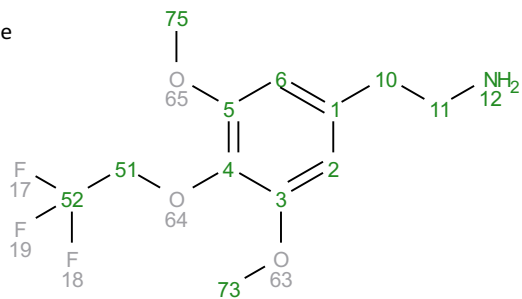
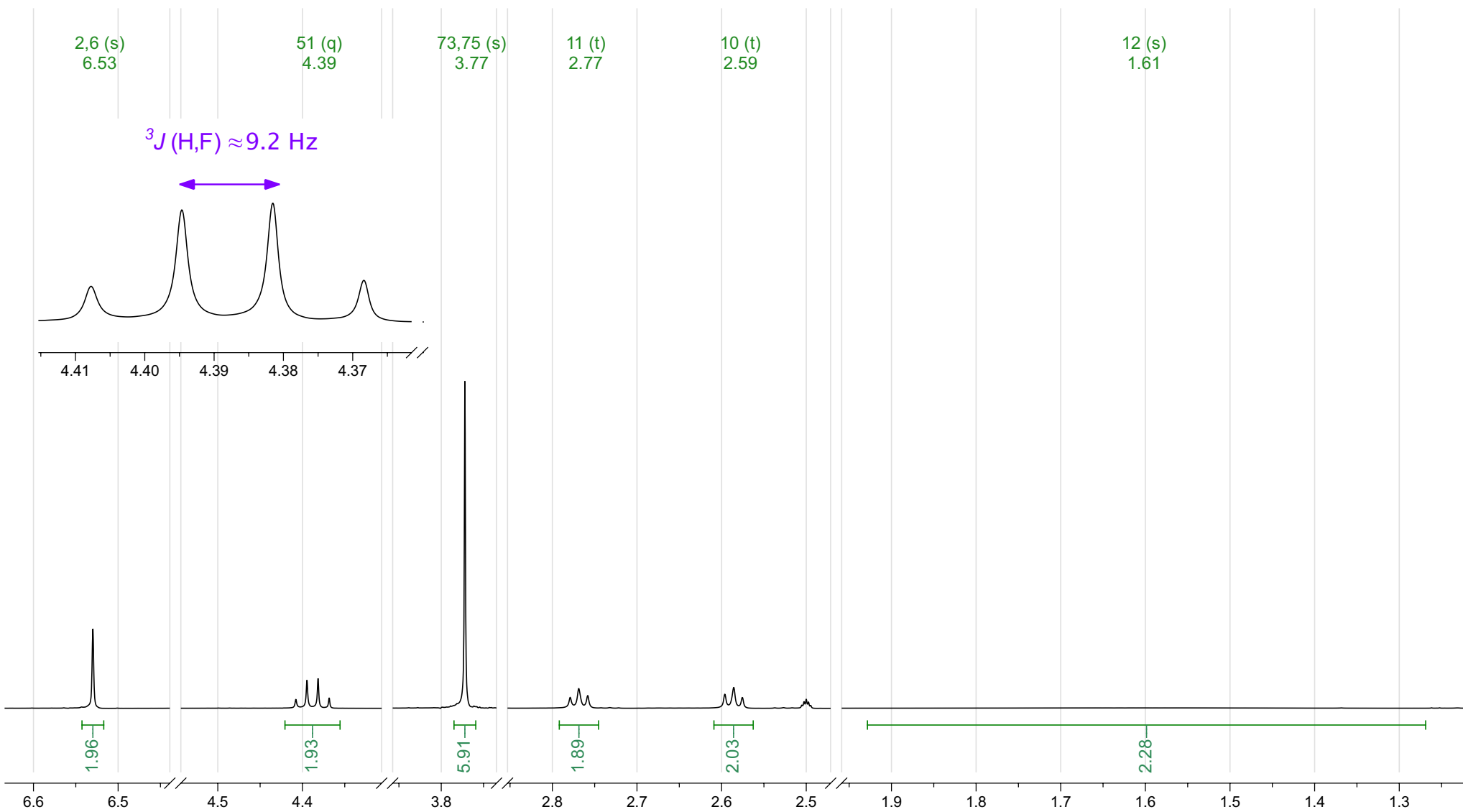


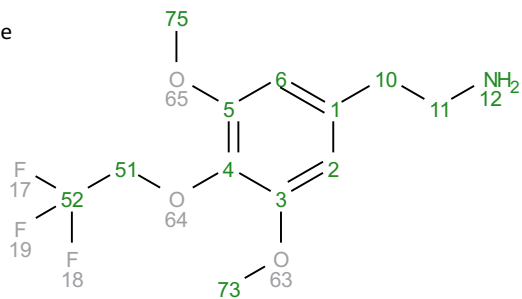
Analyte P23: Trifluoroescaline
 Acquisition Date 2018-08-31T18:10:51
 Solvent dms0
 Temperature 25
 Number of Scans 16
 Relaxation Delay 1
 Experiment 1D
 Spectrometer Frequency 699.81
 Spectral Width 11160.7
 Nucleus 1H
 Acquired Size 50223



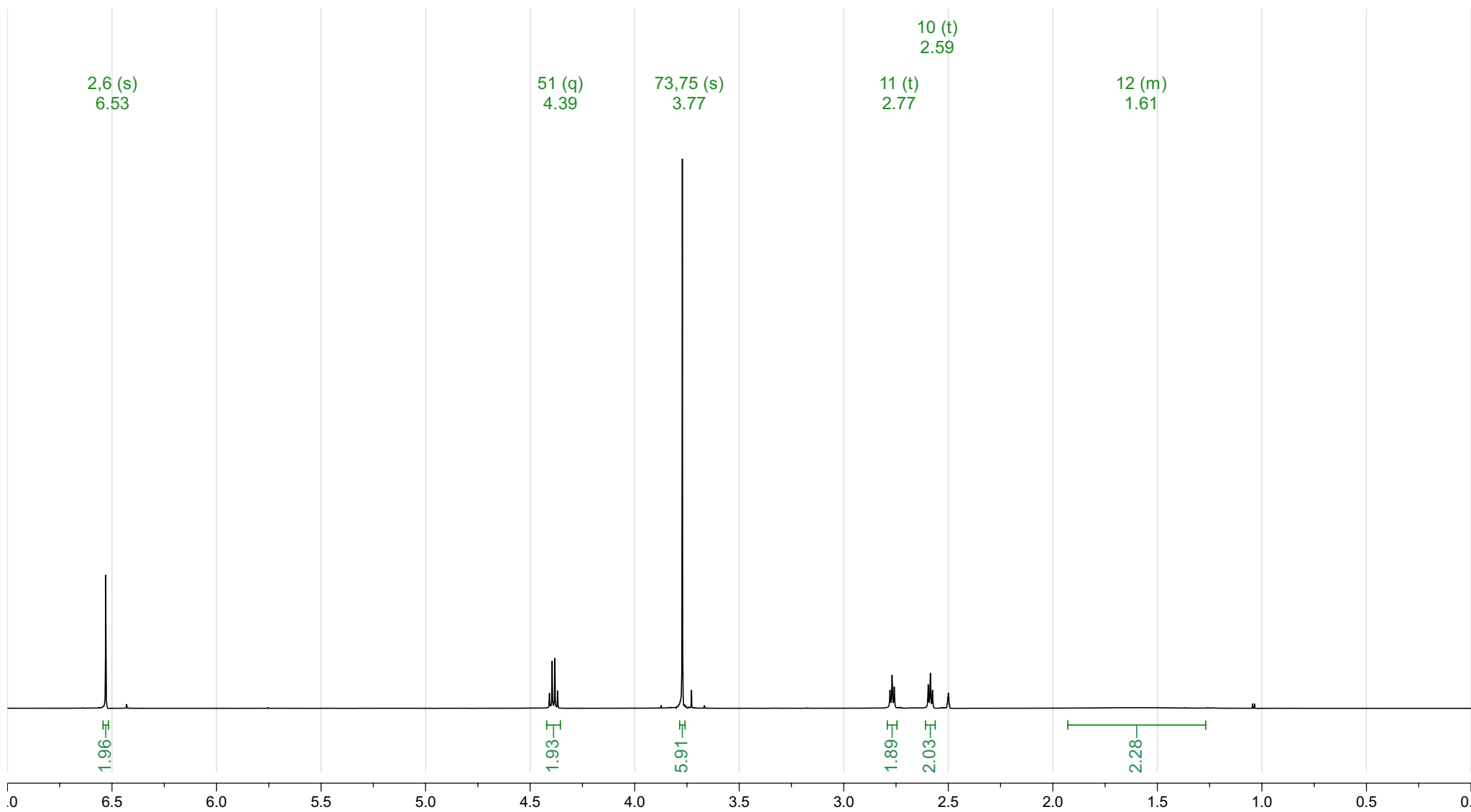
¹H NMR (700 MHz, DMSO-*d*₆) δ 6.53 (s, 2H), 4.39 (q, *J* = 9.2 Hz, 2H), 3.77 (s, 6H), 2.77 (t, *J* = 7.2 Hz, 2H), 2.59 (t, *J* = 7.2 Hz, 2H), 1.61 (s, 2H).



Analyte P23: Trifluoroescaline
Acquisition Date 2018-08-31T18:10:51
Solvent dmso
Temperature 25
Number of Scans 16
Relaxation Delay 1
Experiment 1D
Spectrometer Frequency 699.81
Spectral Width 11160.7
Nucleus 1H
Acquired Size 50223



^1H NMR (700 MHz, $\text{DMSO-}d_6$) δ 6.53 (s, 2H), 4.39 (q, $J = 9.2$ Hz, 2H), 3.77 (s, 6H), 2.77 (t, $J = 7.2$ Hz, 2H), 2.59 (t, $J = 7.2$ Hz, 2H), 1.61 (s, 2H).



Prediction Trifluoroescaline

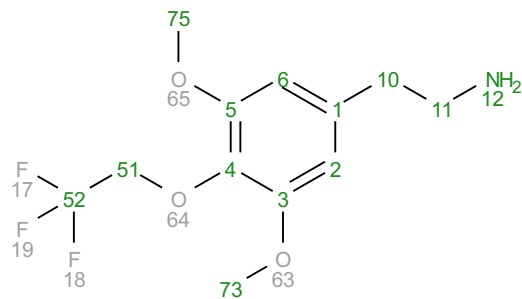
Origin Mnova Best

Solvent DMSO-d6

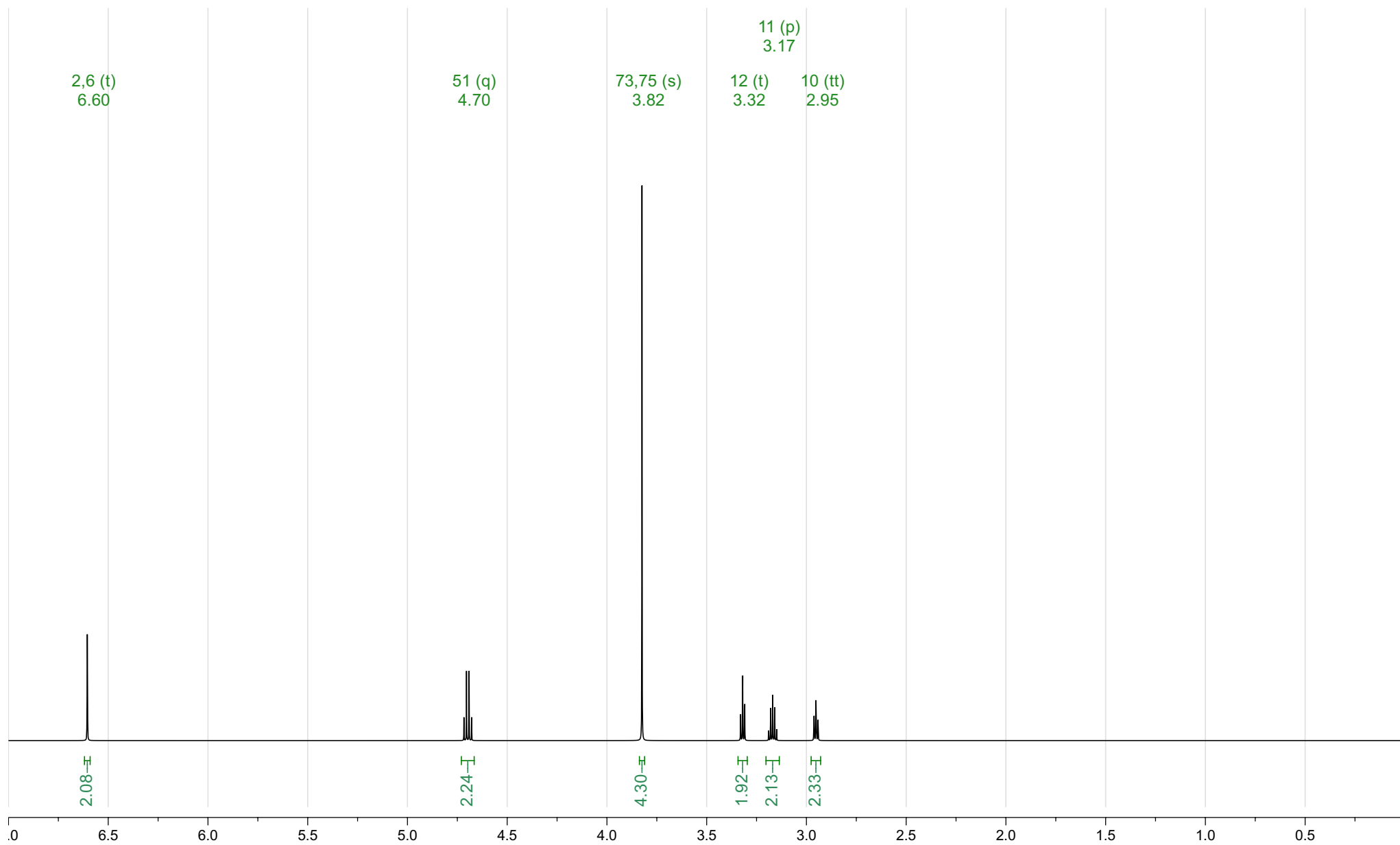
Version 1.0.0

Frequency 700.00

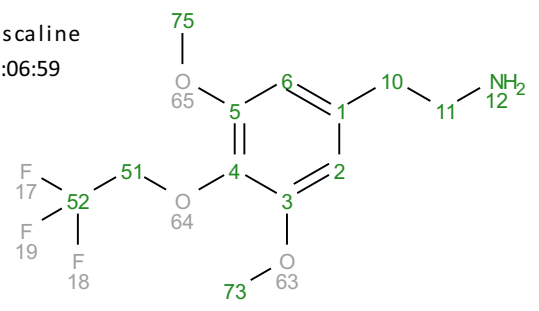
Nucleus 1H



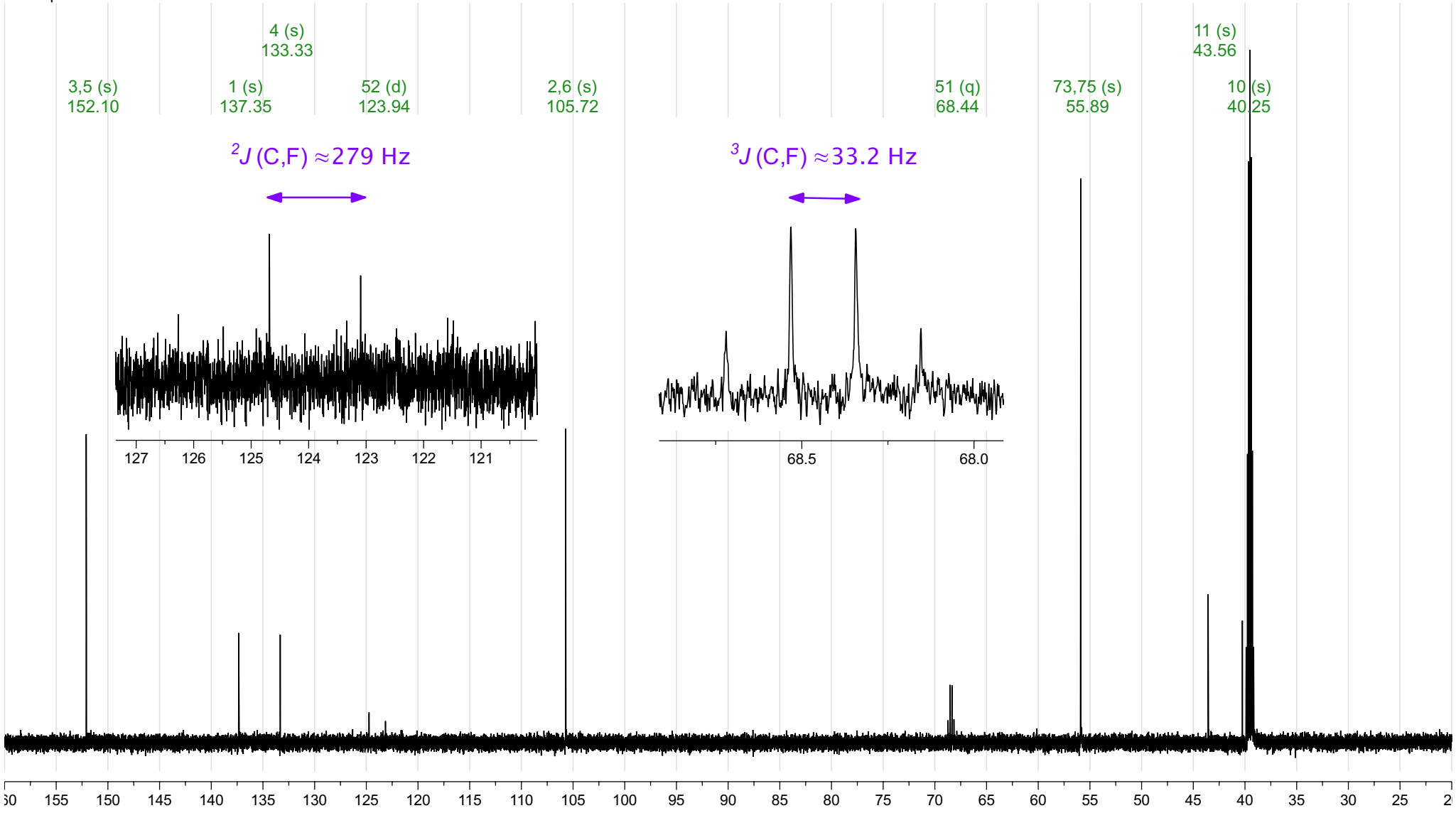
^1H NMR (700 MHz, DMSO- d_6) δ 6.60 (t, J = 0.9 Hz, 2H), 4.70 (q, J = 9.0 Hz, 2H), 3.82 (s, 6H), 3.32 (t, J = 7.2 Hz, 2H), 3.17 (p, J = 7.2 Hz, 2H), 2.95 (tt, J = 7.0, 1.0 Hz, 2H).



Analyte P23: Trifluoroescaline
 Acquisition Date 2018-08-31T20:06:59
 Solvent dms0
 Temperature 25
 Number of Scans 1000
 Relaxation Delay 0
 Experiment 1D
 Spectrometer Frequency 175.98
 Spectral Width 41666.7
 Nucleus 13C
 Acquired Size 125000



¹³C NMR (176 MHz, DMSO-*d*₆) δ 152.10, 137.35, 133.33, 123.94 (d, *J* = 279.1 Hz), 105.72, 68.44 (q, *J* = 33.2 Hz), 55.89, 43.56, 40.25.



Prediction Trifluoroescaline

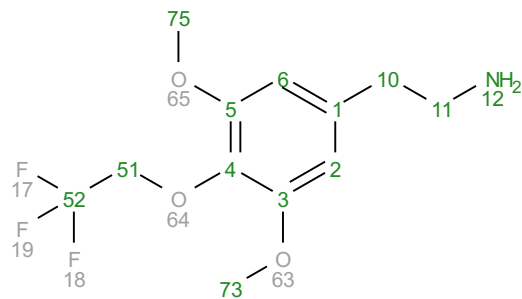
Origin Mnova Best

Solvent DMSO-d6

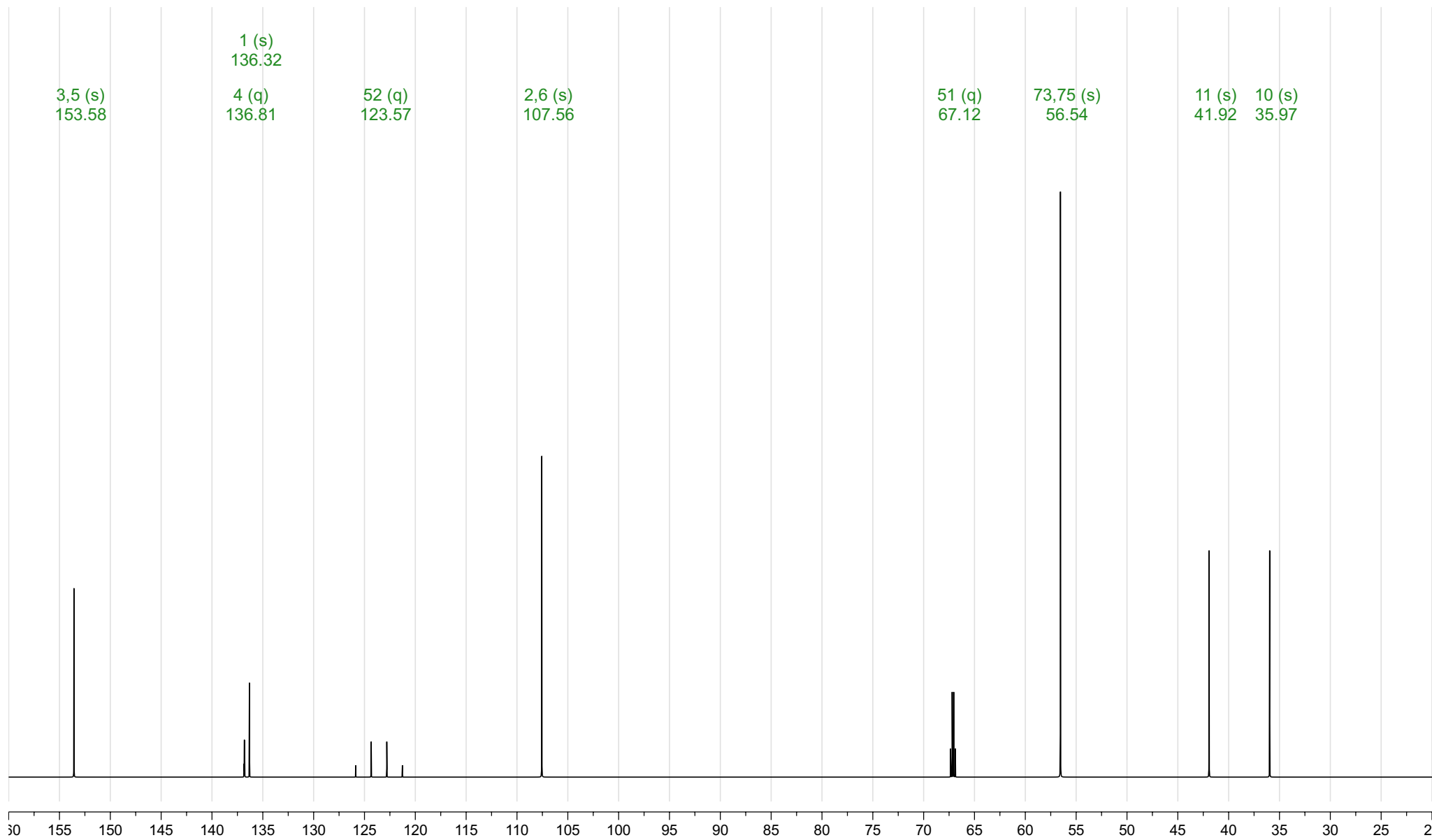
Version 1.0.0

Frequency 175.00

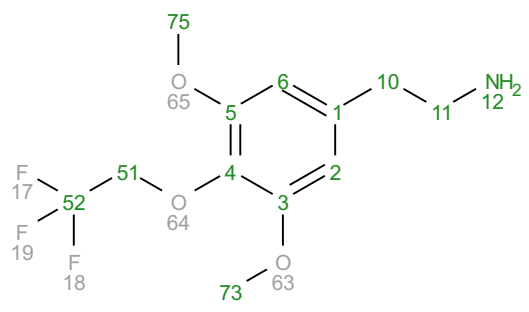
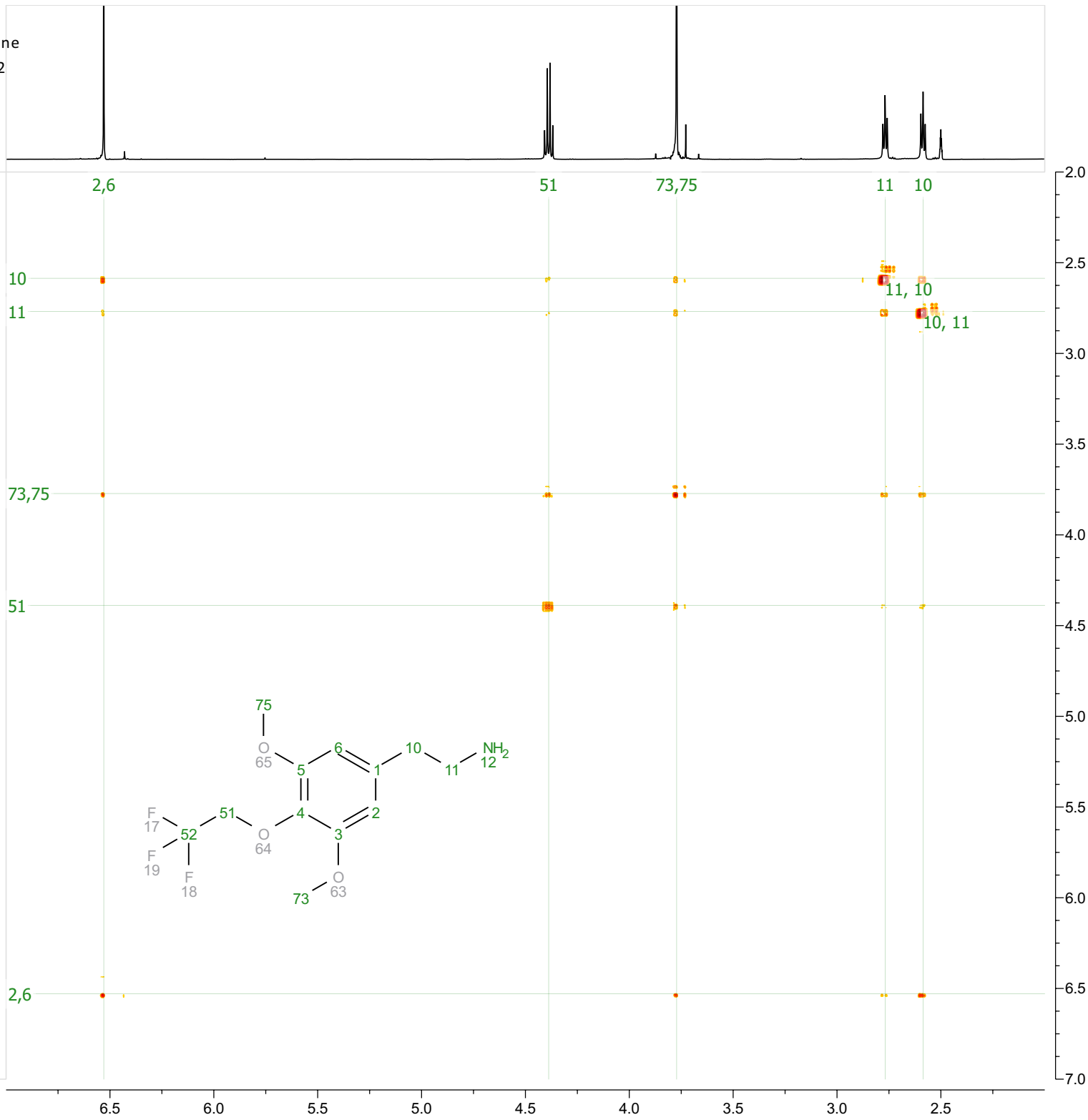
Nucleus ¹³C



¹³C NMR (175 MHz, DMSO-d₆) δ 153.58, 136.81 (q, *J* = 4.0 Hz), 136.32, 123.57 (q, *J* = 268.4, 267.7 Hz), 107.56, 67.12 (q, *J* = 28.1, 27.4 Hz), 56.54, 41.92, 35.97.

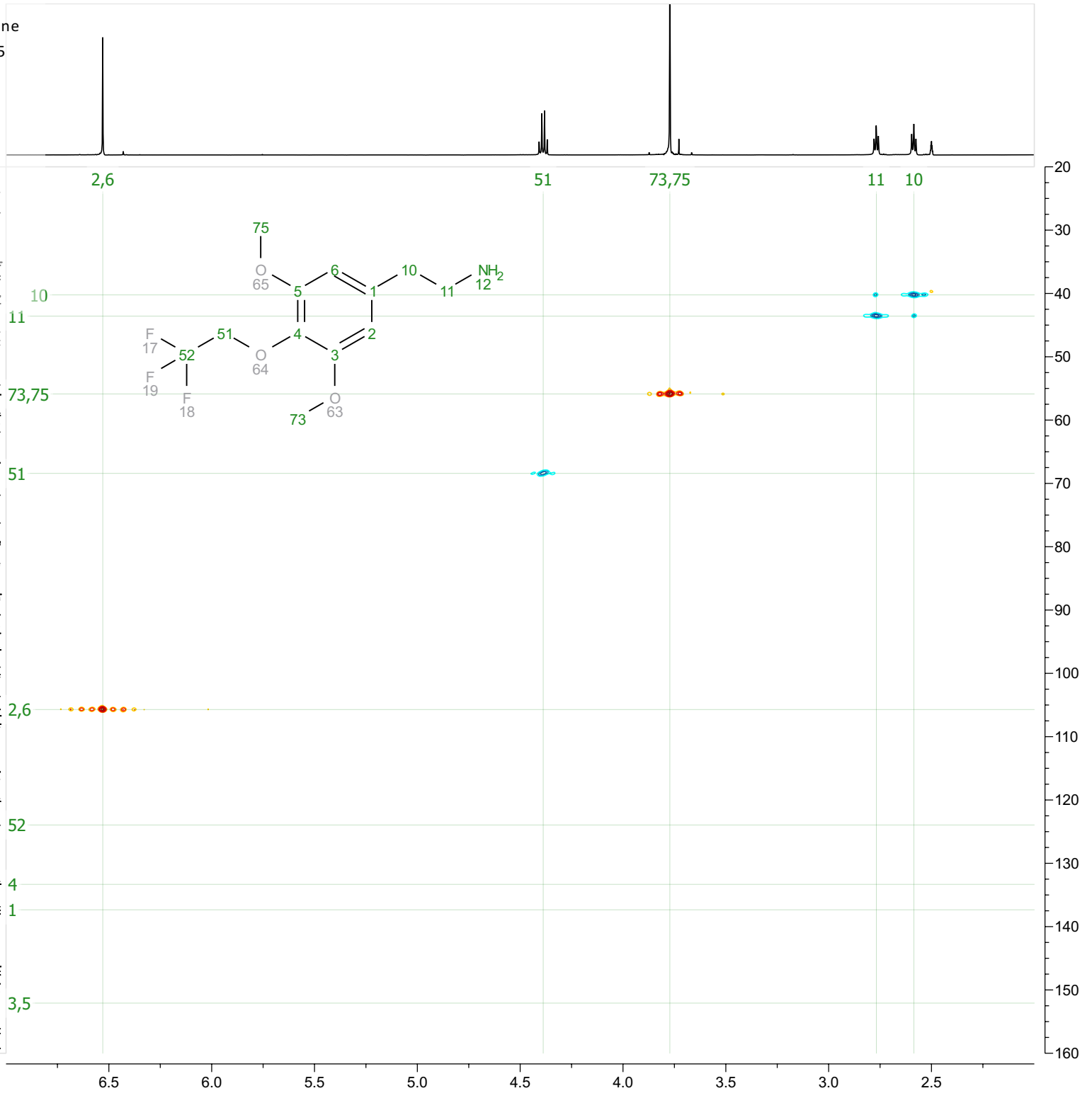


Analyte P23: Trifluoroescaline
 Acquisition Date 2018-08-31T18:13:02
 Solvent dms0
 Temperature 25
 Number of Scans 1
 Relaxation Delay 1
 Experiment COSY
 Spectrometer Frequency (699.80, 699.80)
 Spectral Width (4734.8, 4734.8)
 Nucleus (1H, 1H)
 Acquired Size (2048, 256)



Analyte P23: Trifluoroescaline
Acquisition Date 2018-08-31T18:20:15
Solvent dms0
Temperature 25
Number of Scans 8
Relaxation Delay 1

Experiment HSQC
Spectrometer Frequency (699.81, 175.98)
Spectral Width (11160.7, 35195.8)
Nucleus (1H, 13C)
Acquired Size (1024, 256)



Analyte P23: Trifluoroescaline
Acquisition Date 2018-08-31T19:00:03
Solvent dmsd
Temperature 25
Number of Scans 16
Relaxation Delay 1

Experiment HMBC
Spectrometer Frequency (699.81, 175.98)
Spectral Width (11160.7, 42238.6)
Nucleus (1H, 13C)
Acquired Size (1674, 200)

