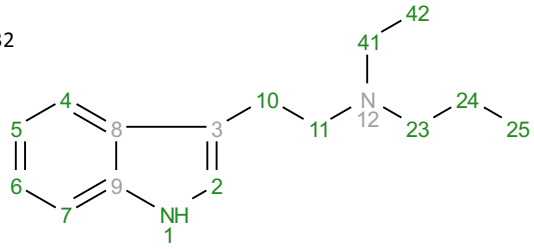
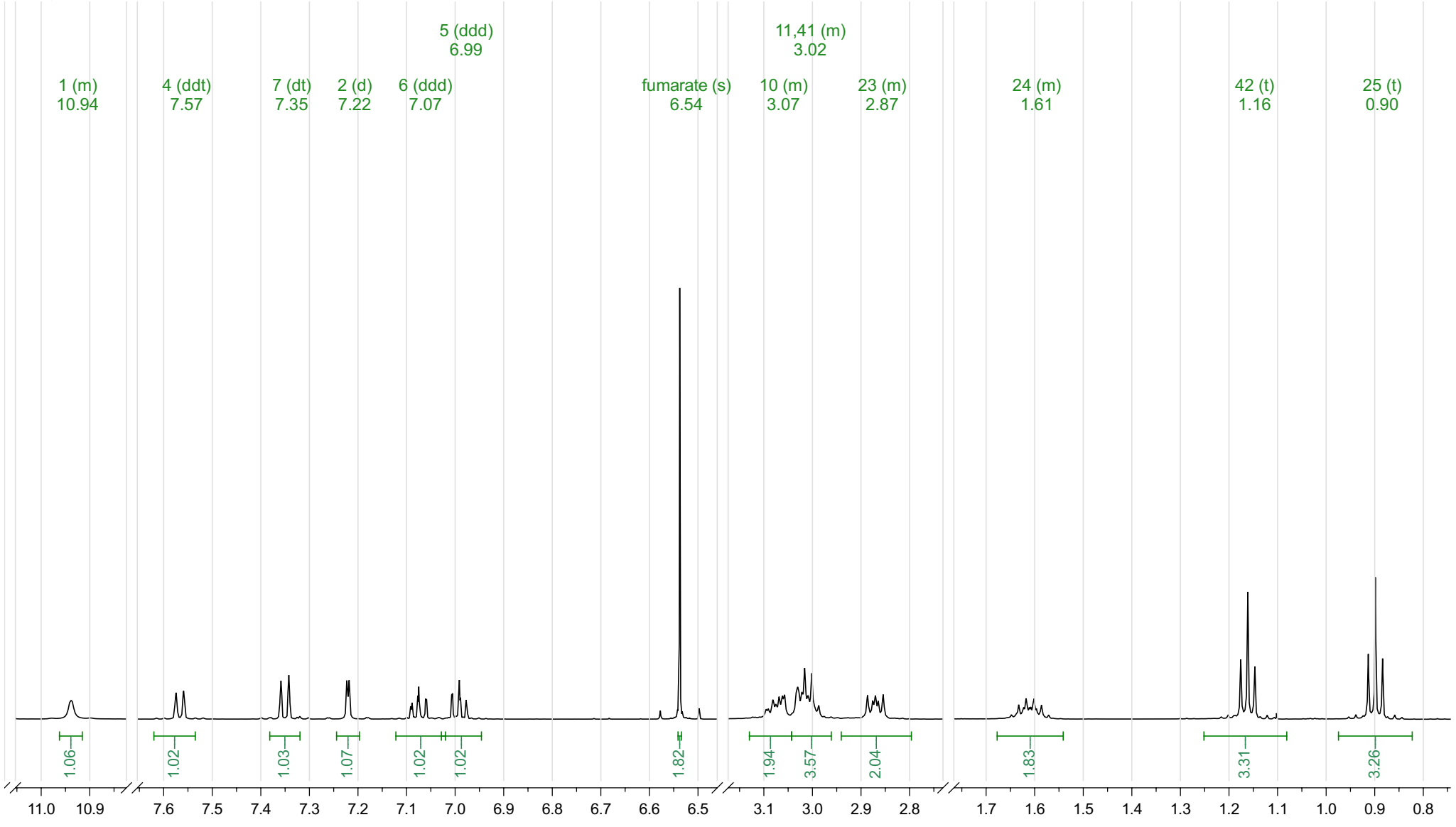
Analyte	T37: EPT fumarate
Acquisition Date	2016-10-13T16:15:32
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	5
Spectrometer Frequency	499.67
Spectral Width	10000.0
Nucleus	1H
Acquired Size	65536



^{1}H NMR (500 MHz, DMSO-d_6) δ 10.96 – 10.92 (m, 1H), 7.57 (ddt, *J* = 7.9, 1.4, 0.7 Hz, 1H), 7.35 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.22 (d, *J* = 2.4 Hz, 1H), 7.07 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 6.99 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 6.54 (s, 2H), 3.13 – 3.04 (m, 2H), 3.04 – 2.96 (m, 4H), 2.94 – 2.80 (m, 2H), 1.68 – 1.54 (m, 2H), 1.16 (t, *J* = 7.2 Hz, 3H), 0.90 (t, *J* = 7.4 Hz, 3H).



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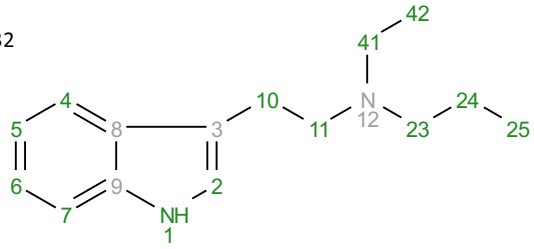
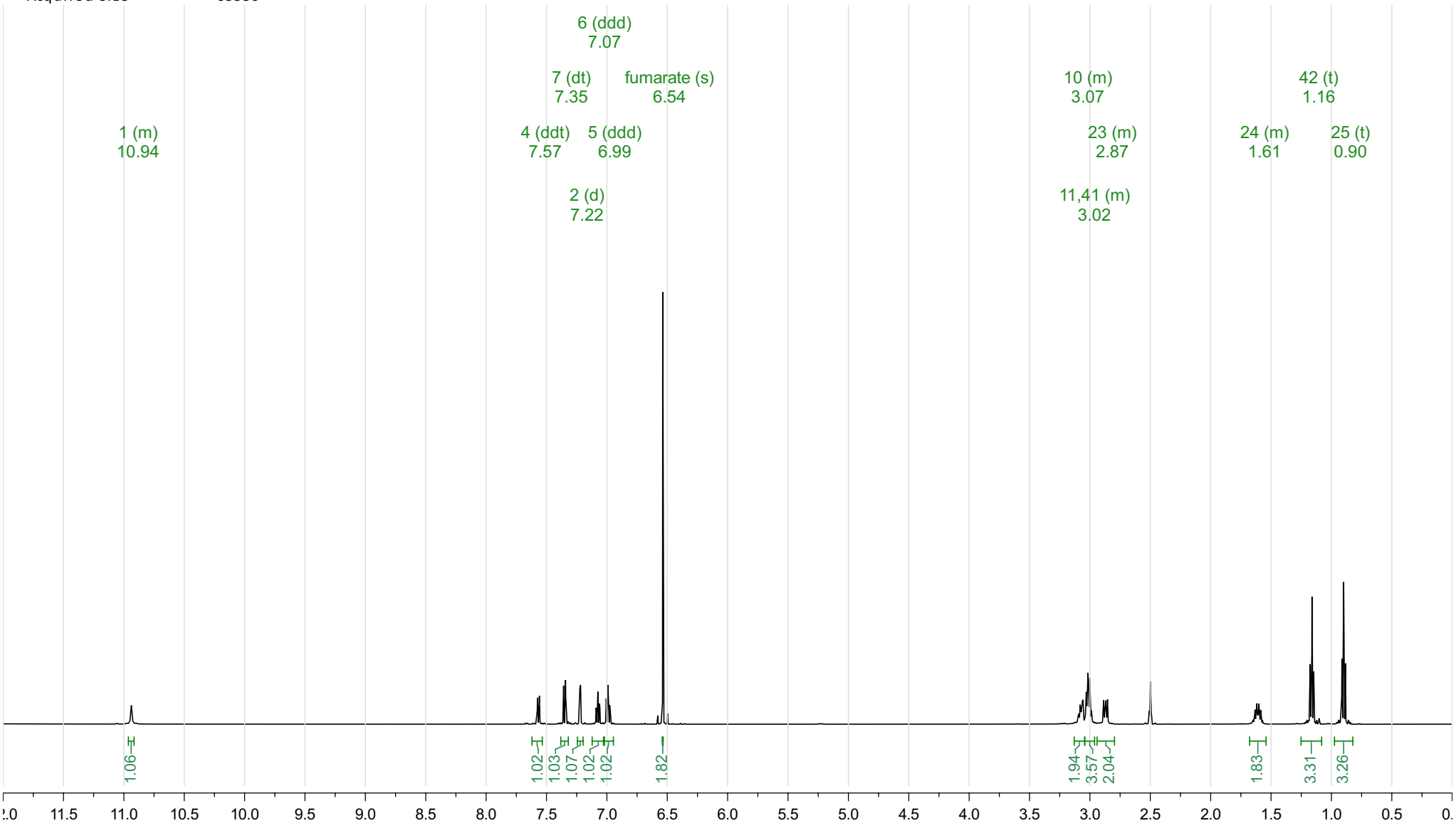
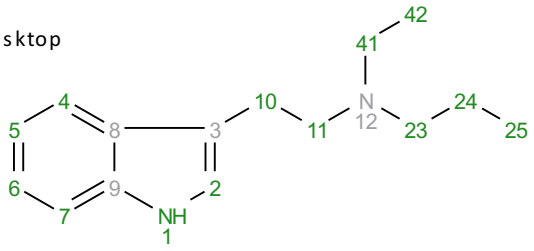
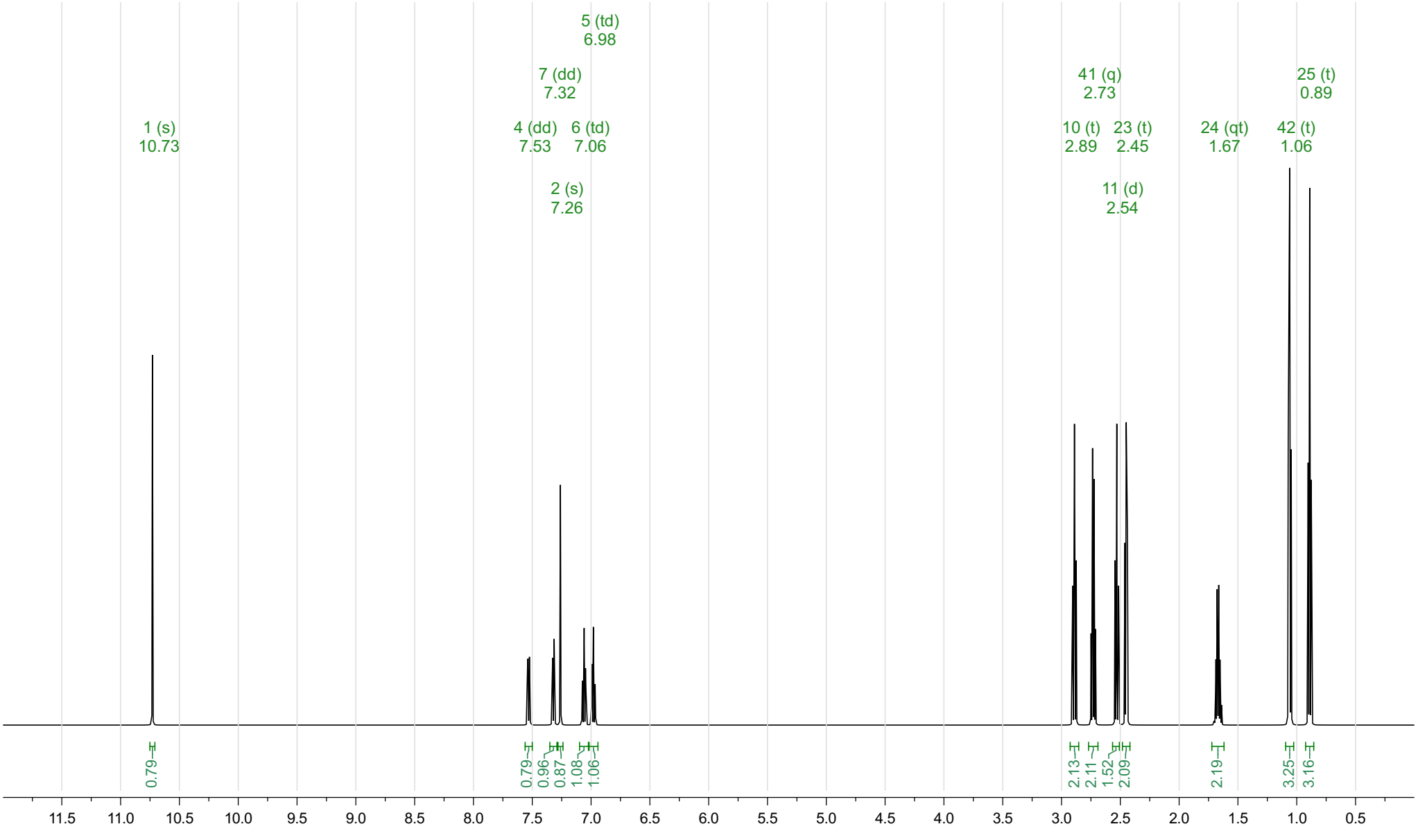


^{1}H NMR (500 MHz, DMSO-d_6) δ 10.96 – 10.92 (m, 1H), 7.57 (ddt, *J* = 7.9, 1.4, 0.7 Hz, 1H), 7.35 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.22 (d, *J* = 2.4 Hz, 1H), 7.07 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 6.99 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 6.54 (s, 2H), 3.13 – 3.04 (m, 2H), 3.04 – 2.96 (m, 4H), 2.94 – 2.80 (m, 2H), 1.68 – 1.54 (m, 2H), 1.16 (t, *J* = 7.2 Hz, 3H), 0.90 (t, *J* = 7.4 Hz, 3H).



Prediction	EPT
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	5
Version	15465
Frequency	500.13
Nucleus	1H



^{1}H NMR (500 MHz, DMSO-d_6) δ 10.73 (s, 1H), 7.53 (dd, *J* = 7.4, 1.9 Hz, 1H), 7.32 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.26 (s, 1H), 7.06 (td, *J* = 7.5, 1.6 Hz, 1H), 6.98 (td, *J* = 7.5, 1.4 Hz, 1H), 2.89 (t, *J* = 7.5 Hz, 2H), 2.73 (q, *J* = 6.3 Hz, 2H), 2.54 (d, *J* = 7.6 Hz, 2H), 2.45 (t, *J* = 5.4 Hz, 2H), 1.67 (qt, *J* = 6.6, 5.2 Hz, 2H), 1.06 (t, *J* = 6.4 Hz, 3H), 0.89 (t, *J* = 6.7 Hz, 3H).