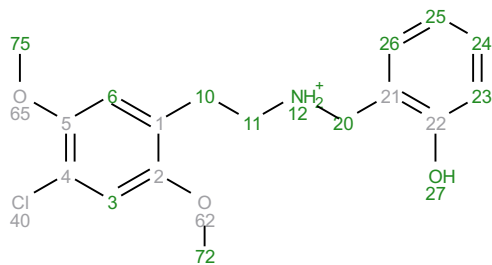
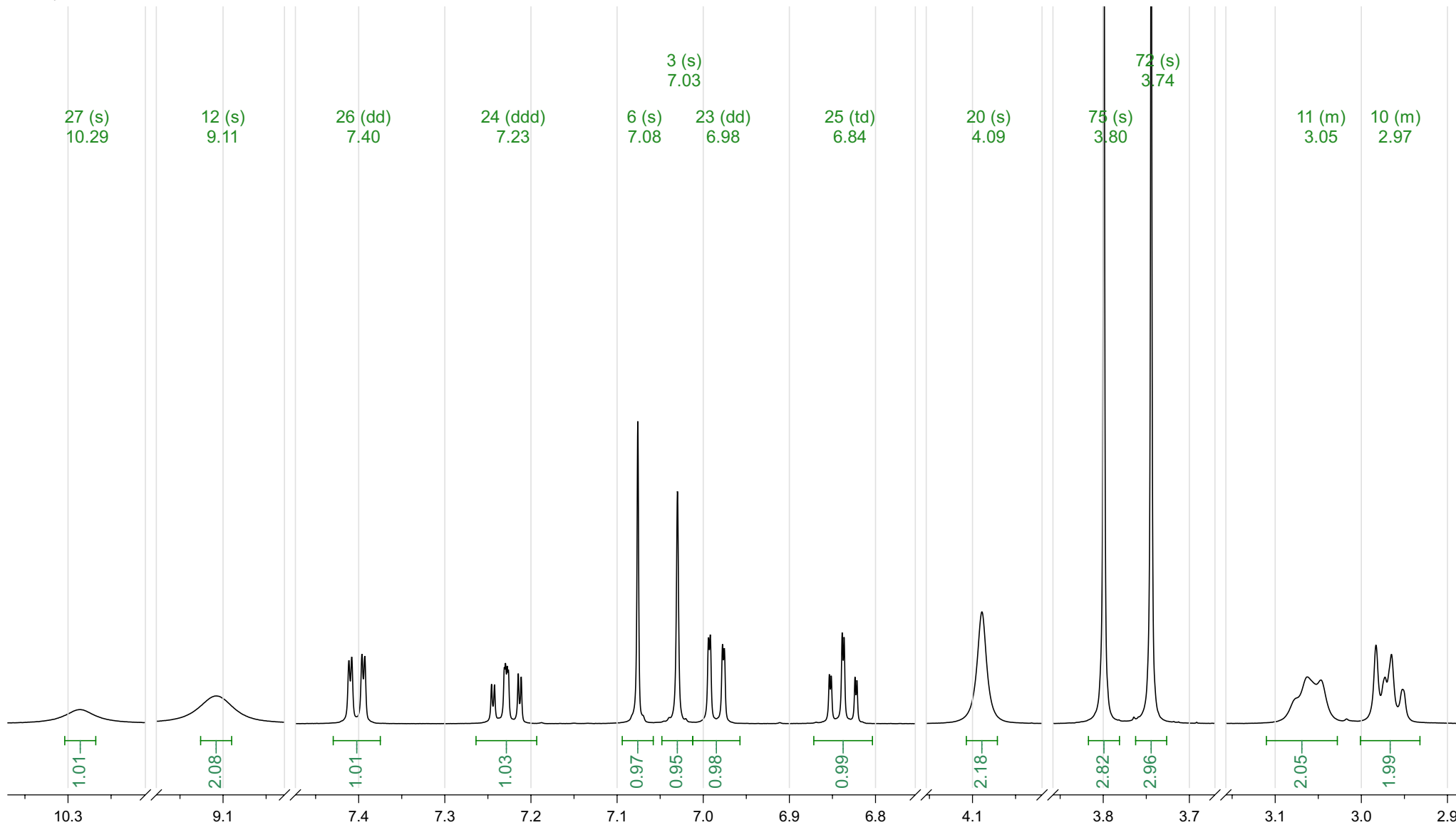


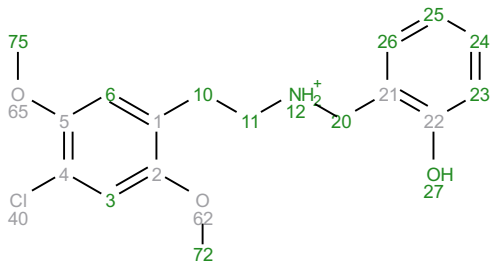
Analyte B14: 25C-NBOH H+
 Acquisition Date 2018-02-21T14:02:23
 Solvent dms0
 Temperature 25
 Number of Scans 16
 Relaxation Delay 10
 Spectrometer Frequency 499.88
 Spectral Width 8012.8
 Nucleus 1H
 Acquired Size 36058



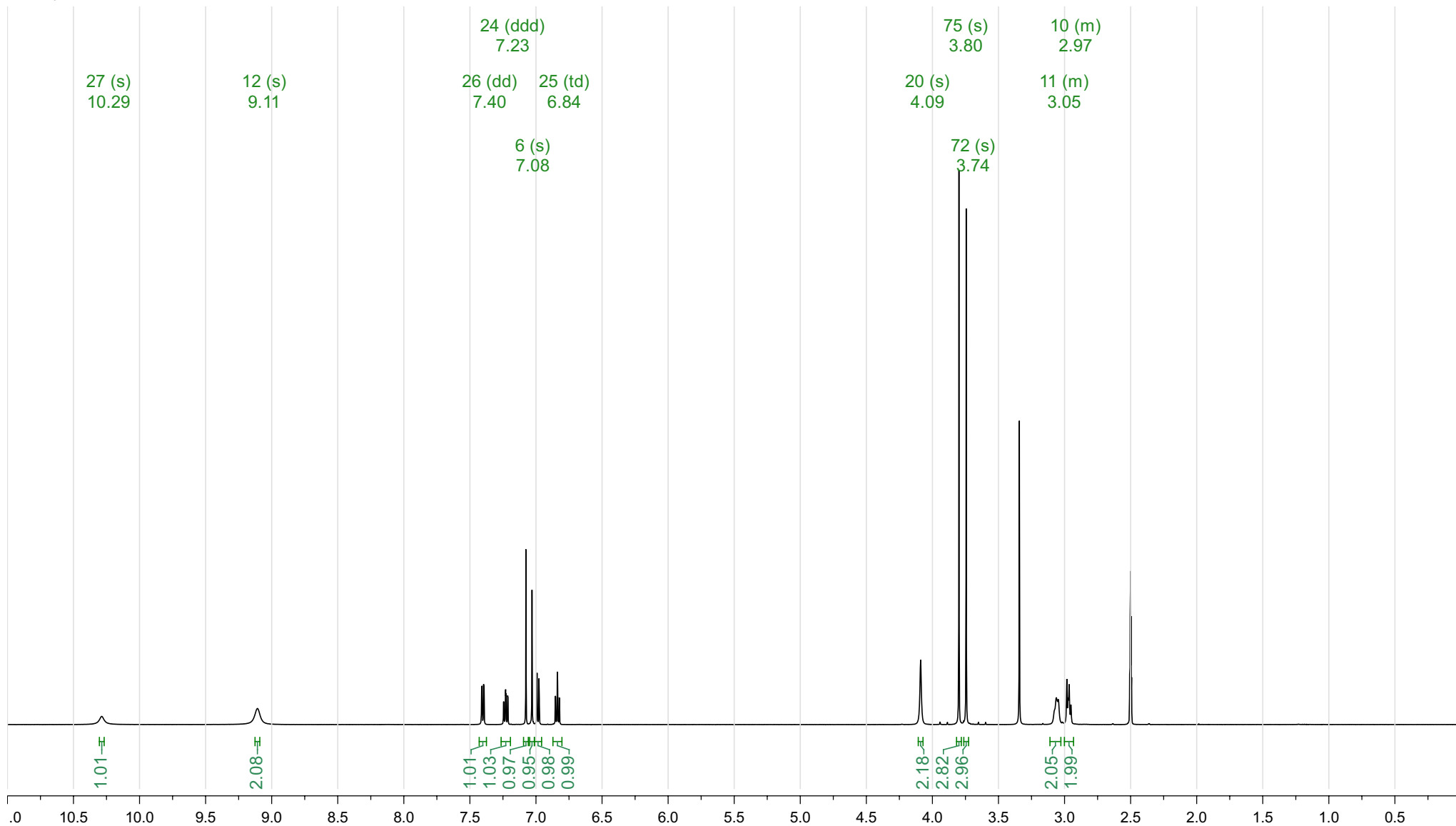
¹H NMR (500 MHz, DMSO-*d*₆) δ 10.29 (s, 1H), 9.11 (s, 2H), 7.40 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.23 (ddd, *J* = 8.2, 7.3, 1.7 Hz, 1H), 7.08 (s, 1H), 7.03 (s, 1H), 6.98 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.84 (td, *J* = 7.4, 1.2 Hz, 1H), 4.09 (s, 2H), 3.80 (s, 3H), 3.74 (s, 3H), 3.11 – 3.03 (m, 2H), 3.00 – 2.93 (m, 2H).



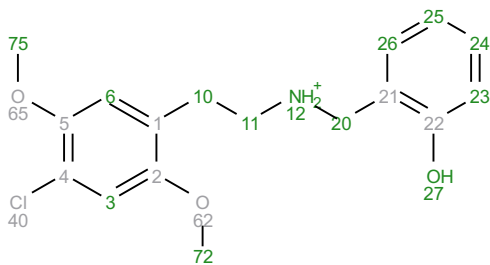
Analyte B14: 25C-NBOH H+
 Acquisition Date 2018-02-21T14:02:23
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 10
 Spectrometer Frequency 499.88
 Spectral Width 8012.8
 Nucleus 1H
 Acquired Size 36058



¹H NMR (500 MHz, DMSO-*d*₆) δ 10.29 (s, 1H), 9.11 (s, 2H), 7.40 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.23 (ddd, *J* = 8.2, 7.3, 1.7 Hz, 1H), 7.08 (s, 1H), 7.03 (s, 1H), 6.98 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.84 (td, *J* = 7.4, 1.2 Hz, 1H), 4.09 (s, 2H), 3.80 (s, 3H), 3.74 (s, 3H), 3.11 – 3.03 (m, 2H), 3.00 – 2.93 (m, 2H).



Prediction 25C-NBOH H+
 Origin Modgraph NMRPredict Desktop
 Solvent DMSO-d6
 Algorithm Best
 GMMX Cycles 5
 Version 20560
 Frequency 500.00
 Nucleus 1H



¹H NMR (500 MHz, DMSO-d₆) δ 9.68 (s, 1H), 7.43 (dq, *J* = 8.1, 1.2 Hz, 1H), 7.20 (tt, *J* = 8.5, 6.5 Hz, 2H), 7.07 (td, *J* = 8.2, 1.7 Hz, 1H), 6.89 (d, *J* = 1.1 Hz, 1H), 6.85 – 6.80 (m, 2H), 6.77 (dd, *J* = 8.3, 1.4 Hz, 1H), 4.11 (td, *J* = 8.5, 1.1 Hz, 2H), 3.87 (s, 3H), 3.84 (s, 3H), 3.37 – 3.29 (m, 2H), 3.25 (tt, *J* = 5.7, 0.9 Hz, 2H).

