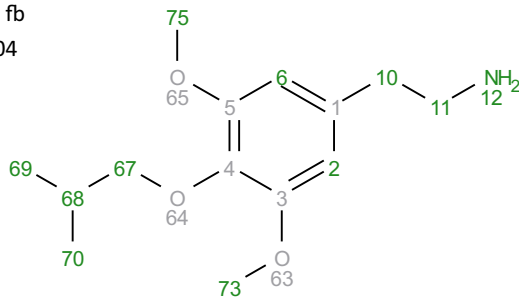
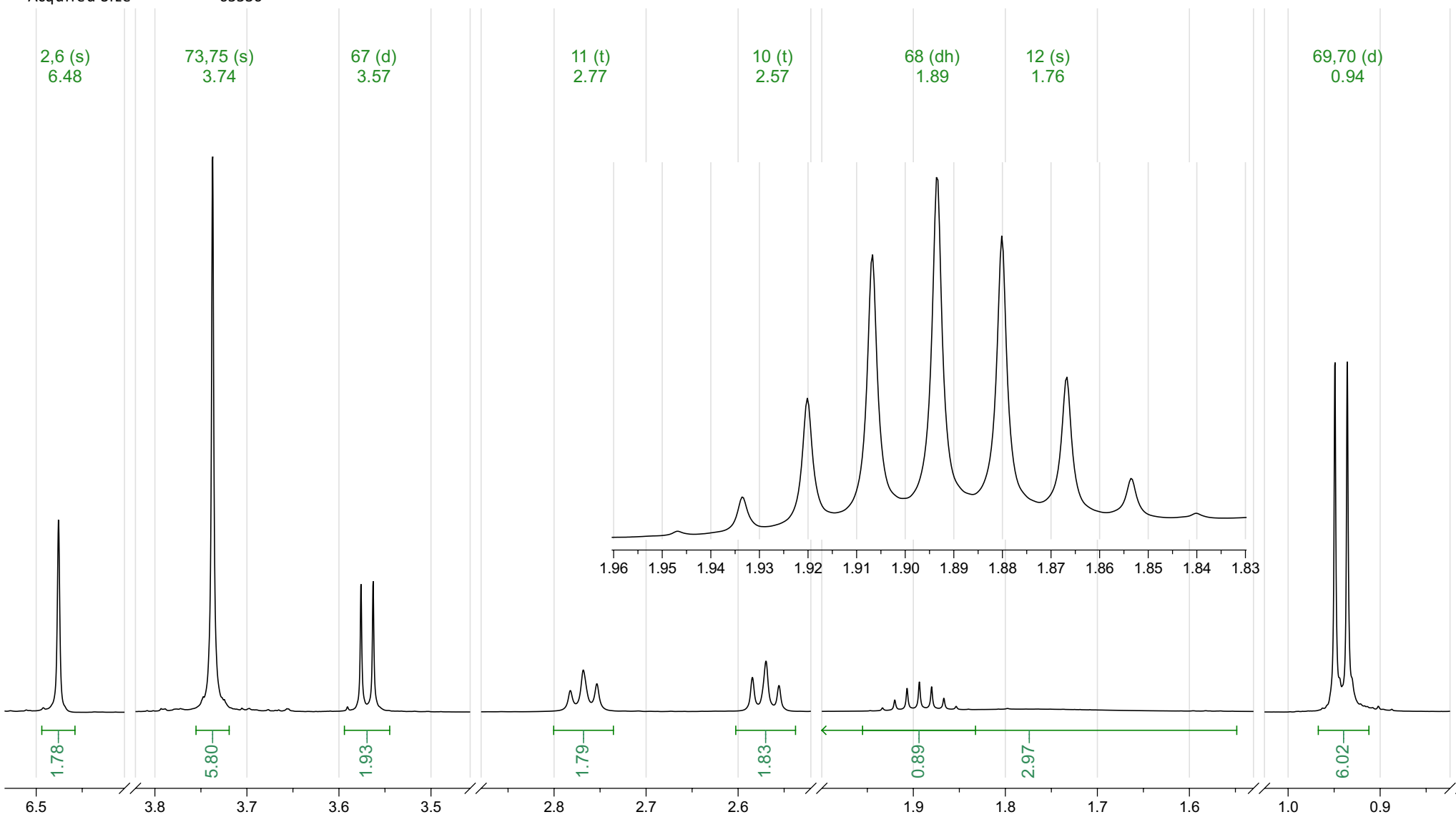


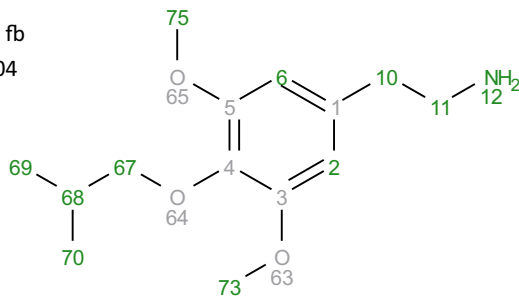
Analyte P24: Isobuscaline fb
 Acquisition Date 2019-01-08T13:08:04
 Solvent dmso
 Temperature 25
 Number of Scans 16
 Relaxation Delay 5
 Experiment 1D
 Spectrometer Frequency 499.67
 Spectral Width 10000.0
 Nucleus 1H
 Acquired Size 65536



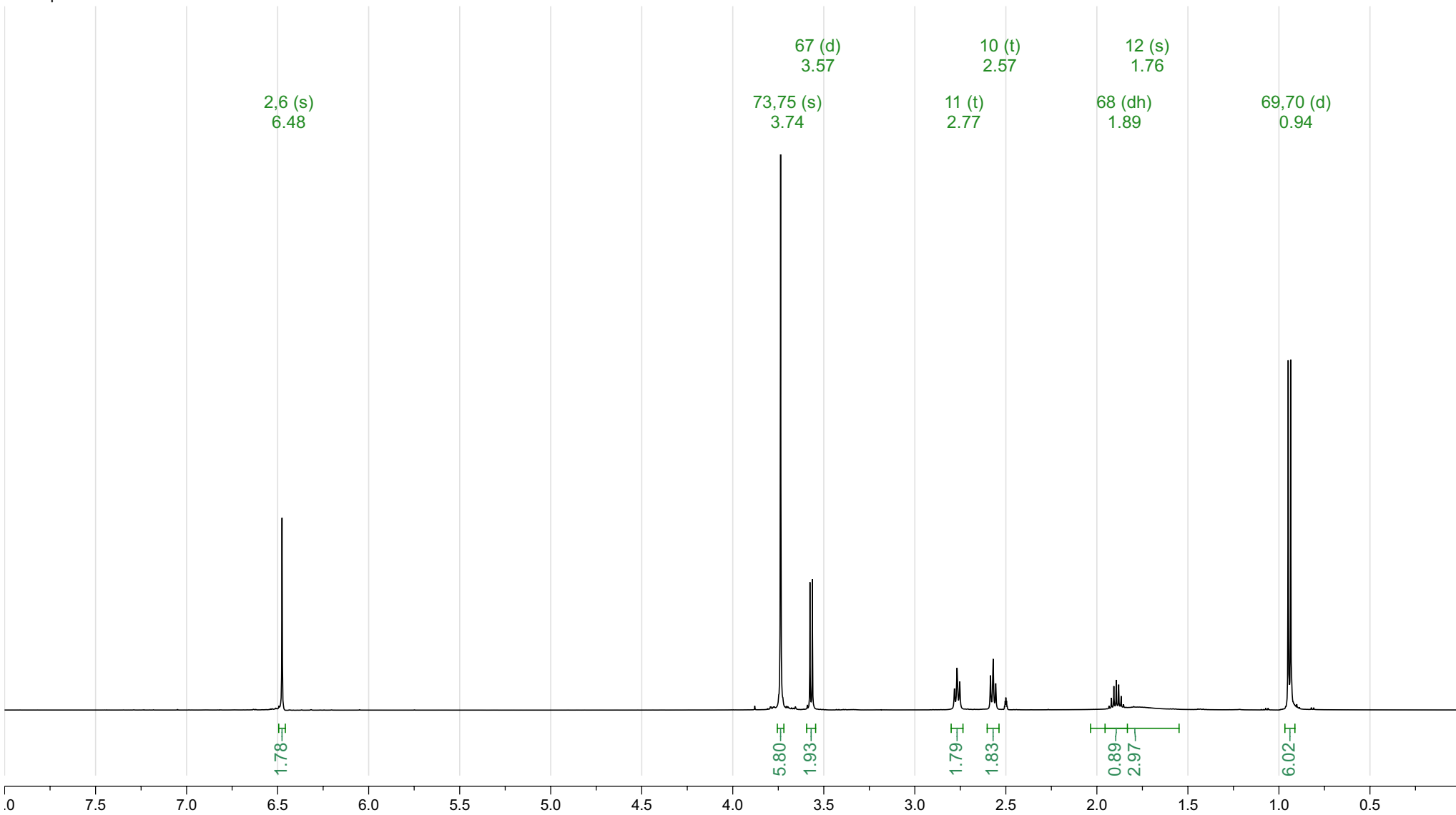
^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 6.48 (s, 2H), 3.74 (s, 6H), 3.57 (d, $J = 6.6$ Hz, 2H), 2.77 (t, $J = 7.2$ Hz, 2H), 2.57 (t, $J = 7.2$ Hz, 2H), 1.89 (dh, $J = 13.3, 6.7$ Hz, 1H), 1.76 (s, 2H), 0.94 (d, $J = 6.7$ Hz, 6H).



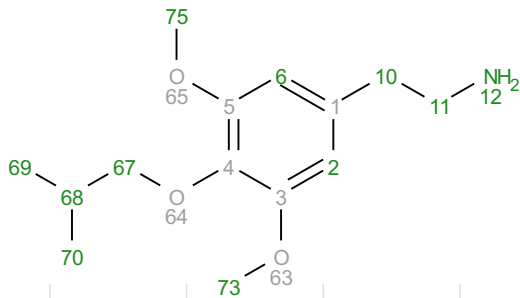
Analyte P24: Isobuscaline fb
Acquisition Date 2019-01-08T13:08:04
Solvent dmso
Temperature 25
Number of Scans 16
Relaxation Delay 5
Experiment 1D
Spectrometer Frequency 499.67
Spectral Width 10000.0
Nucleus 1H
Acquired Size 65536



¹H NMR (500 MHz, DMSO-*d*₆) δ 6.48 (s, 2H), 3.74 (s, 6H), 3.57 (d, *J* = 6.6 Hz, 2H), 2.77 (t, *J* = 7.2 Hz, 2H), 2.57 (t, *J* = 7.2 Hz, 2H), 1.89 (dh, *J* = 13.3, 6.7 Hz, 1H), 1.76 (s, 2H), 0.94 (d, *J* = 6.7 Hz, 6H).



Prediction Isobuscaline
Origin Mnova Best
Solvent DMSO-d6
Version 1.0.0
Frequency 500.00
Nucleus 1H



^1H NMR (500 MHz, DMSO- d_6) δ 6.61 (t, $J = 1.1$ Hz, 2H), 3.87 (s, 6H), 3.86 (d, $J = 6.9$ Hz, 2H), 3.35 – 3.29 (m, 2H), 3.17 (dq, $J = 7.5, 6.9$ Hz, 2H), 2.99 – 2.92 (m, 2H), 2.04 (dh, $J = 13.8, 6.9$ Hz, 1H), 1.03 (d, $J = 6.7$ Hz, 6H).

