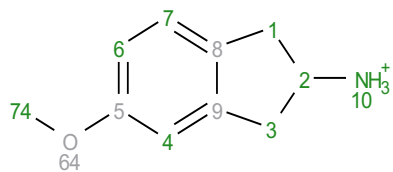
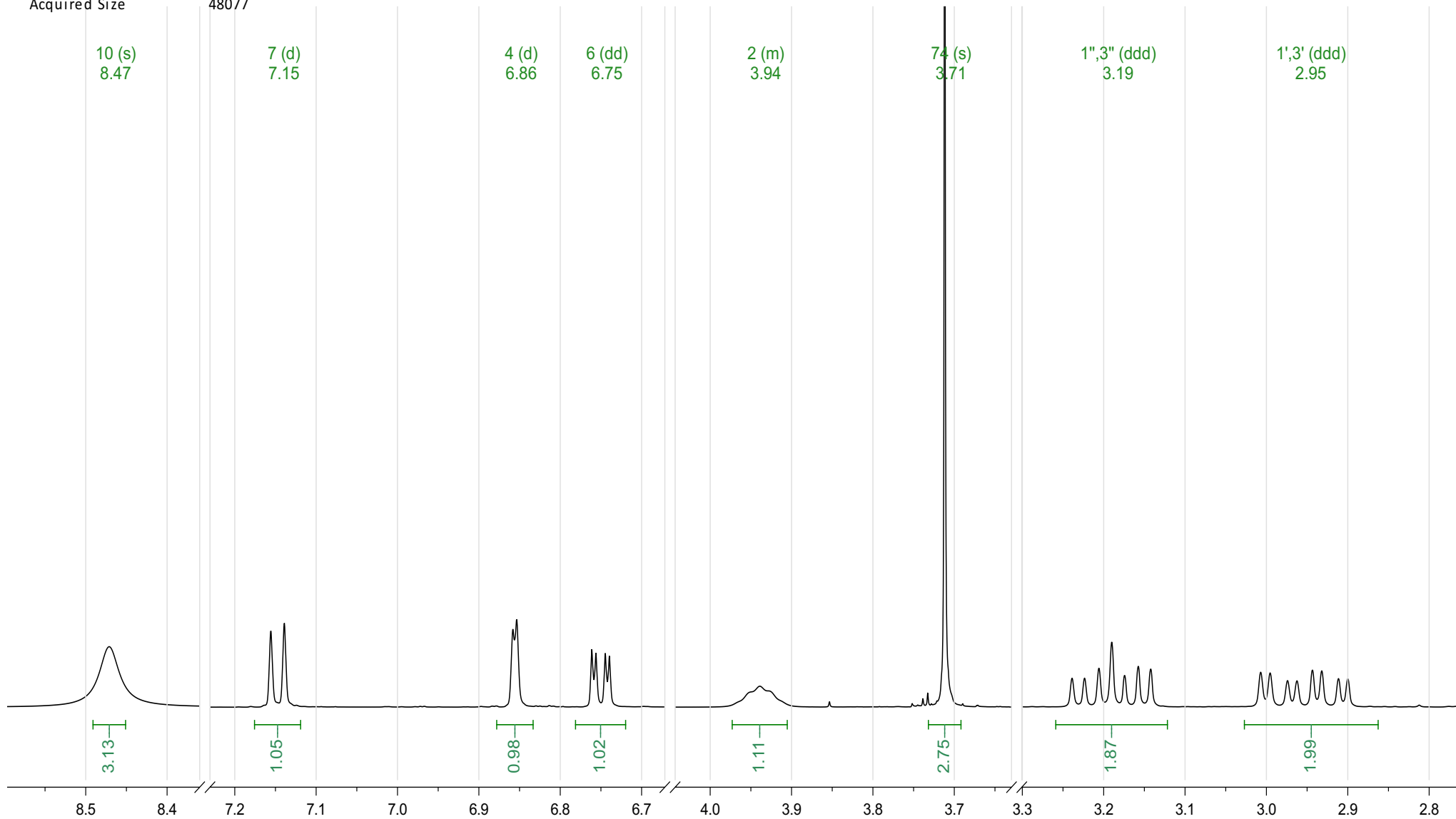


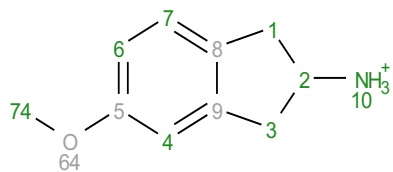
Analyte X39: MEAI
Acquisition Date 2016-12-02T17:55:29
Solvent dms
Temperature 25
Number of Scans 16
Relaxation Delay 1
Spectrometer Frequency 499.66
Spectral Width 8012.8
Nucleus 1H
Acquired Size 48077



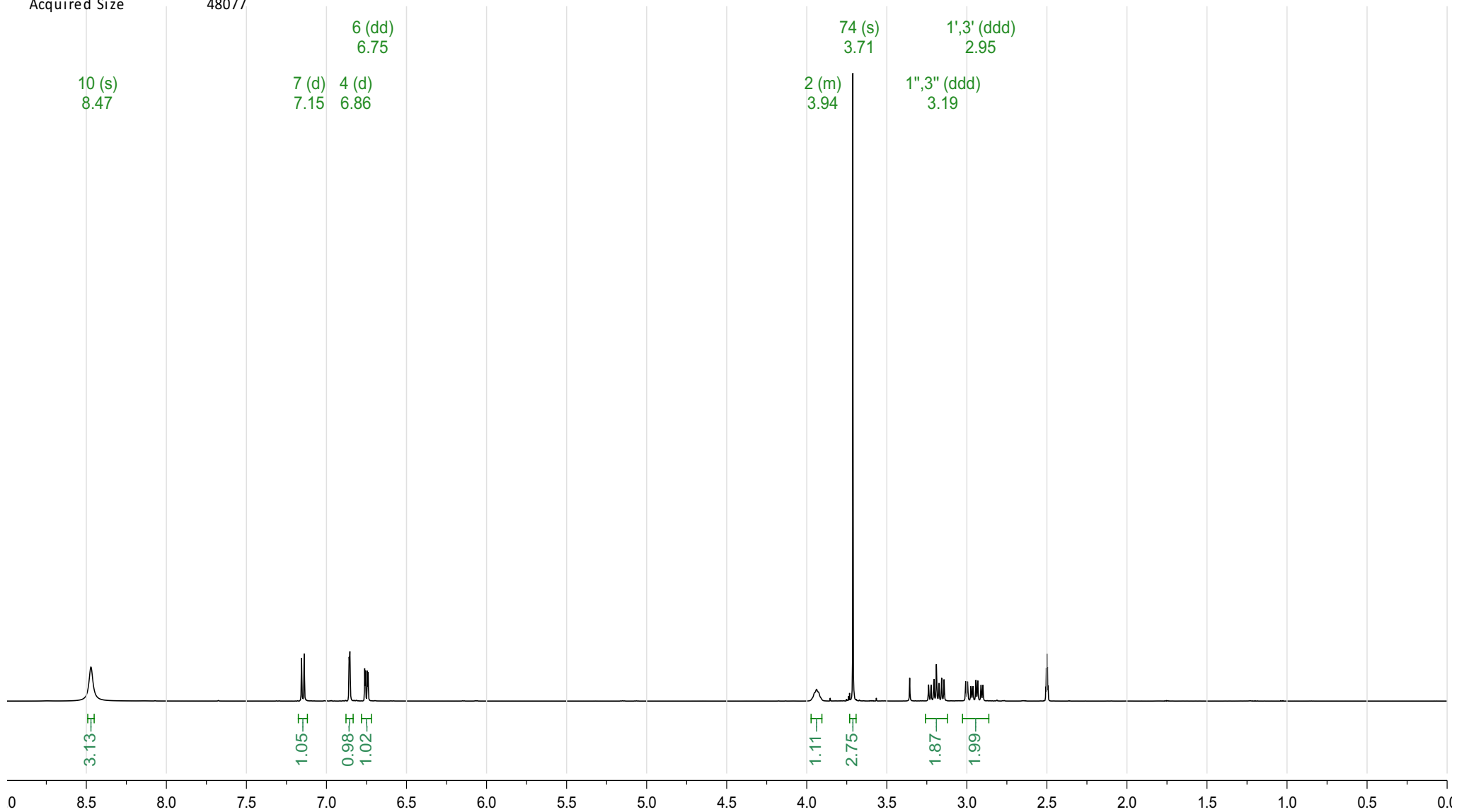
^1H NMR (500 MHz, DMSO- d_6) δ 8.47 (s, 3H), 7.15 (d, $J = 8.3$ Hz, 1H), 6.86 (d, $J = 2.3$ Hz, 1H), 6.75 (dd, $J = 8.3, 2.5$ Hz, 1H), 3.97 – 3.91 (m, 1H), 3.71 (s, 3H), 3.19 (ddd, $J = 24.2, 16.4, 7.6$ Hz, 2H), 2.95 (ddd, $J = 31.2, 16.2, 5.8$ Hz, 2H).



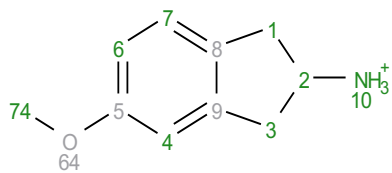
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Acquisition Date 2016-12-02T17:55:29
Solvent dms0
Temperature 25
Number of Scans 16
Relaxation Delay 1
Spectrometer Frequency 499.66
Spectral Width 8012.8
Nucleus 1H
Acquired Size 48077



^1H NMR (500 MHz, DMSO- d_6) δ 8.47 (s, 3H), 7.15 (d, J = 8.3 Hz, 1H), 6.86 (d, J = 2.3 Hz, 1H), 6.75 (dd, J = 8.3, 2.5 Hz, 1H), 3.97 – 3.91 (m, 1H), 3.71 (s, 3H), 3.19 (ddd, J = 24.2, 16.4, 7.6 Hz, 2H), 2.95 (ddd, J = 31.2, 16.2, 5.8 Hz, 2H).



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



^1H NMR (500 MHz, DMSO- d_6) δ 8.62 (s, 3H), 7.20 (dt, $J = 7.5, 1.1$ Hz, 1H), 6.82 (dt, $J = 2.0, 1.0$ Hz, 1H), 6.29 (dd, $J = 7.5, 2.0$ Hz, 1H), 4.11 (q, $J = 8.6$ Hz, 1H), 3.73 (ddd, $J = 13.0, 8.6, 1.0$ Hz, 2H), 3.72 (s, 3H), 3.52 – 3.44 (m, 2H).

