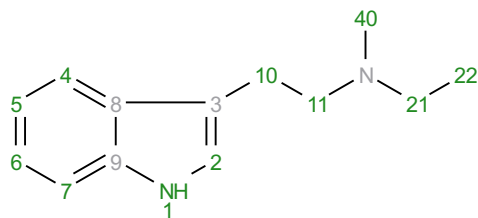
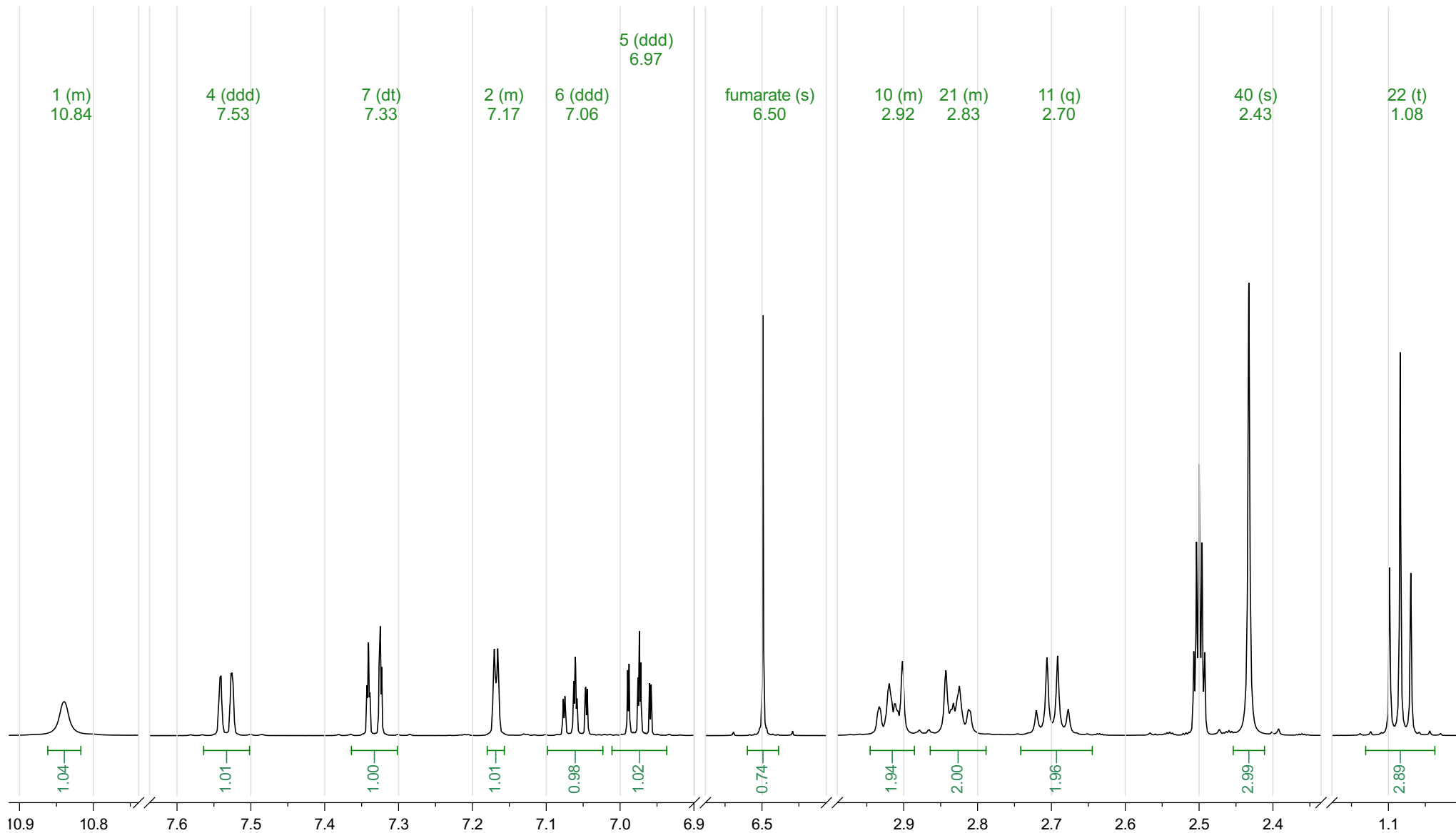


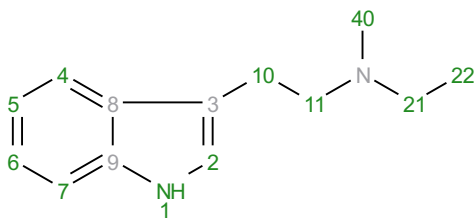
Analyte T5: MET fumarate
 Acquisition Date 2012-12-04T20:27:36
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 8012.8
 Nucleus 1H
 Acquired Size 32768



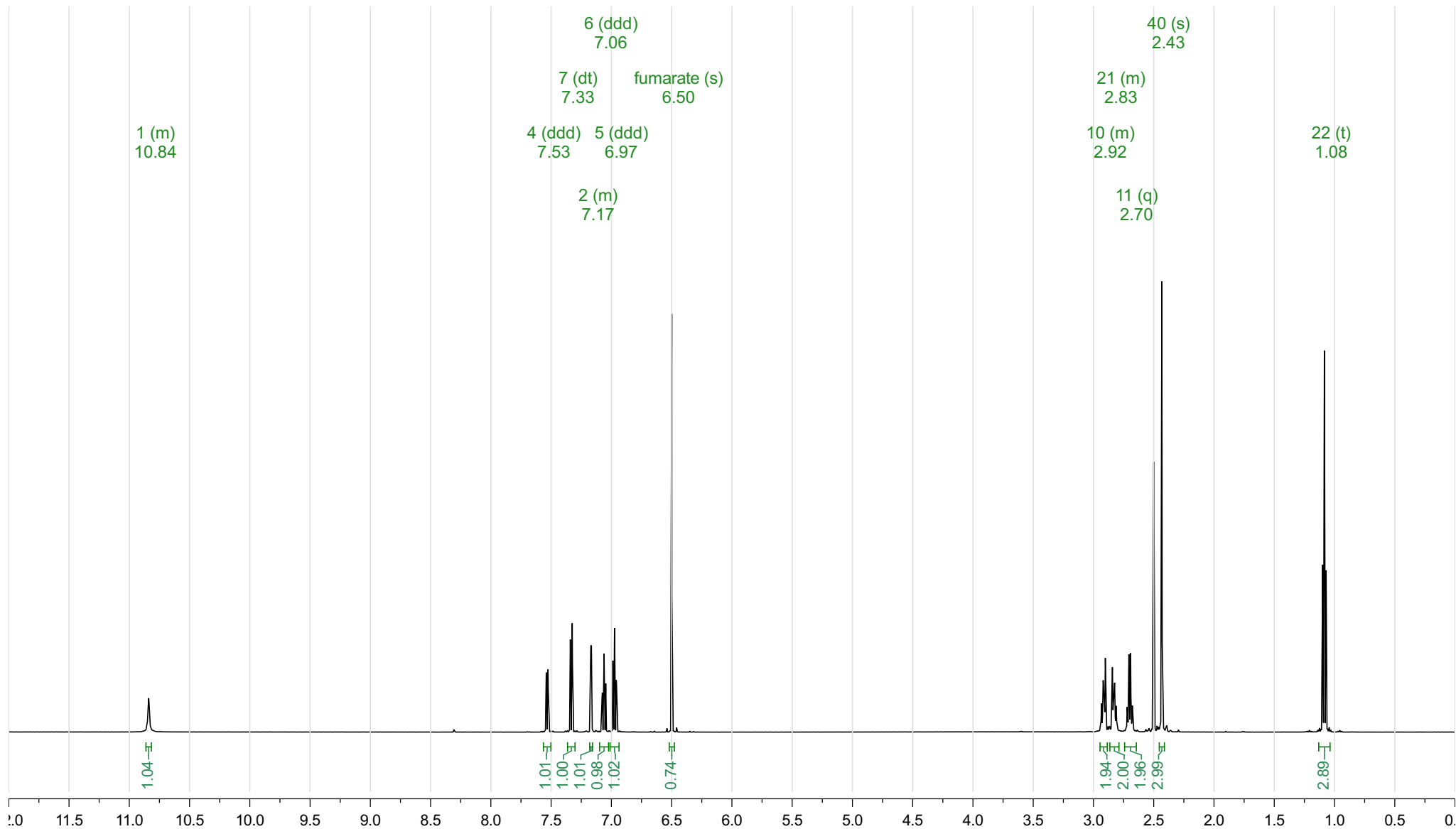
¹H NMR (500 MHz, DMSO-*d*₆) δ 10.86 – 10.82 (m, 1H), 7.53 (ddd, *J* = 7.9, 1.3, 0.7 Hz, 1H), 7.33 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.18 – 7.16 (m, 1H), 7.06 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 6.97 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 6.50 (s, 1H), 2.95 – 2.89 (m, 2H), 2.86 – 2.79 (m, 2H), 2.70 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 1.08 (t, *J* = 7.2 Hz, 3H).



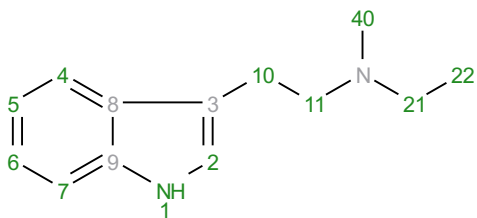
Analyte T5: MET fumarate
 Acquisition Date 2012-12-04T20:27:36
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 8012.8
 Nucleus 1H
 Acquired Size 32768



¹H NMR (500 MHz, DMSO-*d*₆) δ 10.86 – 10.82 (m, 1H), 7.53 (ddd, *J* = 7.9, 1.3, 0.7 Hz, 1H), 7.33 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.18 – 7.16 (m, 1H), 7.06 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 6.97 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 6.50 (s, 1H), 2.95 – 2.89 (m, 2H), 2.86 – 2.79 (m, 2H), 2.70 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 1.08 (t, *J* = 7.2 Hz, 3H).



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



$^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 10.73 (s, 1H), 7.53 (dd, $J = 7.5, 1.8$ Hz, 1H), 7.32 (dd, $J = 7.5, 1.6$ 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, $J = 7.6$ Hz, 2H), 2.64 (q, $J = 6.3$ Hz, 2H), 2.56 (t, $J = 7.6$ Hz, 2H), 2.23 (s, 3H), 1.02 (t, $J = 6.3$ Hz, 3H).

