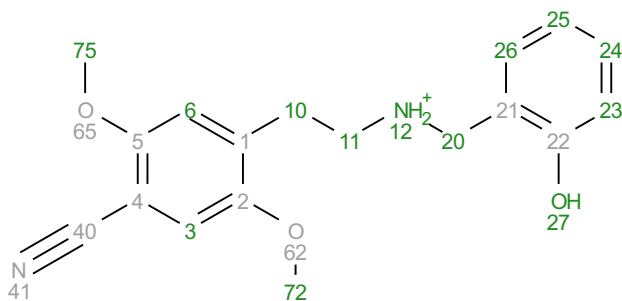
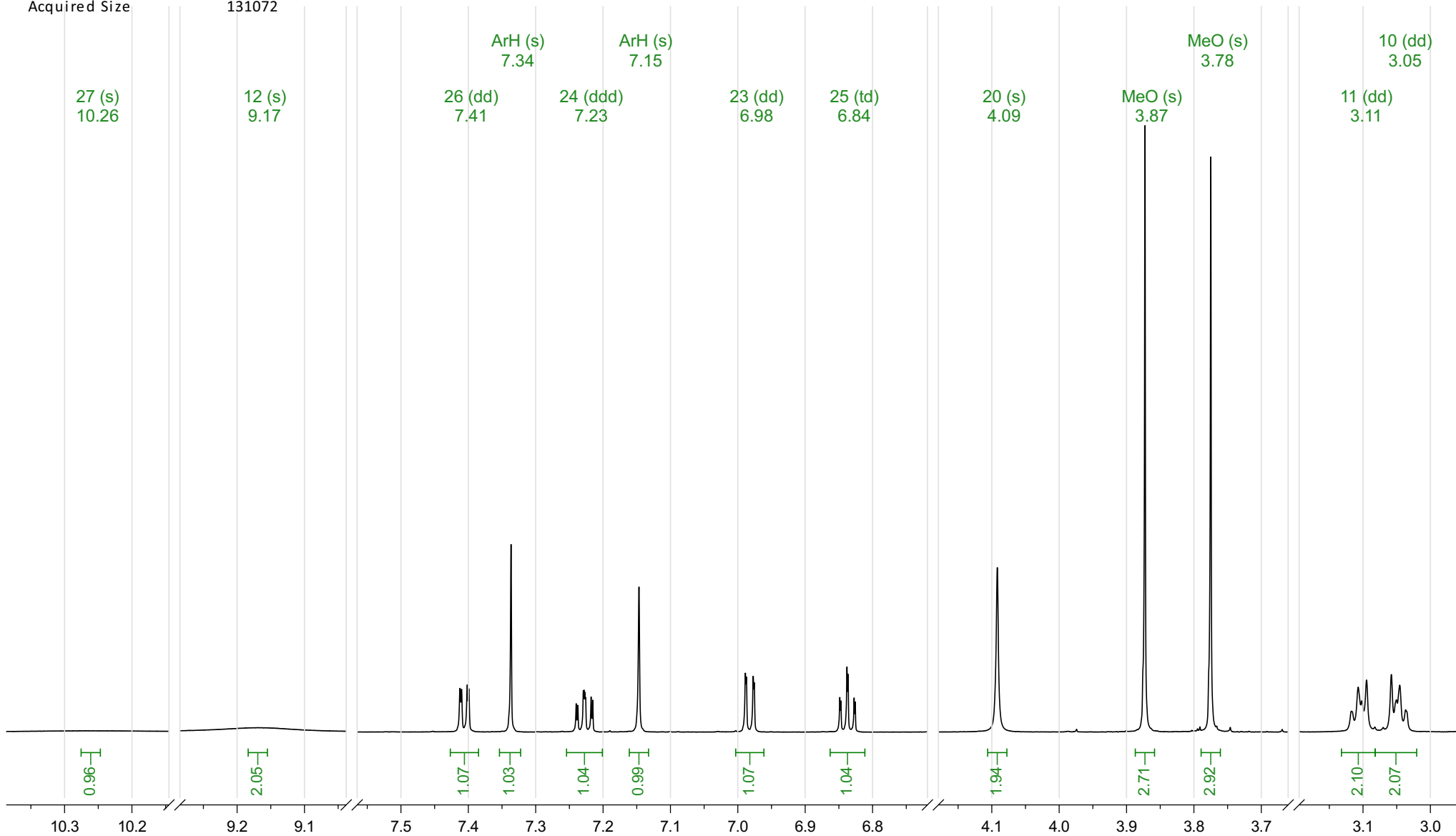


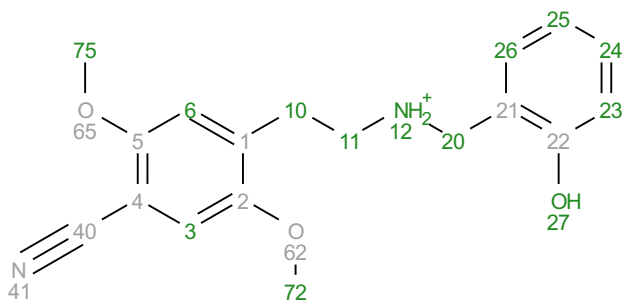
Analyte B13: 25CN-NBOH H+
 Acquisition Date 2016-06-28T15:50:58
 Solvent dms0
 Temperature 27
 Number of Scans 4
 Relaxation Delay 10
 Spectrometer Frequency 699.81
 Spectral Width 14044.9
 Nucleus 1H
 Acquired Size 131072



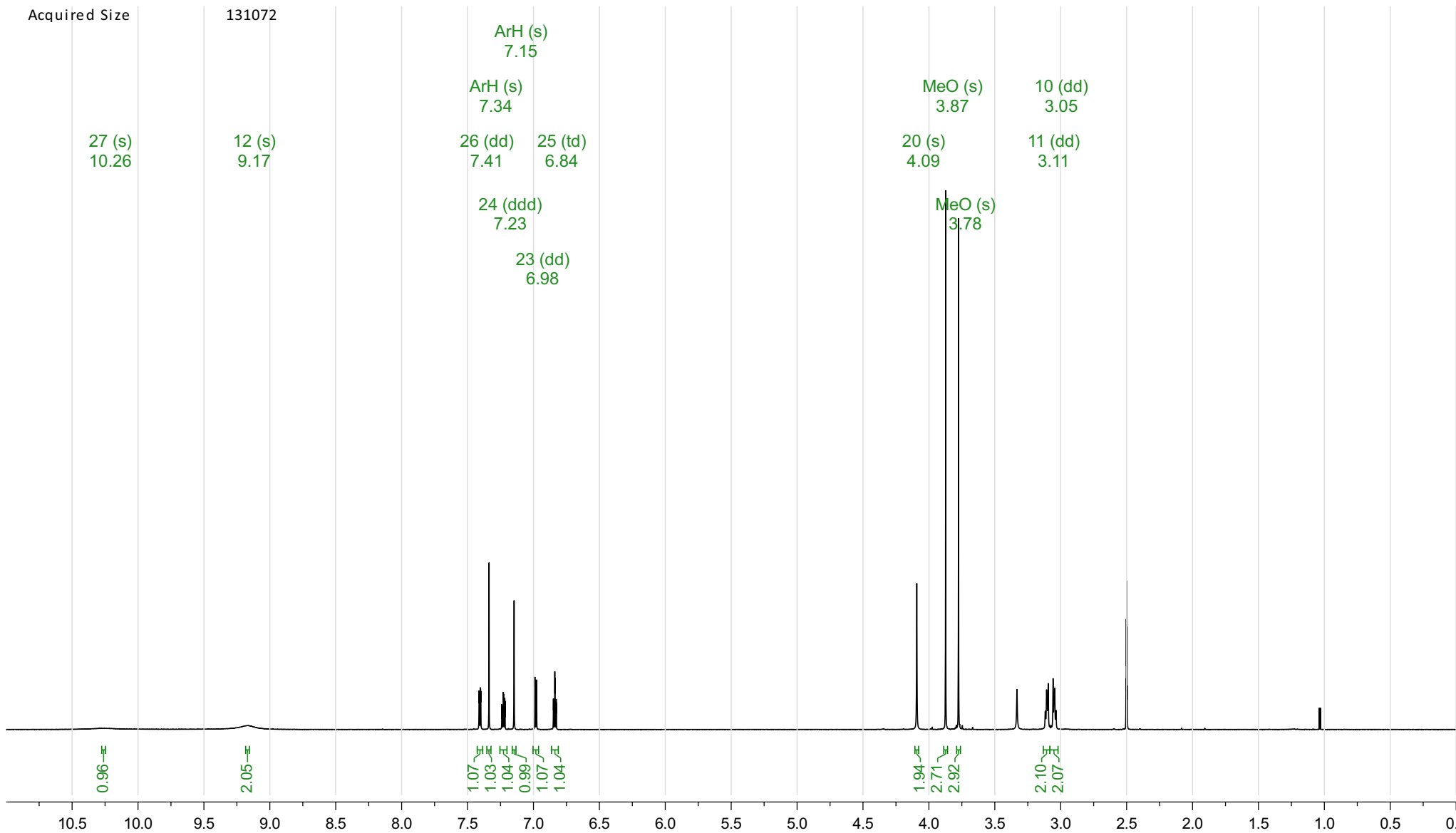
¹H NMR (700 MHz, DMSO-*d*₆) δ 10.26 (s, 1H), 9.17 (s, 2H), 7.41 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.34 (s, 1H), 7.23 (ddd, *J* = 8.1, 7.3, 1.7 Hz, 1H), 7.15 (s, 1H), 6.98 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.84 (td, *J* = 7.4, 1.2 Hz, 1H), 4.09 (s, 2H), 3.87 (s, 3H), 3.78 (s, 3H), 3.11 (dd, *J* = 10.0, 6.1 Hz, 2H), 3.05 (dd, *J* = 9.0, 5.7 Hz, 2H).



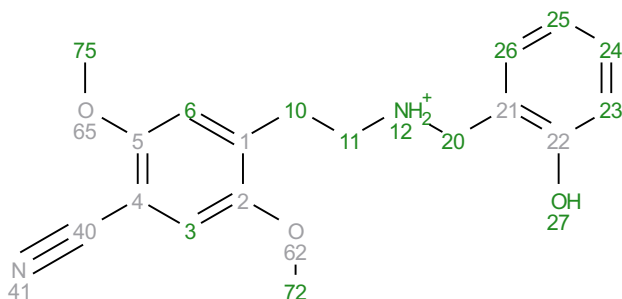
Analyte B13: 25CN-NBOH H+
 Acquisition Date 2016-06-28T15:50:58
 Solvent dms
 Temperature 27
 Number of Scans 4
 Relaxation Delay 10
 Spectrometer Frequency 699.81
 Spectral Width 14044.9
 Nucleus 1H
 Acquired Size 131072



¹H NMR (700 MHz, DMSO-*d*₆) δ 10.26 (s, 1H), 9.17 (s, 2H), 7.41 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.34 (s, 1H), 7.23 (ddd, *J* = 8.1, 7.3, 1.7 Hz, 1H), 7.15 (s, 1H), 6.98 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.84 (td, *J* = 7.4, 1.2 Hz, 1H), 4.09 (s, 2H), 3.87 (s, 3H), 3.78 (s, 3H), 3.11 (dd, *J* = 10.0, 6.1 Hz, 2H), 3.05 (dd, *J* = 9.0, 5.7 Hz, 2H).



Prediction 25CN-NBOH H+
 Origin Modgraph NMRPredict Desktop
 Solvent DMSO-d6
 Algorithm Best
 GMMX Cycles 50
 Version 14011
 Frequency 700.00
 Nucleus 1H



¹H NMR (700 MHz, DMSO-d₆) δ 9.68 (s, 1H), 7.50 (s, 1H), 7.20 (s, 2H), 7.04 (t, *J* = 1.0 Hz, 1H), 7.04 – 6.96 (m, 2H), 6.81 – 6.73 (m, 2H), 3.83 (d, *J* = 0.9 Hz, 2H), 3.80 (s, 3H), 3.74 (s, 3H), 3.33 (t, *J* = 7.1 Hz, 2H), 3.13 (td, *J* = 7.0, 1.0 Hz, 2H).

