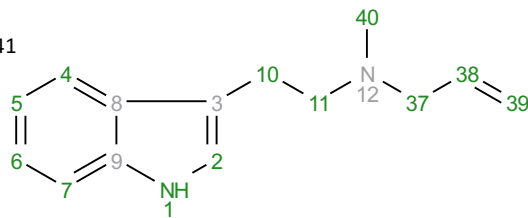
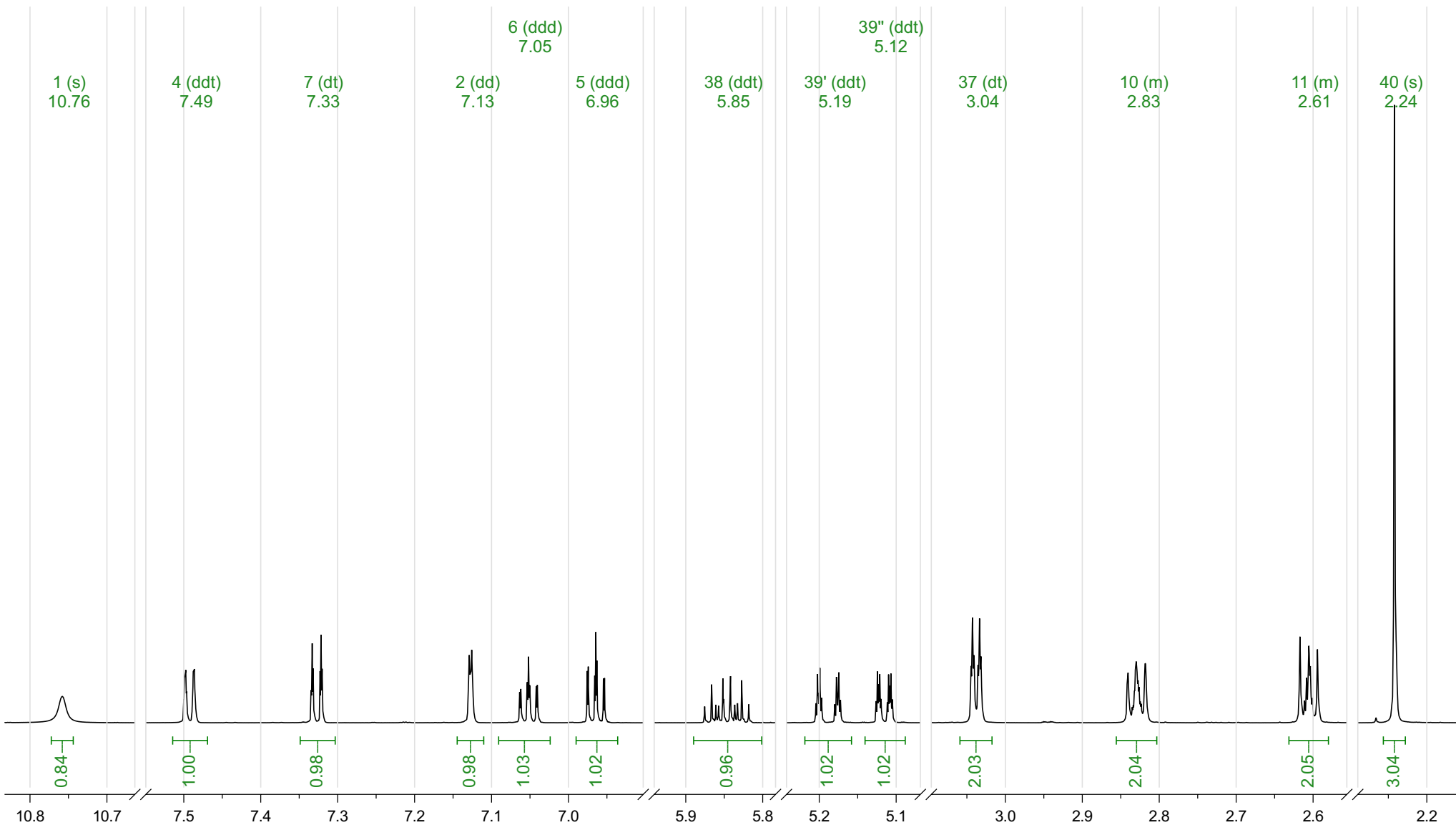


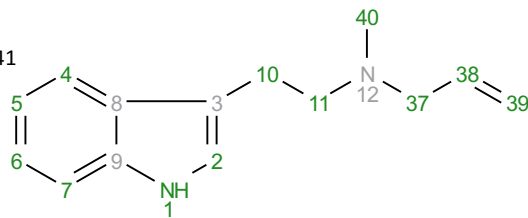
Analyte T41: MALT fb
 Acquisition Date 2017-12-08T22:18:41
 Solvent dms0
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 50223



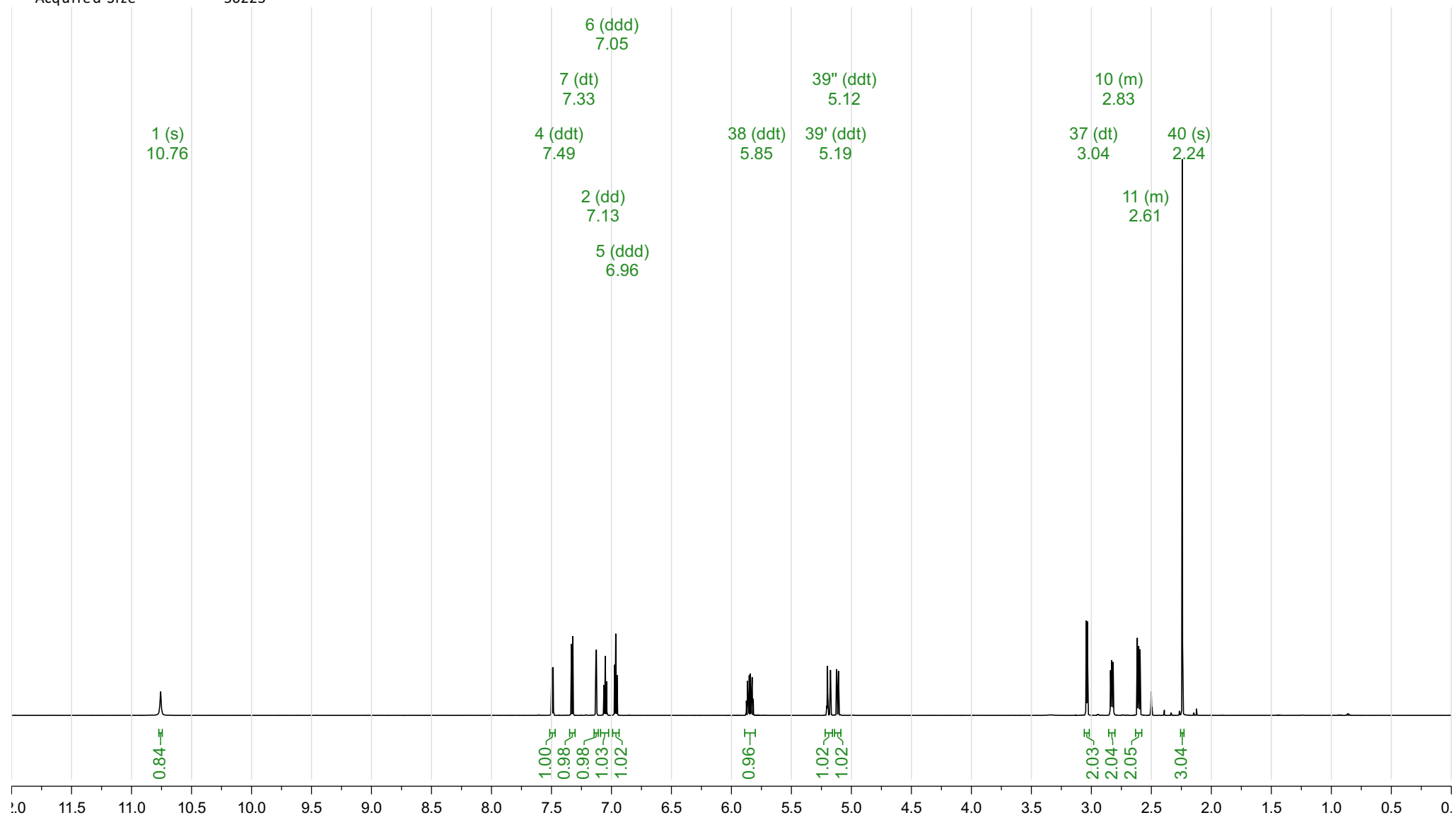
¹H NMR (700 MHz, DMSO-*d*₆) δ 10.76 (s, 1H), 7.49 (ddt, *J* = 7.9, 1.3, 0.8 Hz, 1H), 7.33 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.13 (dd, *J* = 2.2, 1.1 Hz, 1H), 7.05 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 6.96 (ddd, *J* = 7.9, 6.9, 1.0 Hz, 1H), 5.85 (ddt, *J* = 17.3, 10.2, 6.4 Hz, 1H), 5.19 (ddt, *J* = 17.2, 2.2, 1.5 Hz, 1H), 5.12 (ddt, *J* = 10.2, 2.3, 1.2 Hz, 1H), 3.04 (dt, *J* = 6.3, 1.4 Hz, 2H), 2.86 – 2.80 (m, 2H), 2.64 – 2.57 (m, 2H), 2.24 (s, 3H).



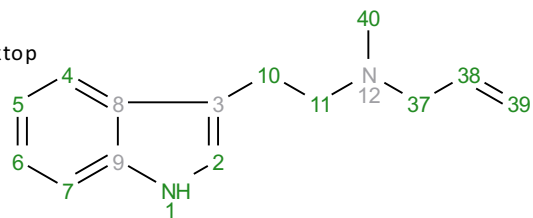
Analyte T41: MALT fb
 Acquisition Date 2017-12-08T22:18:41
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 50223



¹H NMR (700 MHz, DMSO-*d*₆) δ 10.76 (s, 1H), 7.49 (ddt, *J* = 7.9, 1.3, 0.8 Hz, 1H), 7.33 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.13 (dd, *J* = 2.2, 1.1 Hz, 1H), 7.05 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 6.96 (ddd, *J* = 7.9, 6.9, 1.0 Hz, 1H), 5.85 (ddt, *J* = 17.3, 10.2, 6.4 Hz, 1H), 5.19 (ddt, *J* = 17.2, 2.2, 1.5 Hz, 1H), 5.12 (ddt, *J* = 10.2, 2.3, 1.2 Hz, 1H), 3.04 (dt, *J* = 6.3, 1.4 Hz, 2H), 2.86 – 2.80 (m, 2H), 2.64 – 2.57 (m, 2H), 2.24 (s, 3H).



Prediction MALT
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 10.73 (s, 1H), 7.53 (dd, J = 7.8, 1.6 Hz, 1H), 7.32 (dd, J = 7.2, 1.7 Hz, 1H), 7.26 (s, 1H), 7.06 (td, J = 7.5, 1.6 Hz, 1H), 6.98 (td, J = 7.5, 1.6 Hz, 1H), 5.86 (ddt, J = 14.6, 12.1, 6.1 Hz, 1H), 5.18 – 5.10 (m, 2H), 3.04 – 3.00 (m, 2H), 2.89 (t, J = 7.8 Hz, 2H), 2.57 (d, J = 7.6 Hz, 1H), 2.18 (s, 3H).

