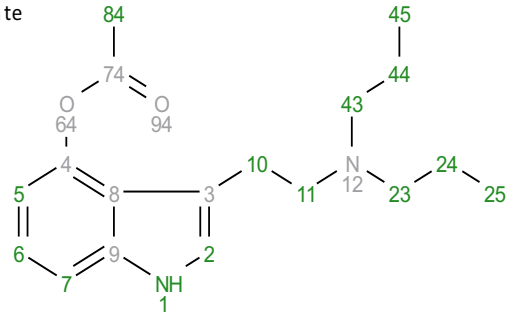
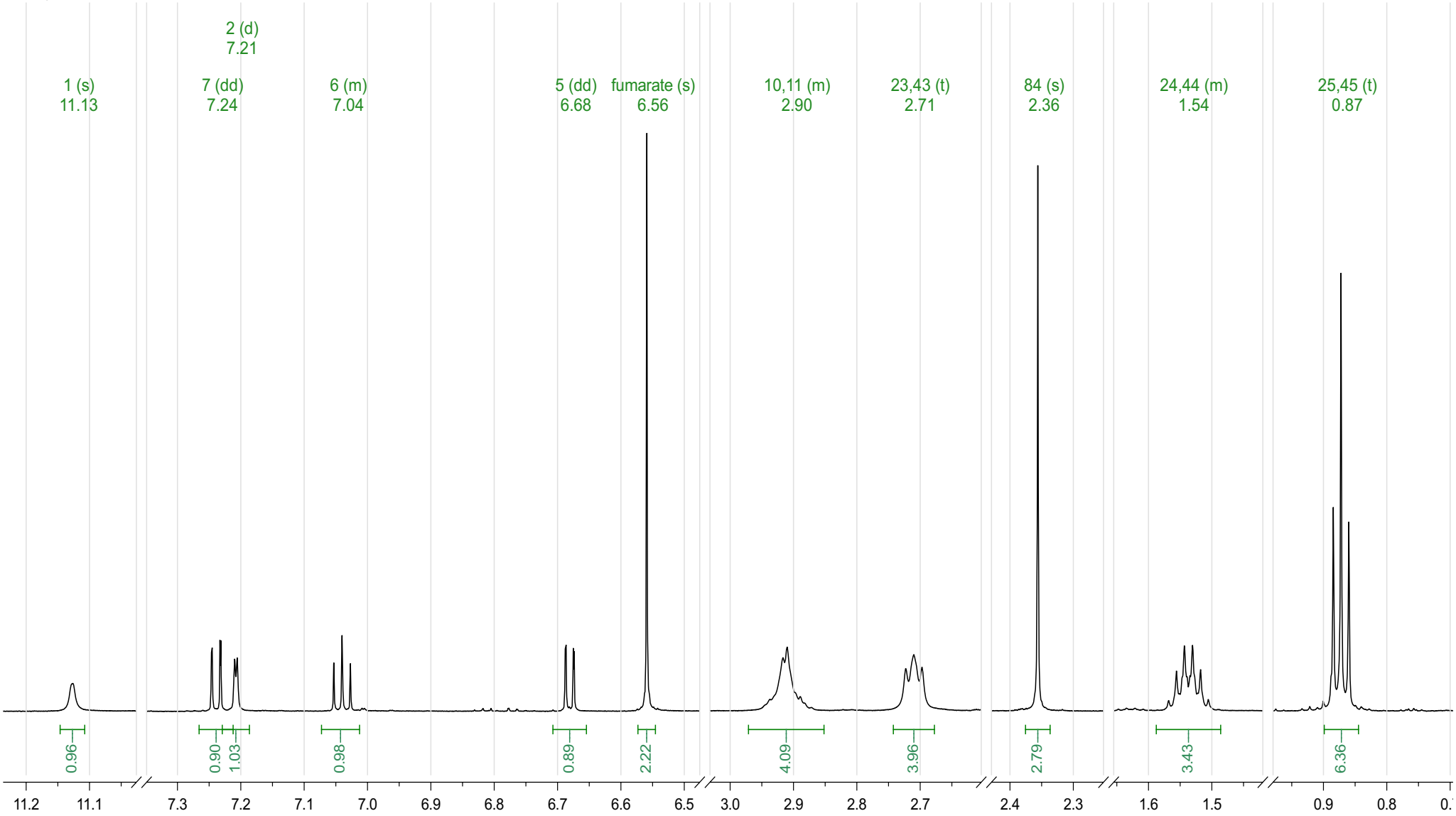
Analyte	T40: 4-AcO-DPT fumarate
Acquisition Date	2017-09-12T07:02:17
Solvent	dmso
Temperature	25
Number of Scans	16
Relaxation Delay	1
Spectrometer Frequency	599.82
Spectral Width	9615.4
Nucleus	1H
Acquired Size	43269



^{1}H NMR (600 MHz, DMSO-d_6) δ 11.13 (s, 1H), 7.24 (dd, J = 8.1, 0.8 Hz, 1H), 7.21 (d, J = 2.4 Hz, 1H), 7.07 – 7.01 (m, 1H), 6.68 (dd, J = 7.6, 0.8 Hz, 1H), 6.56 (s, 2H), 2.97 – 2.85 (m, 4H), 2.71 (t, J = 7.8 Hz, 4H), 2.36 (s, 3H), 1.59 – 1.49 (m, 4H), 0.87 (t, J = 7.3 Hz, 6H).



Analyte	T40: 4-AcO-DPT fumarate
Acquisition Date	2017-09-12T07:02:17
Solvent	dmso
Temperature	25
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Relaxation Delay	1
Spectrometer Frequency	599.82
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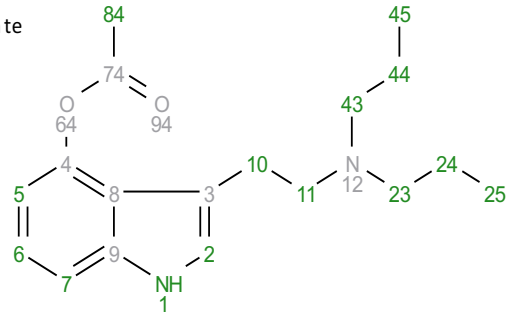
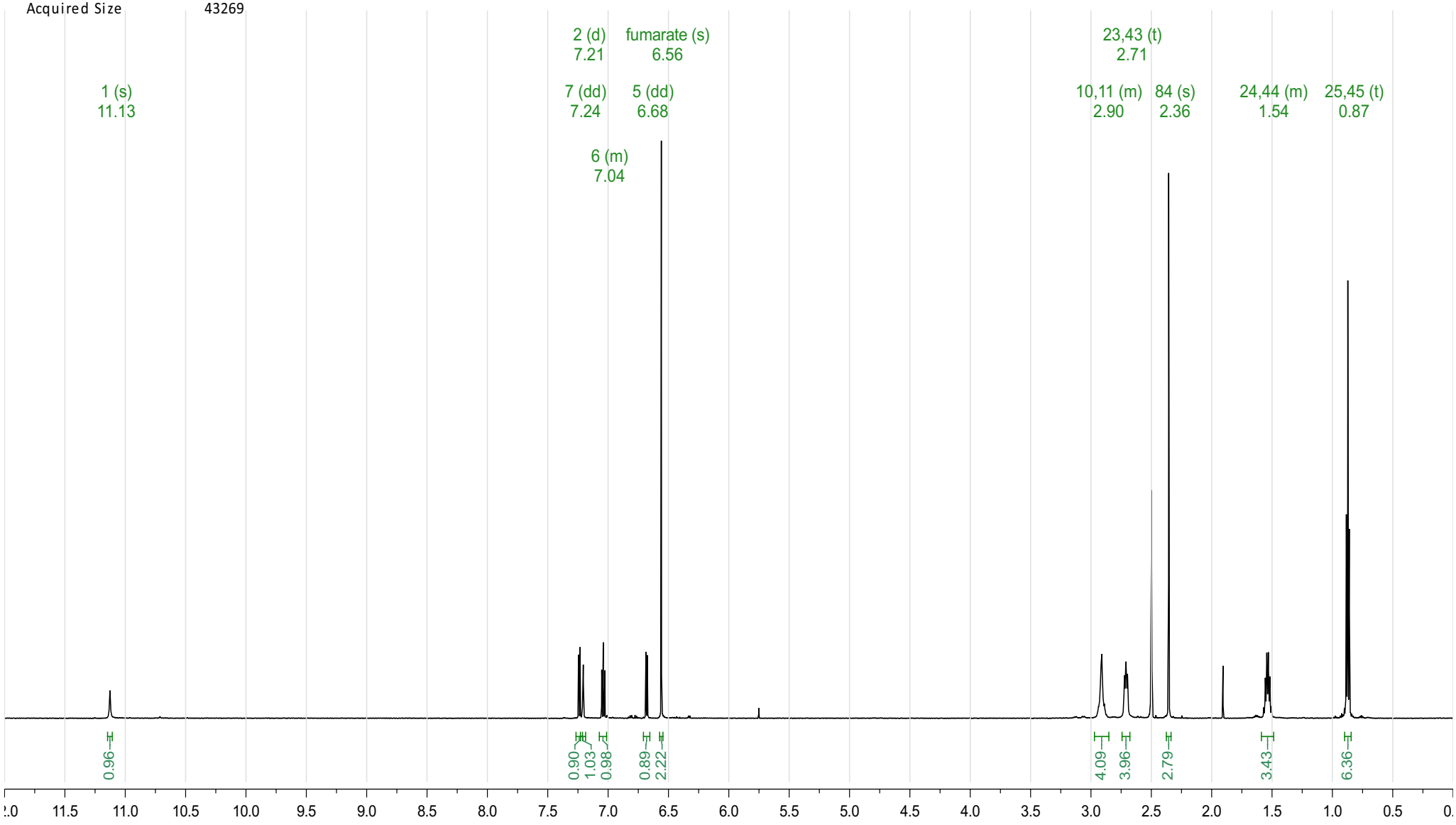
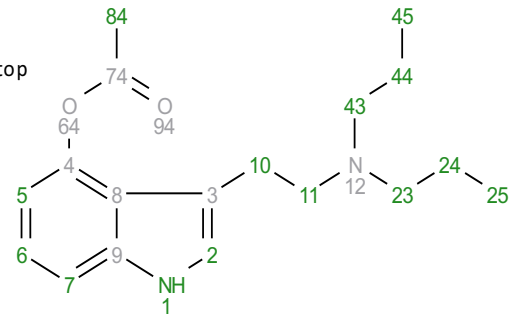
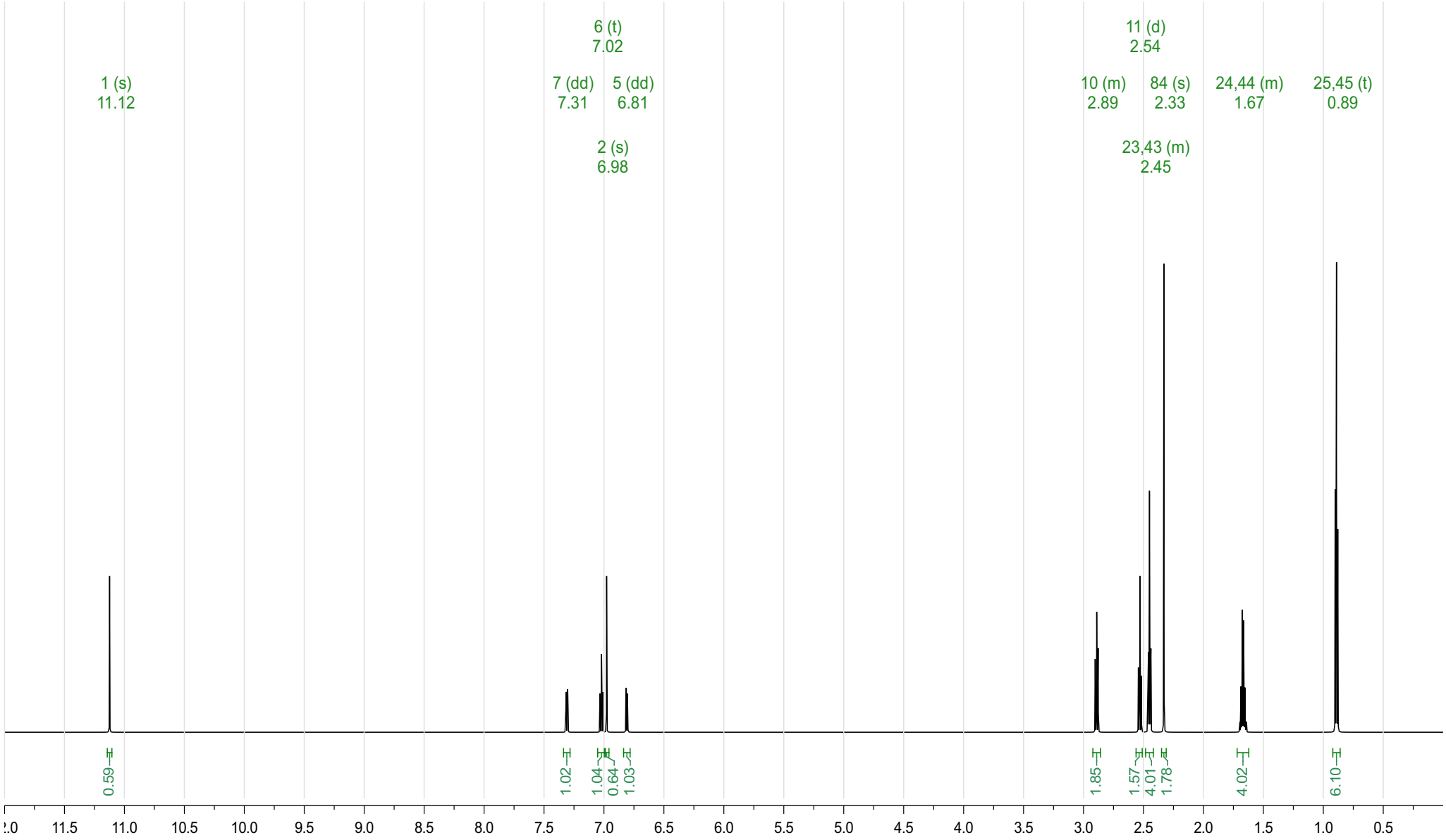


^{1}H NMR (600 MHz, DMSO-d_6) δ 11.13 (s, 1H), 7.24 (dd, J = 8.1, 0.8 Hz, 1H), 7.21 (d, J = 2.4 Hz, 1H), 7.07 – 7.01 (m, 1H), 6.68 (dd, J = 7.6, 0.8 Hz, 1H), 6.56 (s, 2H), 2.97 – 2.85 (m, 4H), 2.71 (t, J = 7.8 Hz, 4H), 2.36 (s, 3H), 1.59 – 1.49 (m, 4H), 0.87 (t, J = 7.3 Hz, 6H).



Prediction	4-AcO-DPT fumarate
Origin	Modgraph NMRPredict Desktop
Solvent	DMSO-d6
Algorithm	Best
GMMX Cycles	5
Version	15465
Frequency	600.00
Nucleus	1H



^{1}H NMR (600 MHz, DMSO-d_6) δ 11.12 (s, 1H), 7.31 (dd, J = 7.5, 1.6 Hz, 1H), 7.02 (t, J = 7.5 Hz, 1H), 6.98 (s, 1H), 6.81 (dd, J = 7.5, 1.6 Hz, 1H), 2.92 – 2.86 (m, 2H), 2.54 (d, J = 7.5 Hz, 2H), 2.48 – 2.42 (m, 4H), 2.33 (s, 3H), 1.72 – 1.62 (m, 4H), 0.89 (t, J = 6.6 Hz, 6H).