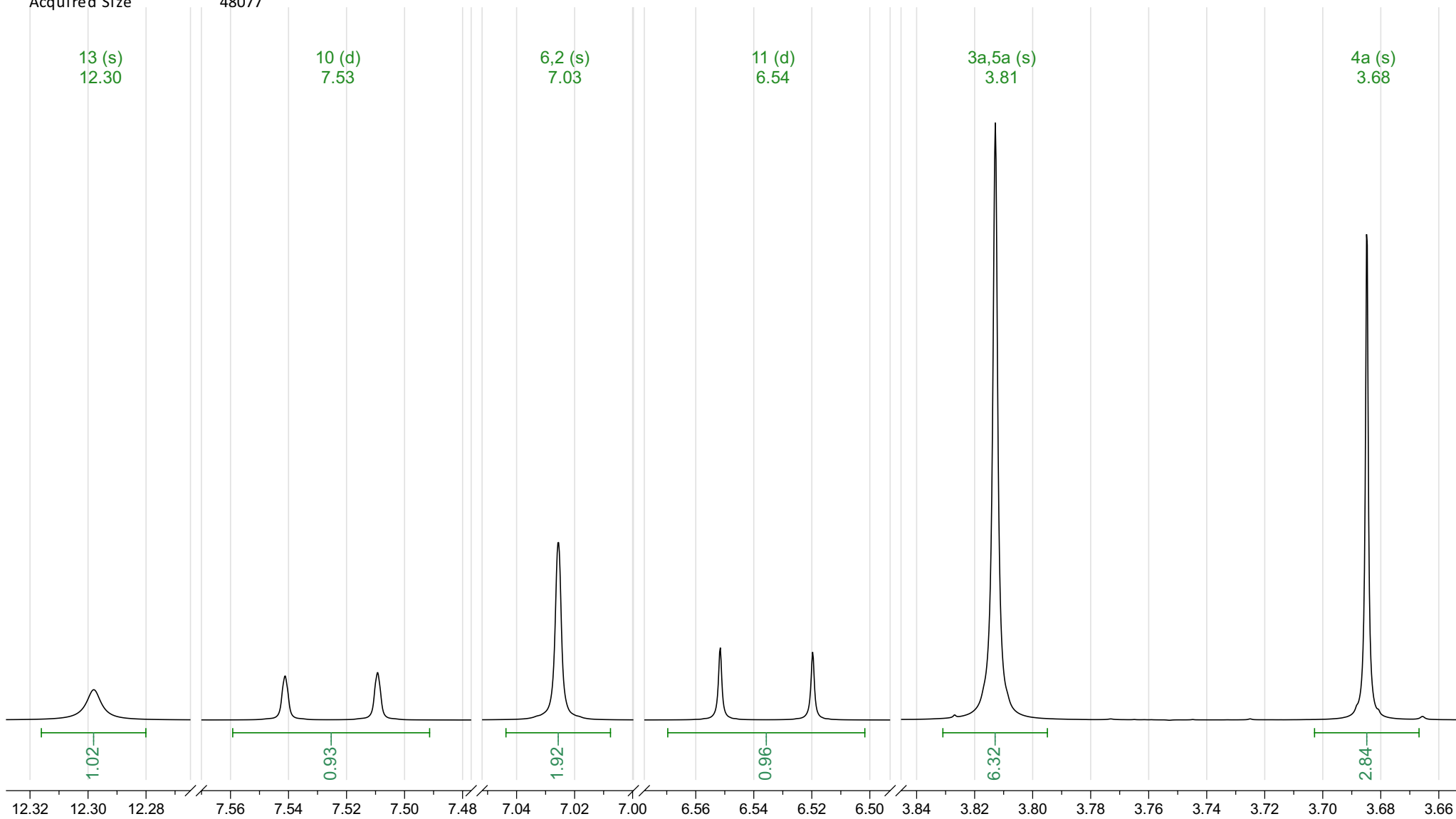
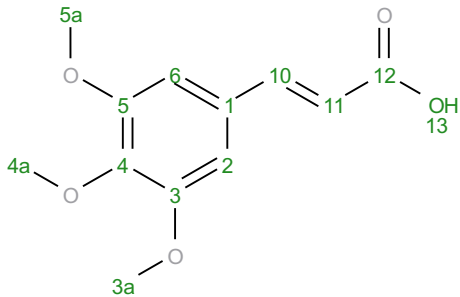


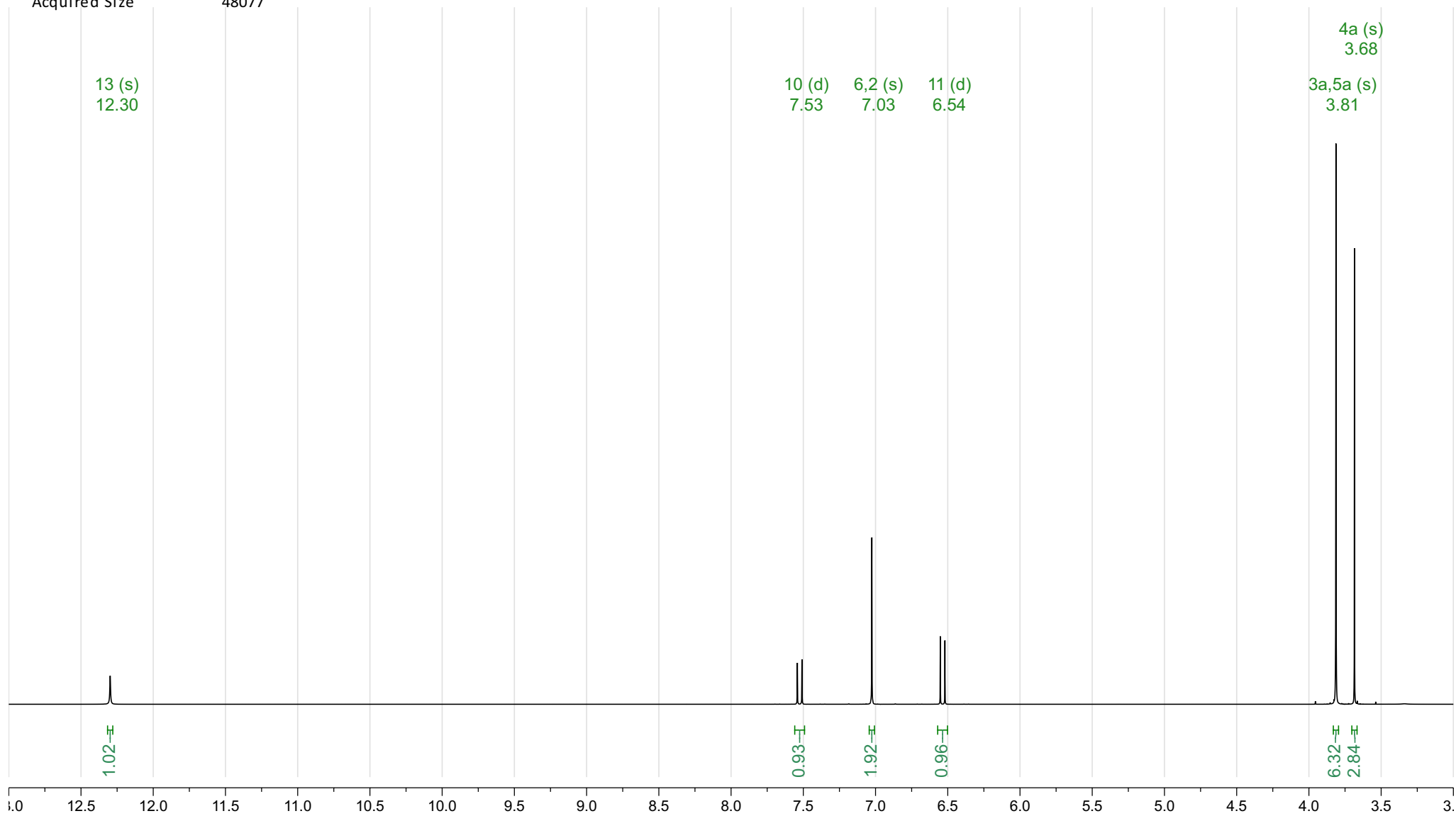
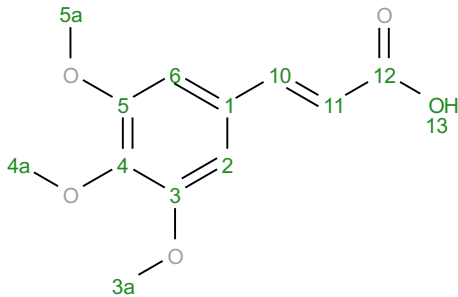
Analyte X62: 3,4,5-MeO-cinnamic acid
Acquisition Date 2019-03-08T15:54:42
Solvent dmso
Temperature 25
Number of Scans 16
Relaxation Delay 1
Experiment 1D
Spectrometer Frequency 499.66
Spectral Width 8012.8
Nucleus 1H
Acquired Size 48077

^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 12.30 (s, 1H), 7.53 (d, $J = 15.9$ Hz, 1H), 7.03 (s, 2H), 6.54 (d, $J = 15.9$ Hz, 1H), 3.81 (s, 6H), 3.68 (s, 3H).



Analyte X62: 3,4,5-MeO-cinnamic acid
Acquisition Date 2019-03-08T15:54:42
Solvent dms
Temperature 25
Number of Scans 16
Relaxation Delay 1
Experiment 1D
Spectrometer Frequency 499.66
Spectral Width 8012.8
Nucleus 1H
Acquired Size 48077

^1H NMR (500 MHz, DMSO- d_6) δ 12.30 (s, 1H), 7.53 (d, J = 15.9 Hz, 1H), 7.03 (s, 2H), 6.54 (d, J = 15.9 Hz, 1H), 3.81 (s, 6H), 3.68 (s, 3H).



Prediction 3,4,5-MeO-cinnamic acid

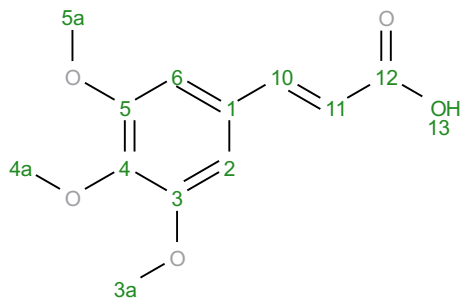
Origin Mnova Best

Solvent DMSO-d6

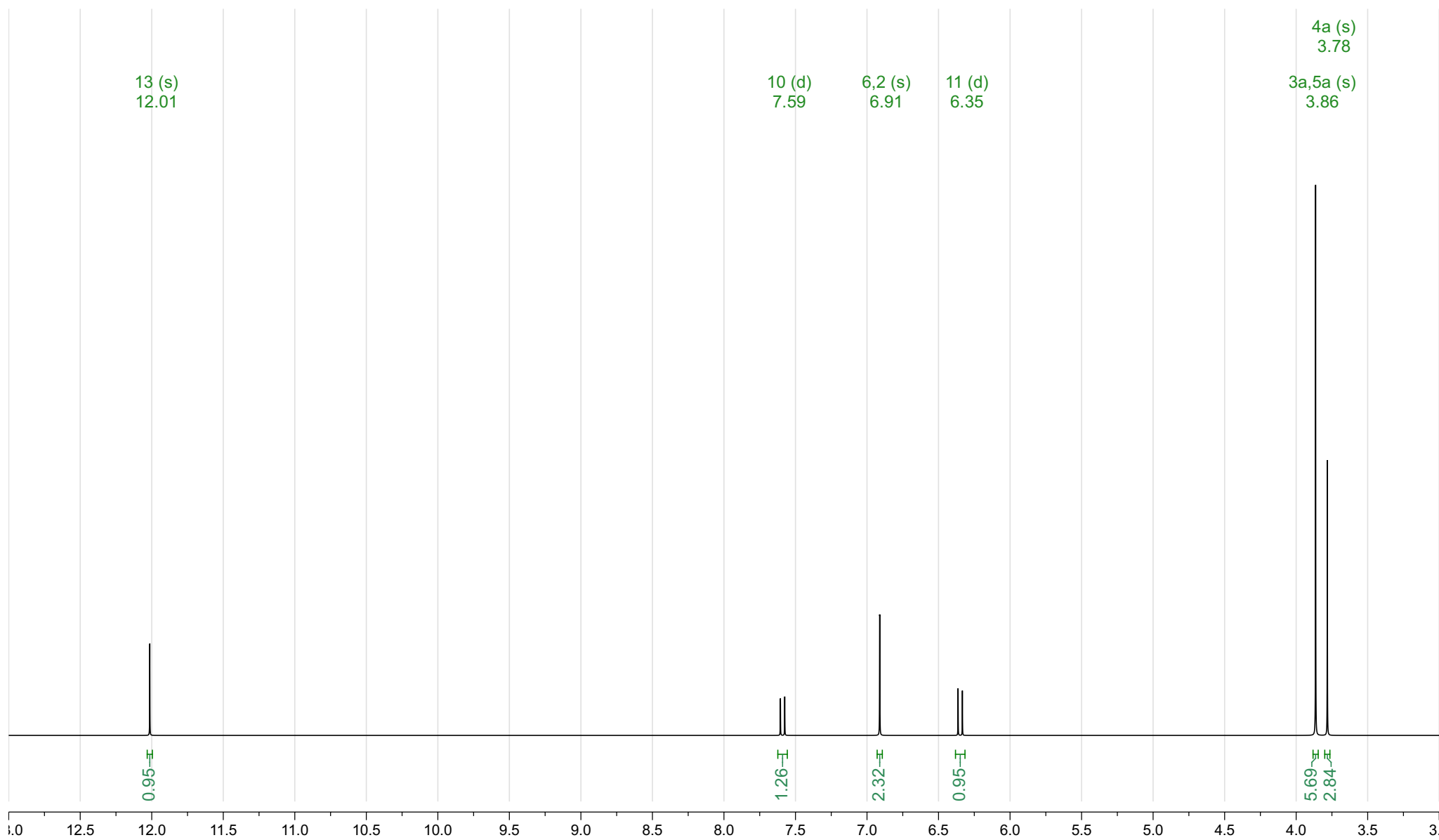
Version 1.0.0

Frequency 500.00

Nucleus 1H

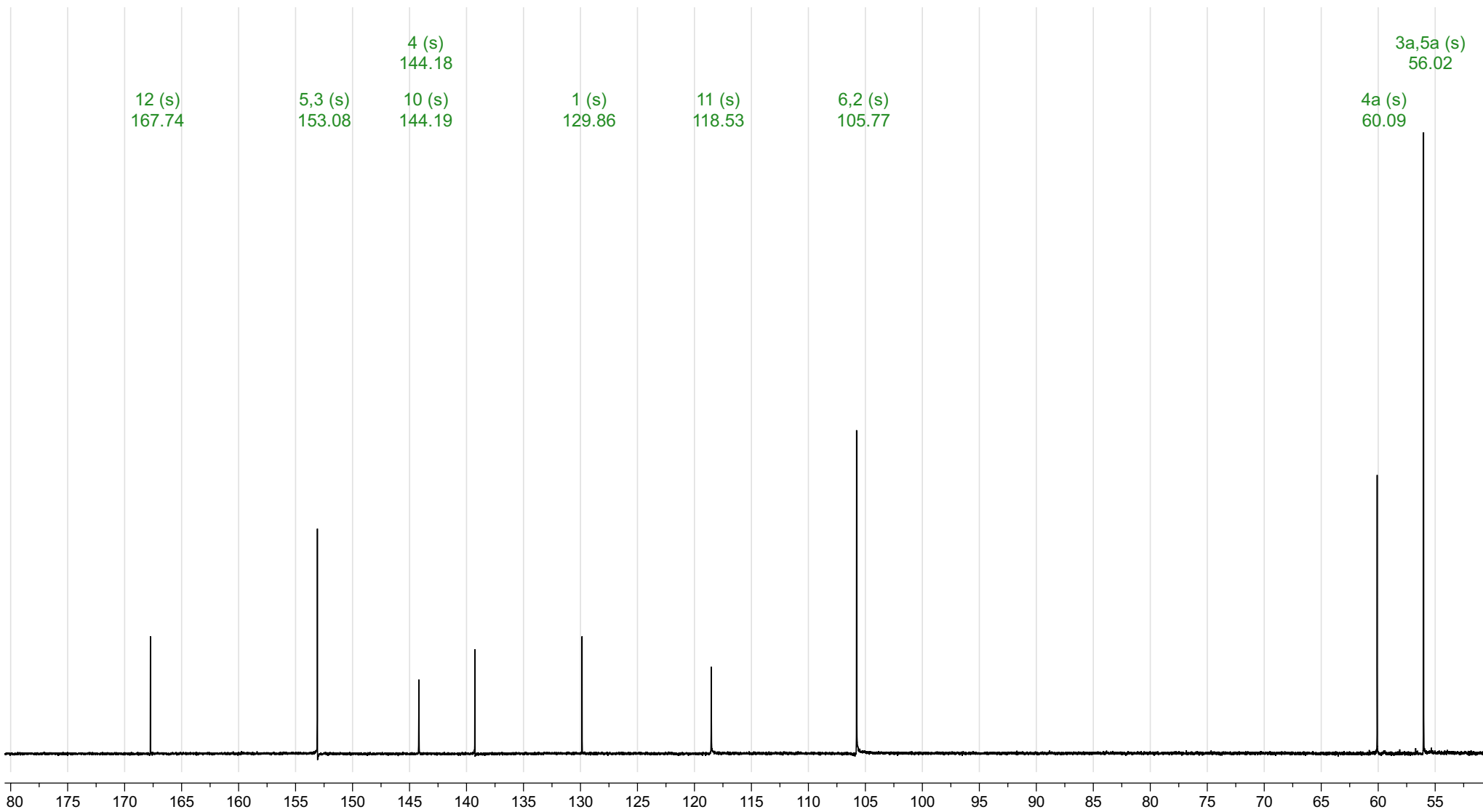
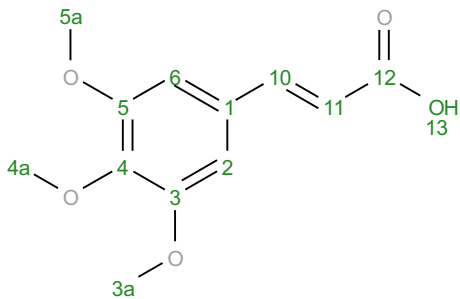


$^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 12.01 (s, 1H), 7.59 (d, $J = 15.1$ Hz, 1H), 6.91 (s, 2H), 6.35 (d, $J = 15.1$ Hz, 1H), 3.86 (s, 6H), 3.78 (s, 3H).



Analyte X61: 3,4,5-MeO-cinnamic acid
Acquisition Date 2019-03-20T09:24:52
Solvent dmso
Temperature 25
Number of Scans 256
Relaxation Delay 0
Experiment 1D
Spectrometer Frequency 125.65
Spectral Width 30487.8
Nucleus ¹³C
Acquired Size 60976

¹³C NMR (126 MHz, DMSO-*d*₆) δ 167.74, 153.08, 144.19, 144.18, 129.86, 118.53, 105.77, 60.09, 56.02.



Prediction 3,4,5-MeO-cinnamic acid

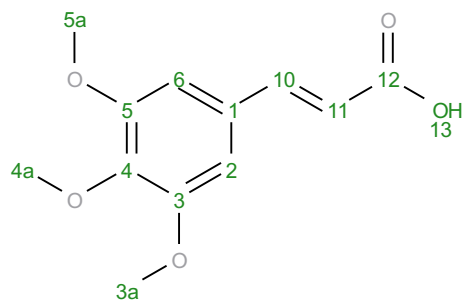
Origin Mnova Best

Solvent DMSO-d6

Version 1.0.0

Frequency 125.00

Nucleus ¹³C



¹³C NMR (125 MHz, DMSO-*d*₆) δ 168.46, 153.33, 144.54, 140.27, 129.47, 118.68, 106.18, 60.80, 56.24.

