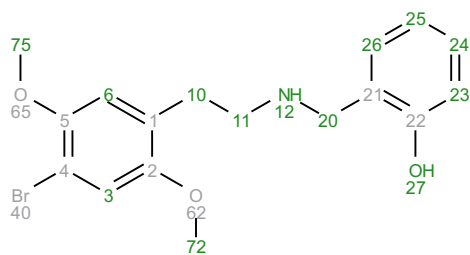
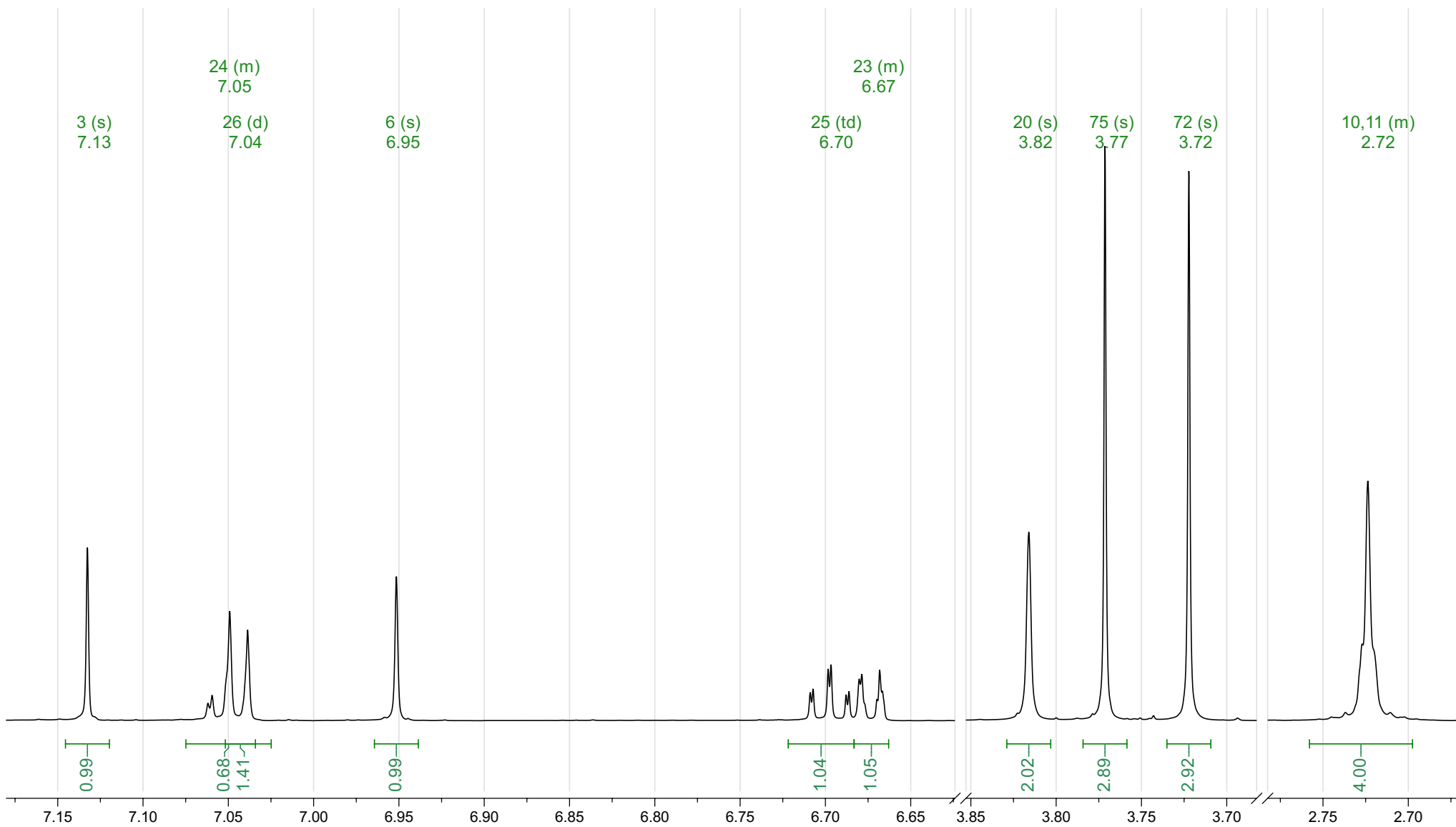


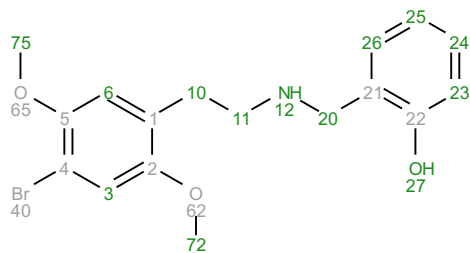
Analyte B15: 25B-NBOH
 Acquisition Date 2018-03-21T15:27:45
 Solvent dmso
 Temperature 25
 Number of Scans 64
 Relaxation Delay 1
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 71429



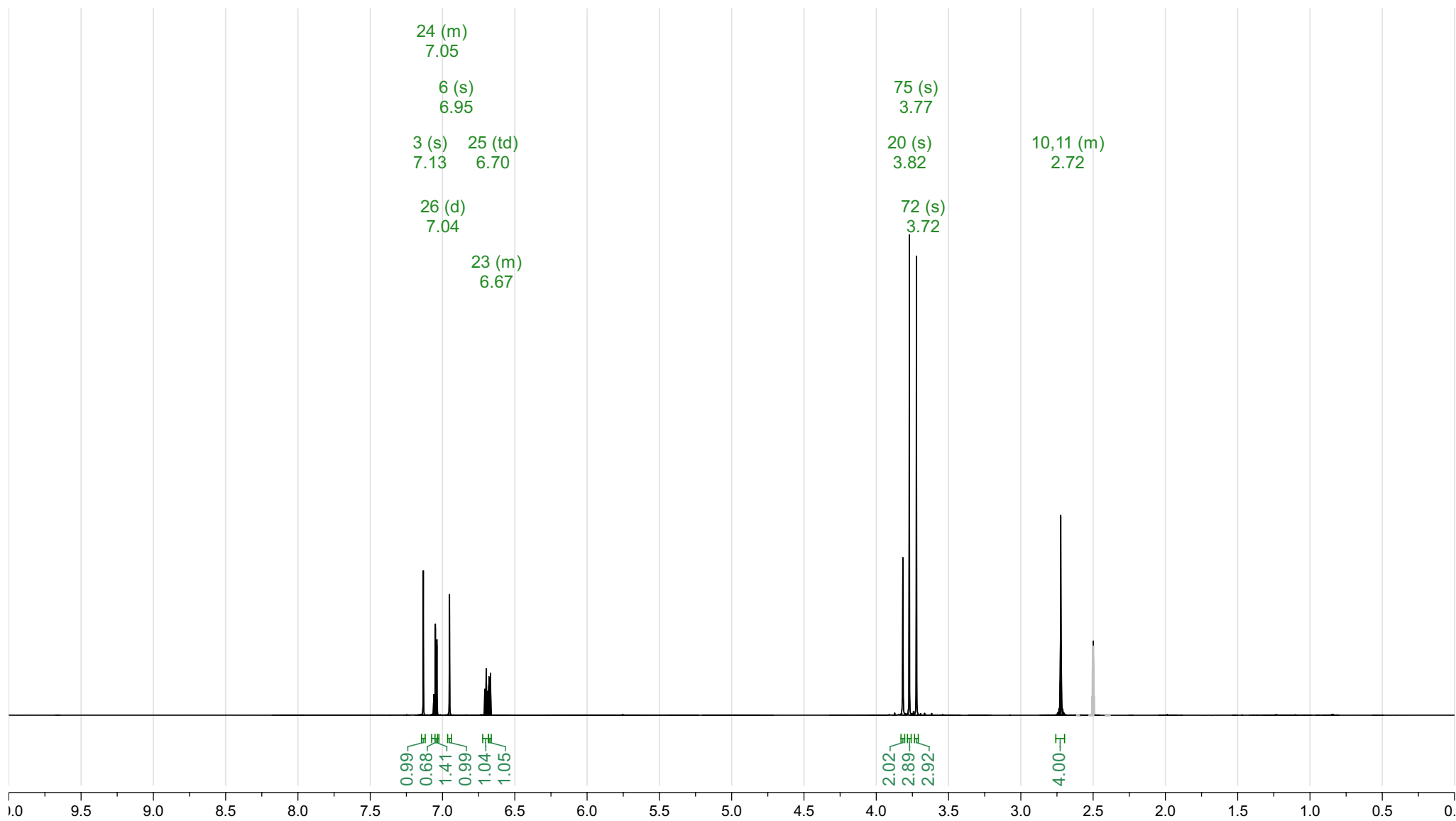
¹H NMR (700 MHz, DMSO-*d*₆) δ 7.13 (s, 1H), 7.07 – 7.02 (m, 1H), 7.04 (d, *J* = 7.3 Hz, 1H), 6.95 (s, 1H), 6.70 (td, *J* = 7.4, 1.2 Hz, 1H), 6.68 – 6.66 (m, 1H), 3.82 (s, 2H), 3.77 (s, 3H), 3.72 (s, 3H), 2.76 – 2.70 (m, 4H).



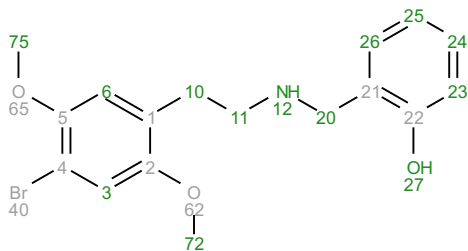
Analyte B15: 25B-NBOH
 Acquisition Date 2018-03-21T15:27:45
 Solvent dmso
 Temperature 25
 Number of Scans 64
 Relaxation Delay 1
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 71429



^1H NMR (700 MHz, DMSO- d_6) δ 7.13 (s, 1H), 7.07 – 7.02 (m, 1H), 7.04 (d, J = 7.3 Hz, 1H), 6.95 (s, 1H), 6.70 (td, J = 7.4, 1.2 Hz, 1H), 6.68 – 6.66 (m, 1H), 3.82 (s, 2H), 3.77 (s, 3H), 3.72 (s, 3H), 2.76 – 2.70 (m, 4H).



Prediction 25B-NBOH
 Origin Modgraph NMRPredict Desktop
 Solvent DMSO-d6
 Algorithm Best
 GMMX Cycles 10
 Version 20560
 Frequency 700.00
 Nucleus 1H



¹H NMR (700 MHz, DMSO-d₆) δ 9.23 (s, 1H), 7.25 (s, 1H), 7.20 (dq, *J* = 7.5, 1.1 Hz, 1H), 7.05 (td, *J* = 7.5, 1.5 Hz, 1H), 6.95 (t, *J* = 1.0 Hz, 1H), 6.92 (td, *J* = 7.5, 1.5 Hz, 1H), 6.87 (tt, *J* = 8.4, 6.3 Hz, 1H), 6.77 (dd, *J* = 7.5, 1.6 Hz, 1H), 4.10 (dd, *J* = 8.5, 1.0 Hz, 2H), 3.86 (s, 3H), 3.77 (s, 3H), 3.24 (q, *J* = 6.9 Hz, 2H), 2.99 (td, *J* = 7.2, 1.2 Hz, 2H).

