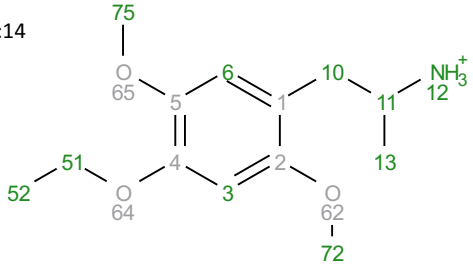
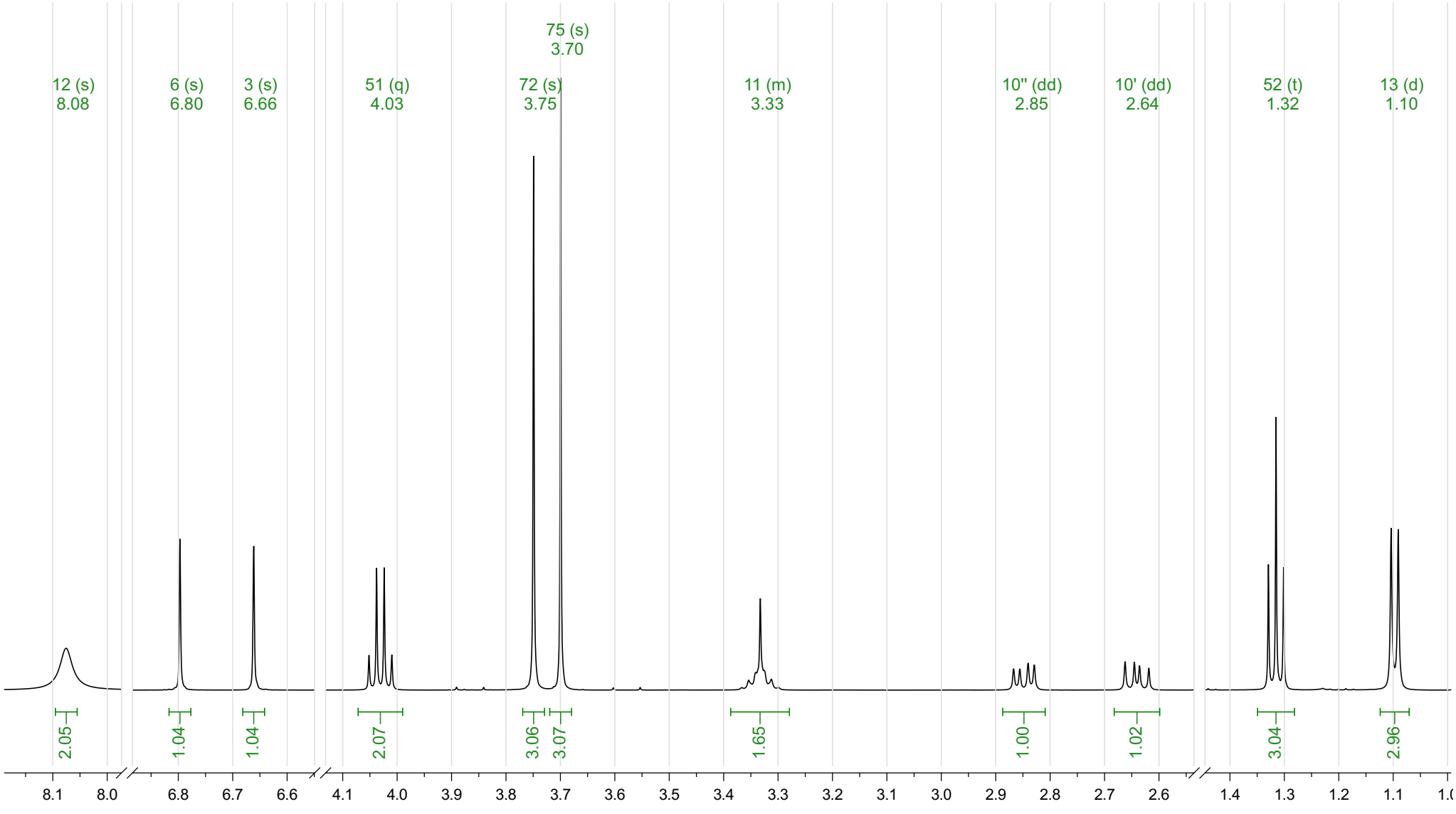
Analyte	SB3: MEM H+
Acquisition Date	2016-12-02T16:48:14
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	1
Spectrometer Frequency	499.66
Spectral Width	8012.8
Nucleus	1H
Acquired Size	48077



^{1}H NMR (500 MHz, DMSO-d_6) δ 8.08 (s, 3H), 6.80 (s, 1H), 6.66 (s, 1H), 4.03 (q, J = 7.0 Hz, 2H), 3.75 (s, 3H), 3.70 (s, 3H), 3.39 – 3.28 (m, 1H), 2.85 (dd, J = 13.3, 5.7 Hz, 1H), 2.64 (dd, J = 13.3, 8.5 Hz, 1H), 1.32 (t, J = 7.0 Hz, 3H), 1.10 (d, J = 6.5 Hz, 3H).



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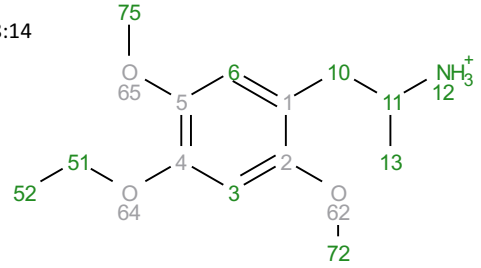
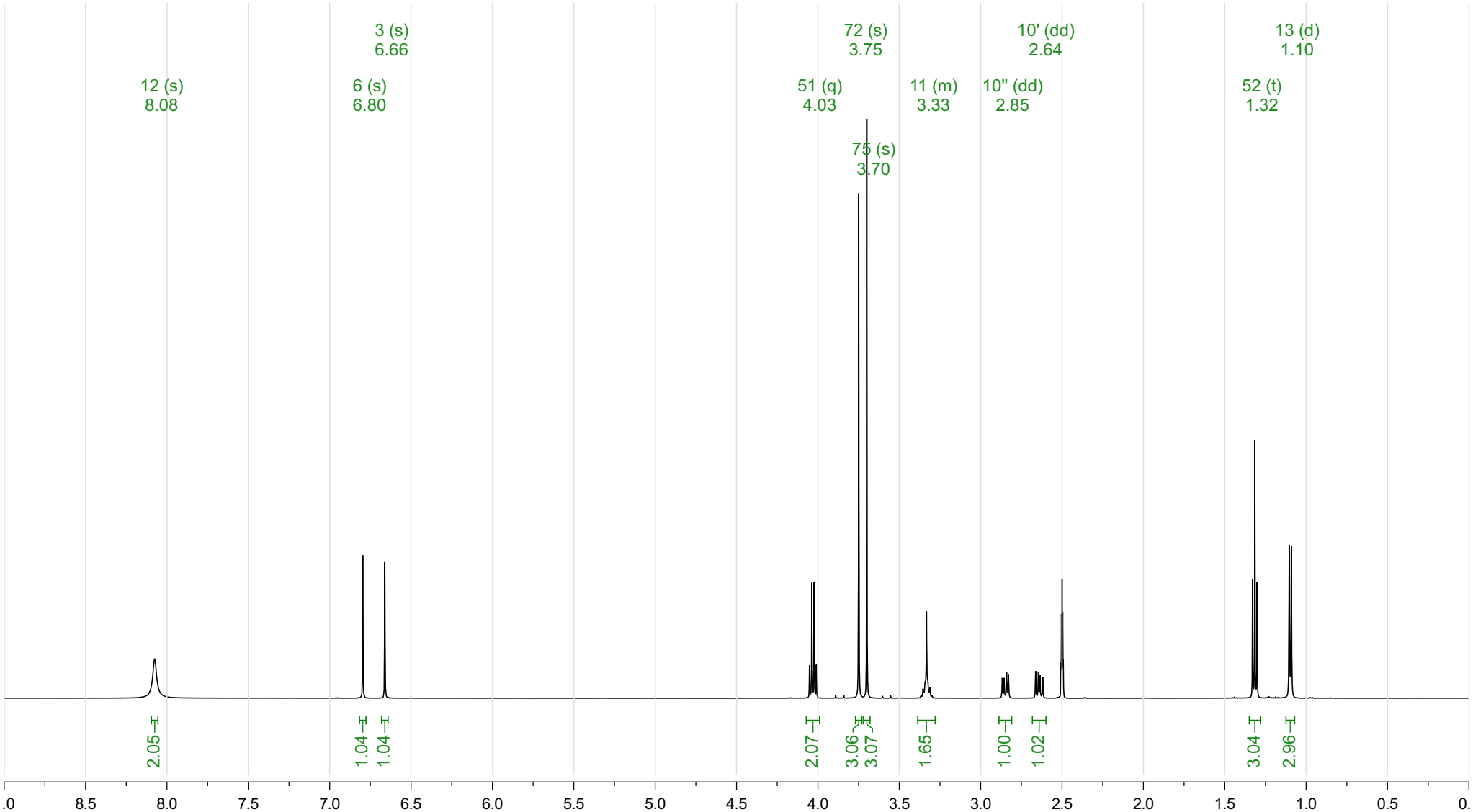
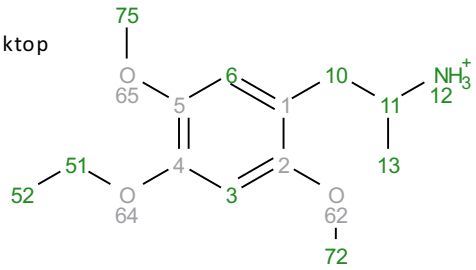


^{1}H NMR (500 MHz, DMSO-d_6) δ 8.08 (s, 3H), 6.80 (s, 1H), 6.66 (s, 1H), 4.03 (q, J = 7.0 Hz, 2H), 3.75 (s, 3H), 3.70 (s, 3H), 3.39 – 3.28 (m, 1H), 2.85 (dd, J = 13.3, 5.7 Hz, 1H), 2.64 (dd, J = 13.3, 8.5 Hz, 1H), 1.32 (t, J = 7.0 Hz, 3H), 1.10 (d, J = 6.5 Hz, 3H).



Prediction	MEM H+
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	25
Version	18153
Frequency	500.13
Nucleus	1H



^{1}H NMR (500 MHz, DMSO-d_6) δ 8.25 (d, J = 5.3 Hz, 3H), 6.92 (t, J = 1.0 Hz, 1H), 6.84 (s, 1H), 4.19 (dq, J = 10.1, 7.0 Hz, 1H), 3.95 (dq, J = 10.1, 6.9 Hz, 1H), 3.80 (s, 3H), 3.73 (s, 3H), 3.48 (dtt, J = 10.8, 6.4, 5.4 Hz, 1H), 2.99 (ddd, J = 15.5, 6.4, 1.0 Hz, 1H), 2.88 (ddd, J = 15.5, 6.3, 0.9 Hz, 1H), 1.40 (t, J = 6.9 Hz, 3H), 1.11 (d, J = 5.5 Hz, 3H).