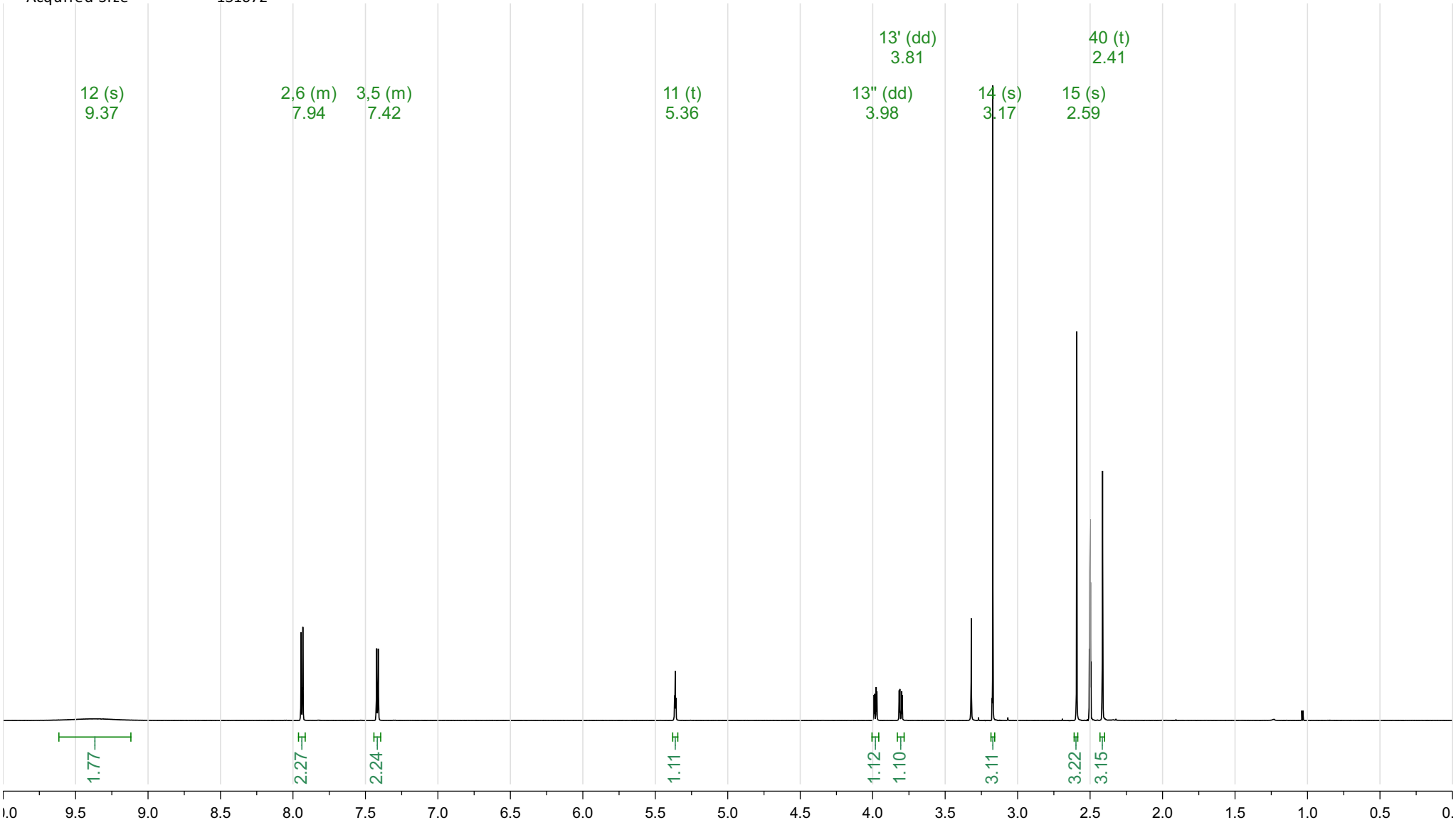
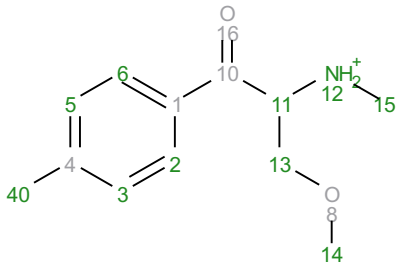


^{1}H NMR (700 MHz, DMSO-d_6) δ 9.37 (s, 2H), 7.96 – 7.92 (m, 2H), 7.44 – 7.39 (m, 2H), 5.36 (t, J = 3.3 Hz, 1H), 3.98 (dd, J = 11.4, 3.2 Hz, 1H), 3.81 (dd, J = 11.5, 3.4 Hz, 1H), 3.17 (s, 3H), 2.59 (s, 3H), 2.41 (t, J = 0.7 Hz, 3H).



Prediction	Mexedrone H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	5
Version	20560
Frequency	500.00
Nucleus	1H



^{1}H NMR (500 MHz, DMSO-d_6) δ 7.98 – 7.92 (m, 2H), 7.41 (dd, J = 8.3, 1.1 Hz, 2H), 7.20 (dq, J = 9.7, 3.3 Hz, 2H), 5.28 (p, J = 9.3 Hz, 1H), 4.42 – 4.34 (m, 1H), 4.17 – 4.09 (m, 1H), 3.27 (s, 3H), 2.55 (t, J = 3.3 Hz, 3H), 2.39 (d, J = 1.1 Hz, 3H).