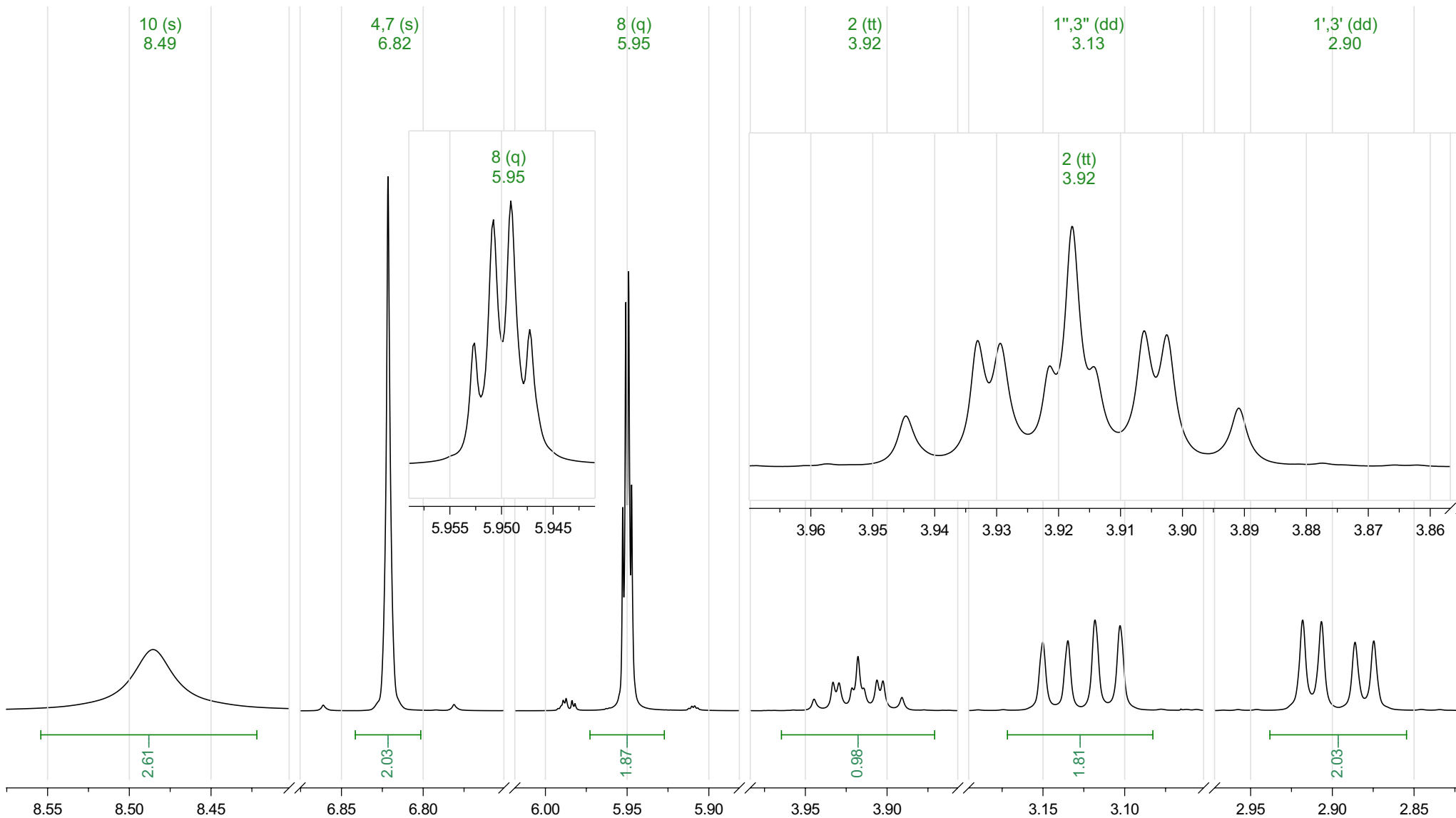
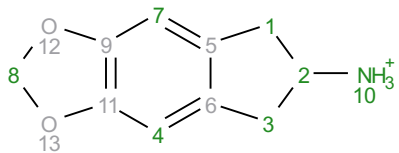


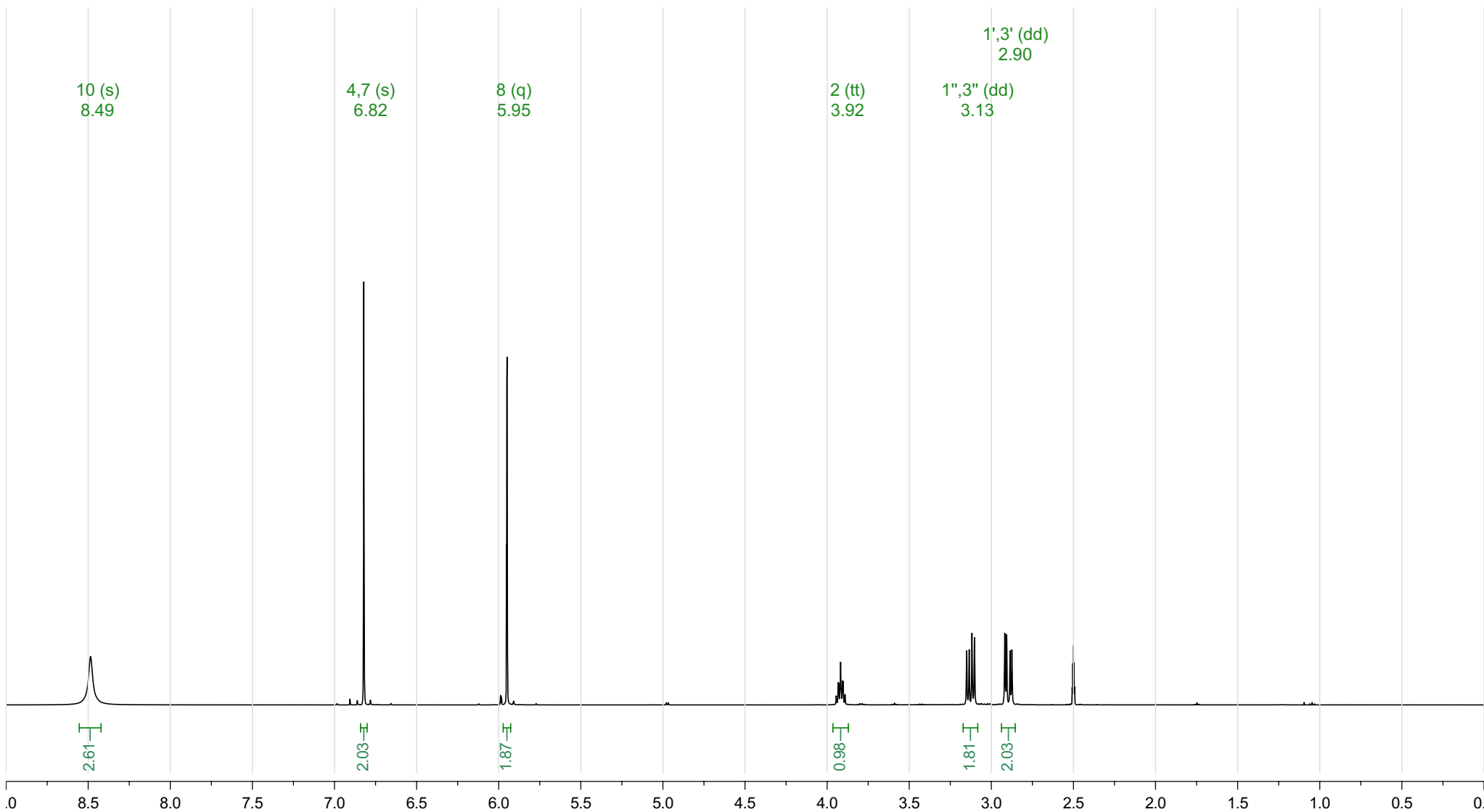
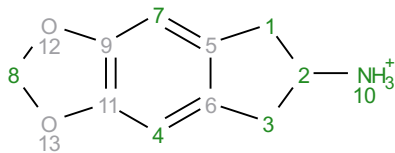
Analyte SB4a: MDAI H+
 Acquisition Date 2017-06-08T12:33:32
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536

¹H NMR (500 MHz, DMSO-d₆) δ 8.49 (s, 3H), 6.82 (s, 2H), 5.95 (q, J = 0.9 Hz, 2H), 3.92 (tt, J = 7.7, 5.8 Hz, 1H), 3.13 (dd, J = 15.8, 7.7 Hz, 2H), 2.90 (dd, J = 16.1, 5.7 Hz, 2H).



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Acquisition Date 2017-06-08T12:33:32
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Spectrometer Frequency 499.67
Spectral Width 10000.0
Nucleus 1H
Acquired Size 65536

¹H NMR (500 MHz, DMSO-*d*₆) δ 8.49 (s, 3H), 6.82 (s, 2H), 5.95 (q, *J* = 0.9 Hz, 2H), 3.92 (tt, *J* = 7.7, 5.8 Hz, 1H), 3.13 (dd, *J* = 15.8, 7.7 Hz, 2H), 2.90 (dd, *J* = 16.1, 5.7 Hz, 2H).



Prediction MDAI H+
Origin Modgraph NMRPredict Desktop
Solvent DMSO-d6
Algorithm Best
GMMX Cycles 5
Version 15465
Frequency 500.00
Nucleus 1H

^1H NMR (500 MHz, DMSO- d_6) δ 8.62 (s, 3H), 6.82 (t, $J = 1.0$ Hz, 2H), 6.03 (s, 2H), 4.11 (q, $J = 8.6$ Hz, 1H), 3.73 (ddd, $J = 13.0, 8.5, 1.0$ Hz, 2H), 3.52 – 3.45 (m, 2H).

