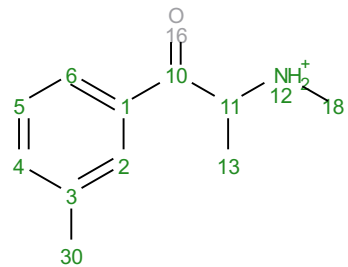
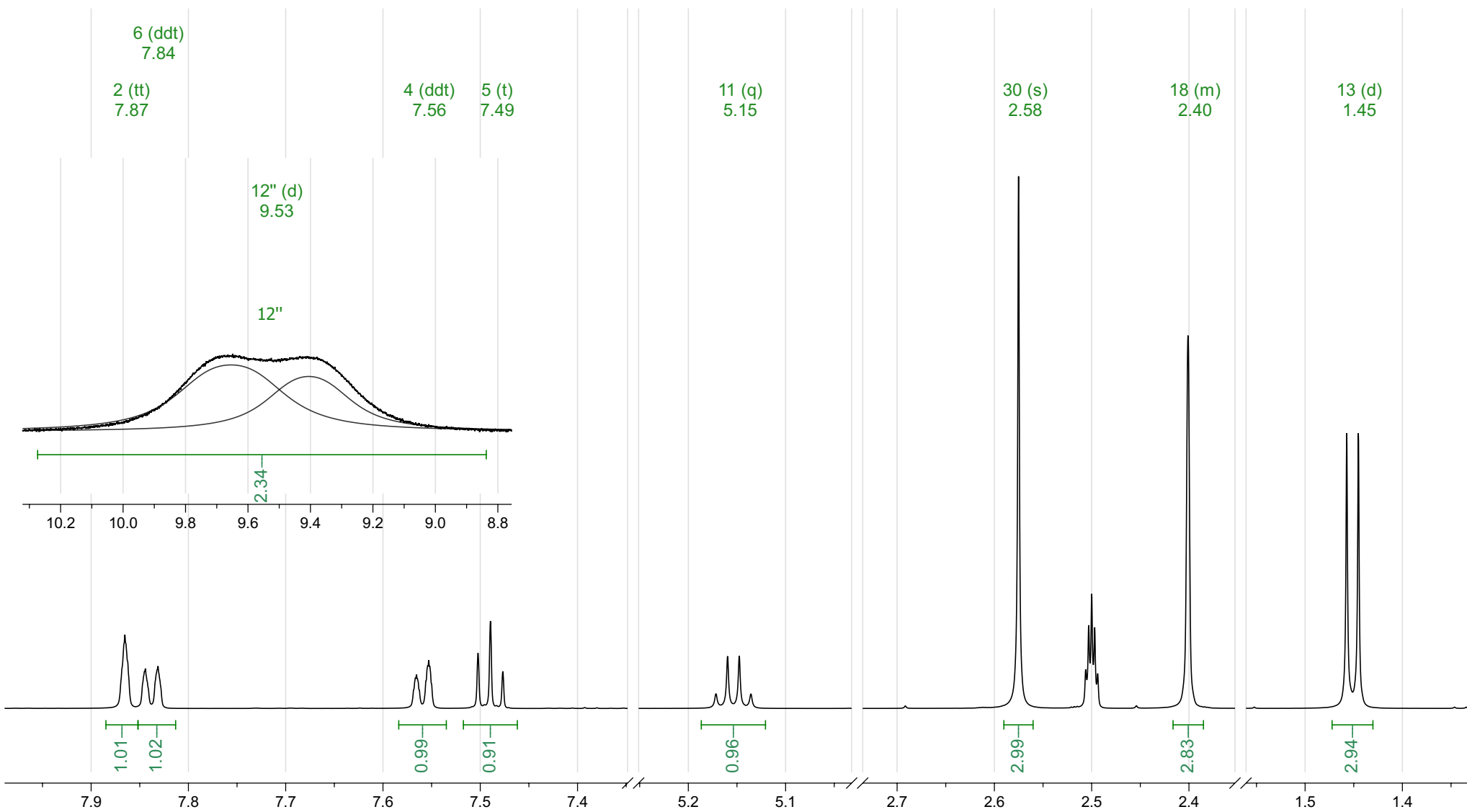


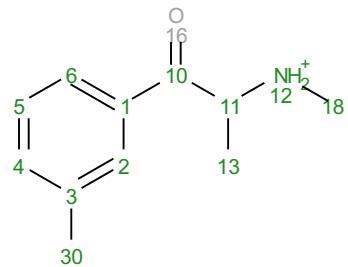
Analyte X59: 3-MMC H+
 Acquisition Date 2018-11-02T09:53:40
 Solvent dms0
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Experiment 1D
 Spectrometer Frequency 599.82
 Spectral Width 9615.4
 Nucleus 1H
 Acquired Size 43269



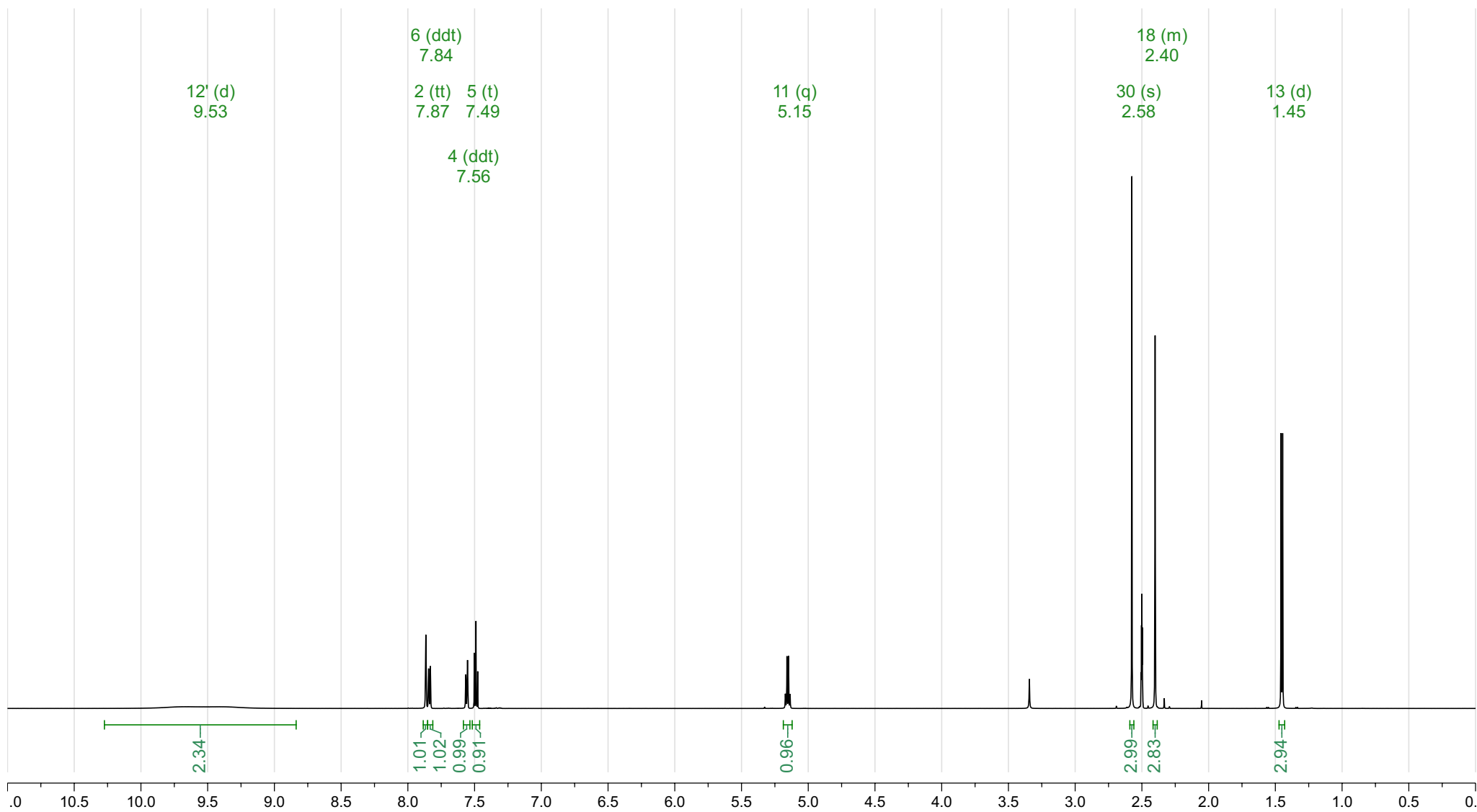
^1H NMR (600 MHz, $\text{DMSO-}d_6$) δ 9.53 (d, $J = 149.4$ Hz, 2H), 7.87 (tt, $J = 1.6, 0.8$ Hz, 1H), 7.84 (ddt, $J = 7.8, 1.8, 0.9$ Hz, 1H), 7.56 (ddt, $J = 7.5, 1.9, 1.0$ Hz, 1H), 7.49 (t, $J = 7.6$ Hz, 1H), 5.15 (q, $J = 7.2$ Hz, 3H), 2.58 (s, 3H), 2.42 – 2.39 (m, 3H), 1.45 (d, $J = 7.2$ Hz, 3H).



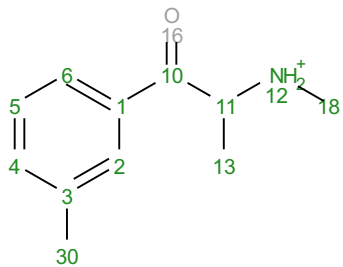
Analyte X59: 3-MMC H⁺
 Acquisition Date 2018-11-02T09:53:40
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Experiment 1D
 Spectrometer Frequency 599.82
 Spectral Width 9615.4
 Nucleus 1H
 Acquired Size 43269



¹H NMR (600 MHz, DMSO-*d*₆) δ 9.53 (d, *J* = 149.4 Hz, 2H), 7.87 (tt, *J* = 1.6, 0.8 Hz, 1H), 7.84 (ddt, *J* = 7.8, 1.8, 0.9 Hz, 1H), 7.56 (ddt, *J* = 7.5, 1.9, 1.0 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 5.15 (q, *J* = 7.2 Hz, 1H), 2.58 (s, 3H), 2.42 – 2.39 (m, 3H), 1.45 (d, *J* = 7.2 Hz, 3H).



Prediction 3-MMCH⁺
Origin Mnova Best
Solvent DMSO-d₆
Version 1.0.0
Frequency 700.00
Nucleus ¹H



¹H NMR (700 MHz, DMSO-d₆) δ 7.86 (dt, *J* = 7.8, 1.6 Hz, 1H), 7.75 – 7.71 (m, 1H), 7.71 – 7.69 (m, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.33 – 7.29 (m, 1H), 7.31 – 7.28 (m, 1H), 5.02 – 4.94 (m, 1H), 2.44 (td, *J* = 3.6, 1.5 Hz, 3H), 2.34 (s, 3H), 1.41 (d, *J* = 6.9 Hz, 3H).

