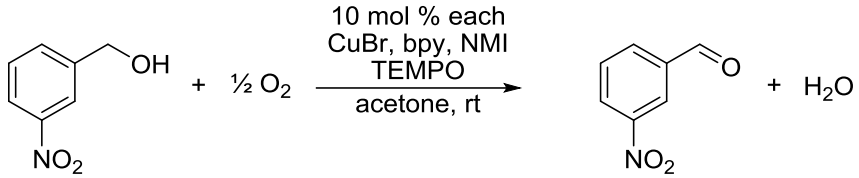
**Name:** **CHEM 344 Fall 2014**

**Spectroscopy Problem Set**

**TA:**

**Due at start of discussion Monday/Tuesday the 22nd/23rd September**

1) Assign all of the integrated signals in the $^1$H-NMR spectrum of the crude reaction mixture from the aerobic oxidation reaction shown below. Use the standard labeling ($H_a$, $H_b$, $H_c$, etc.) shown in the NMR lectures and problem sets. Justify your assignments by use of the empirical (Curphy-Morrison) parameters found in the appendix of the laboratory manual.




Use the $^1$H-NMR spectrum of the crude product mixture to determine the % conversion of this reaction (assume there are no side reactions). Note that one of the signals of the low abundance molecule is completely obscured. (**10 pts)**

2) Use the supplied spectral data to identify Compound 2, $C_{14}H_{12}O_2$. **(14 pts)**

3) Use the supplied spectral data to identify Compound 3, $C_5H_7BrO_2$. **(14 pts)**

4) Use the supplied spectral data to identify Compound 4, $C_{11}H_{14}O_2$. **(12 pts)**

**Questions 2 - 4 require you to use a combination of molecular formula, NMR and MS data in order to identify each unknown compound; use all data supplied and hand in all spectra for each question.**

- Clearly provide your calculation of the unsaturation number (IHD, DBE) value for each compound.

- **Draw all molecules or fragments directly onto the provided spectra**. Show all lone pairs and charges for each structure. Write and sketch clearly!

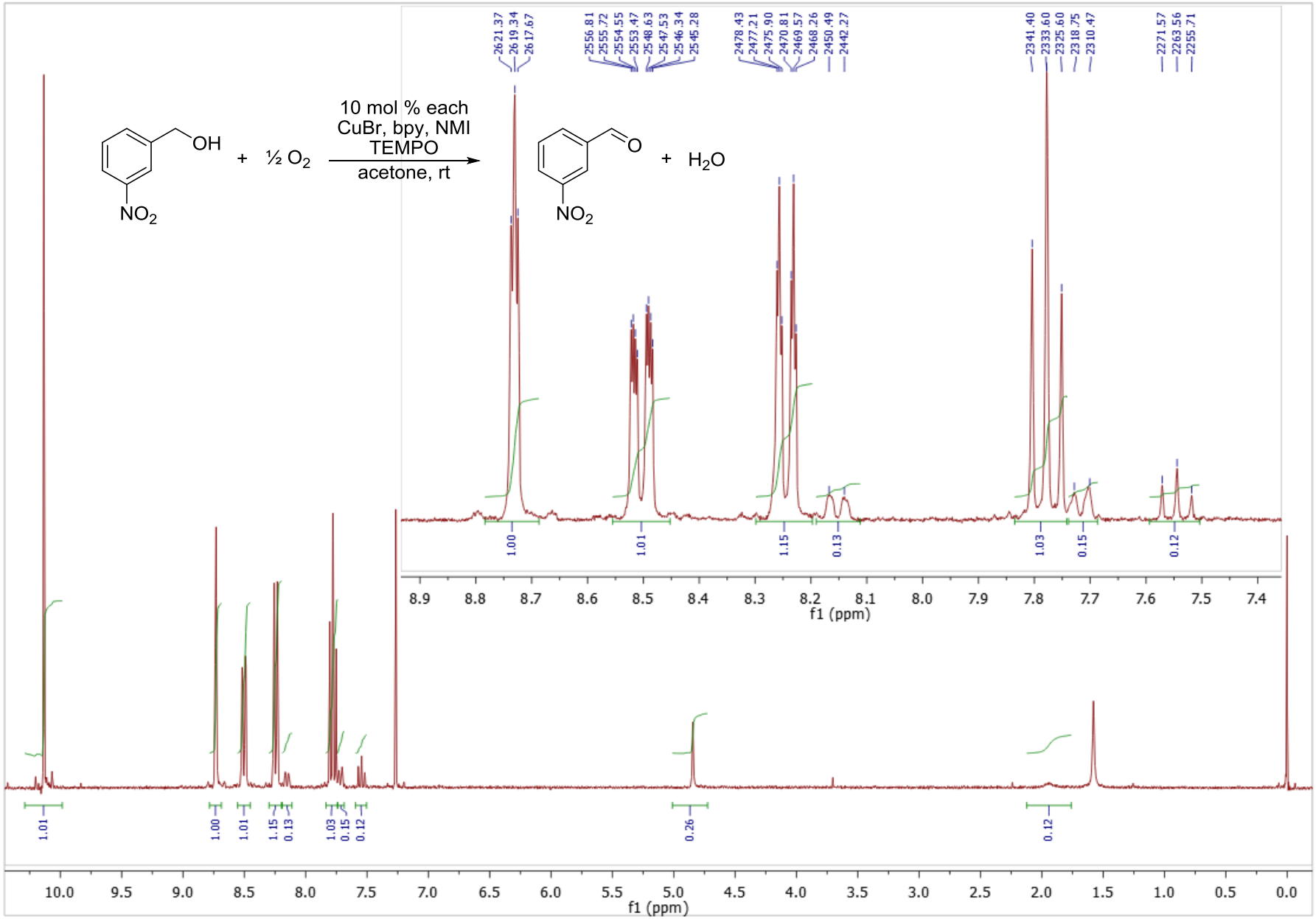
- Label each set of equivalent protons using the $H_a$, $H_b$, $H_c$ etc. labeling system shown in the $^1$H-NMR lectures and practice problem sets. Assign each **$^1$H-NMR** signal and write your assignments directly onto the spectrum. Justify your assignments by use of the empirical (Curphy-Morrison) parameters found in the laboratory manual.

- Identify each **$^{13}$C-NMR** signal as either alkyl, vinyl, alkynyl, aryl, nitrile, imine, or carbonyl (you do not need to assign individual carbon atoms to each signal).

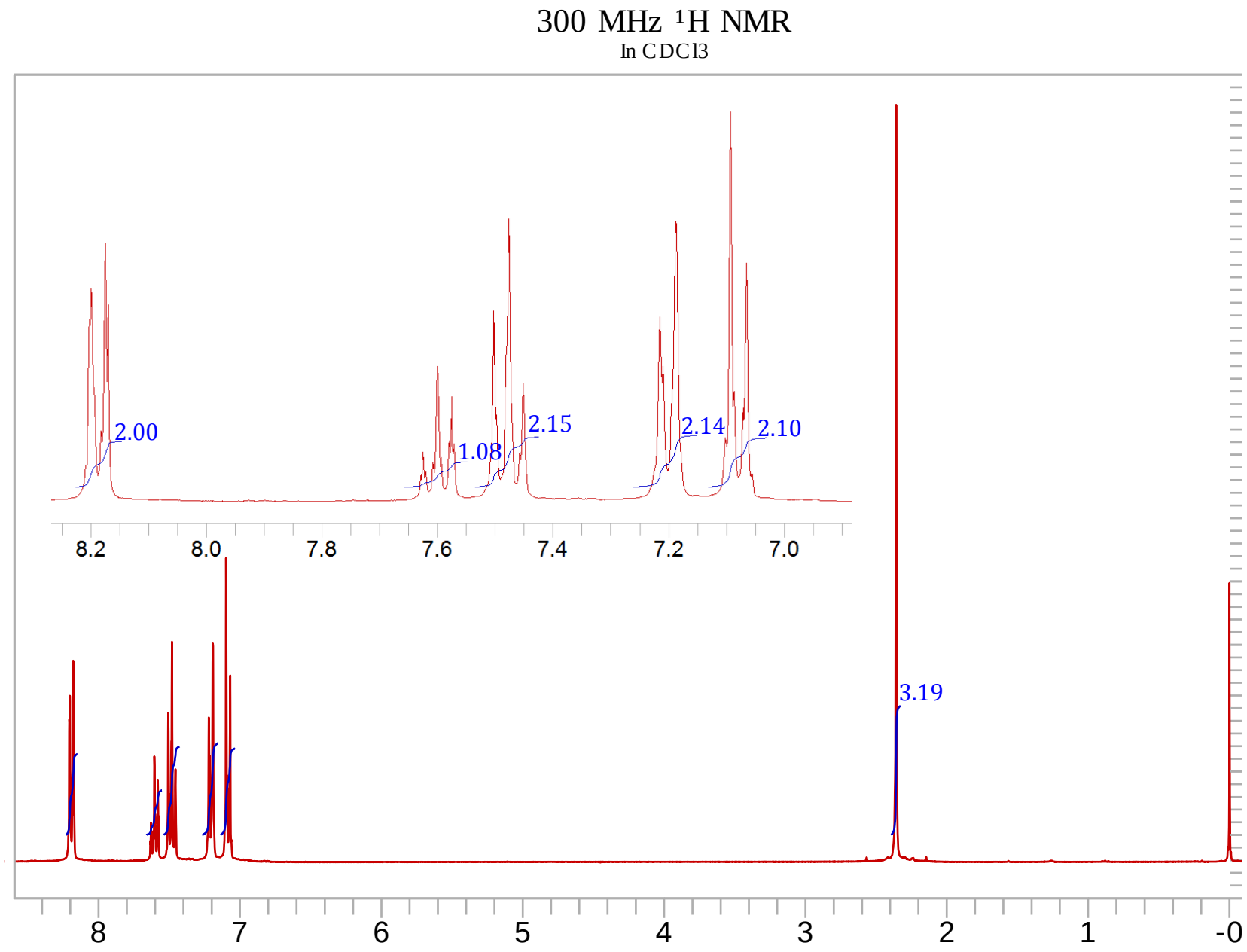
- Assign each key **IR** absorption band >1500 $cm^{-1}$ to a specific functional group.

- Draw fragments for all labeled peaks in the **EI-MS** directly onto the spectrum (you do not need to show the fragmentation mechanism).

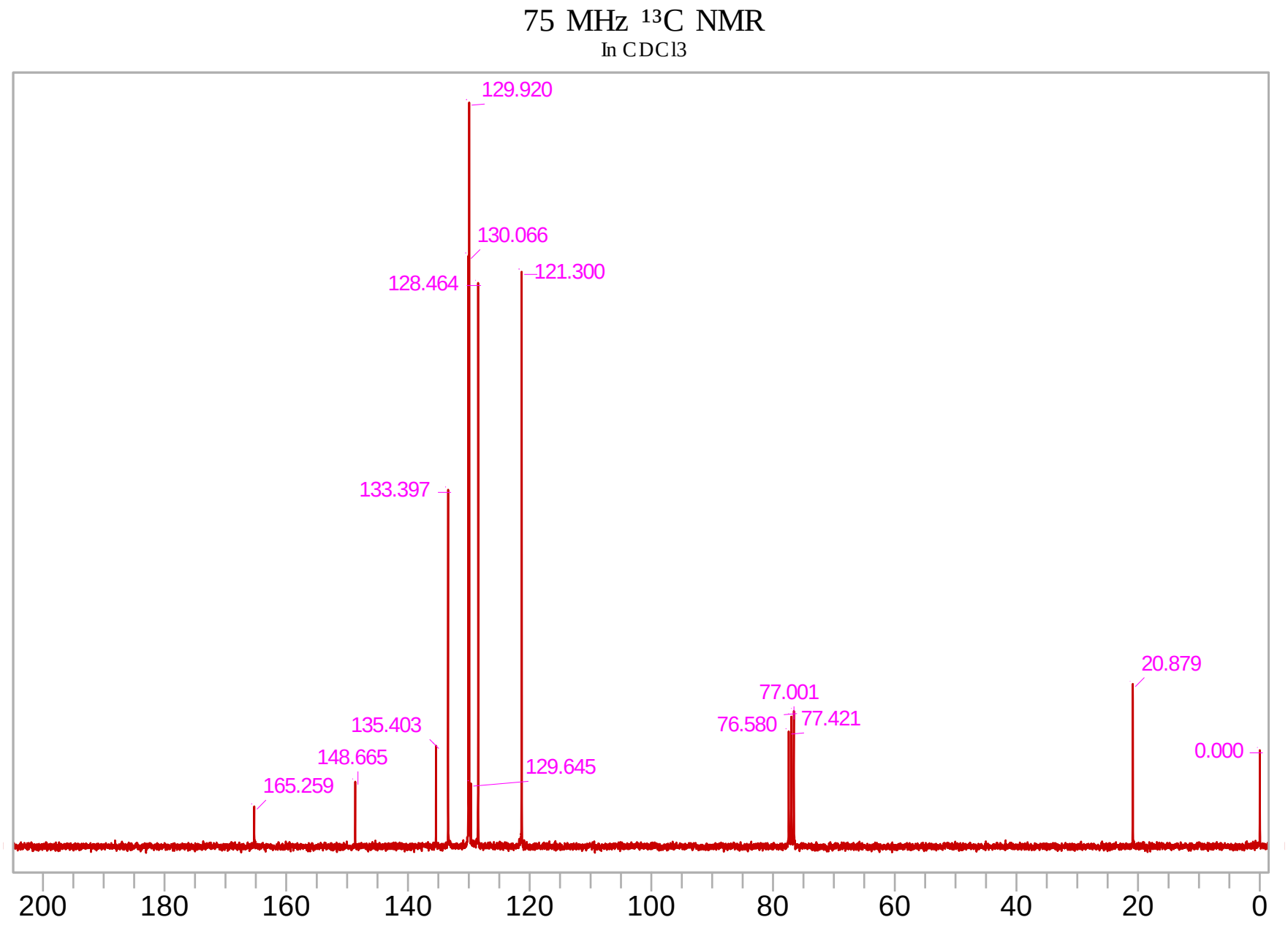
1) Aerobic Oxidation Crude Product Mixture $^{1}$H-NMR



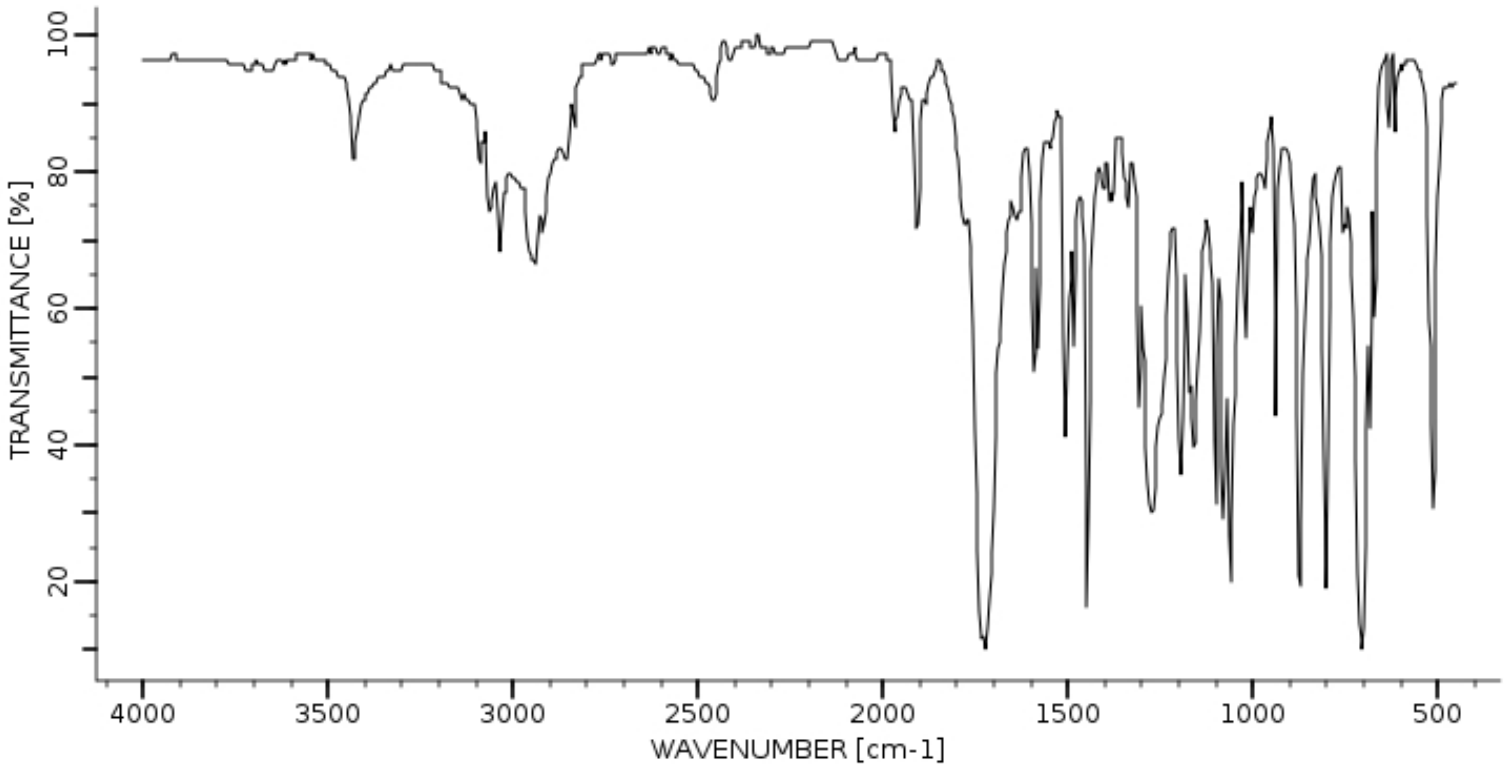
2) Compound 2 ($C_{14}H_{12}O_2$): $^1$H-NMR



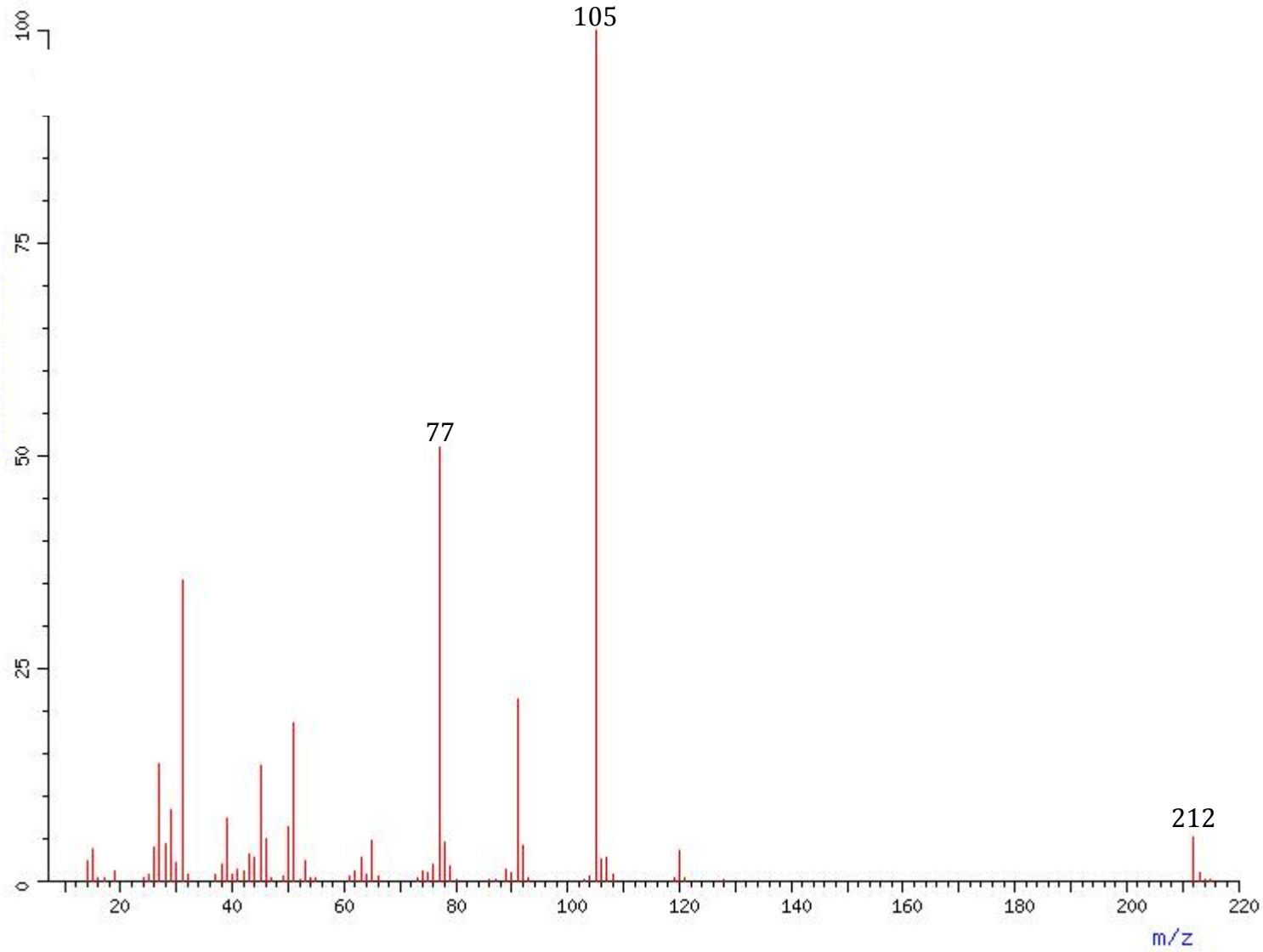
2) Compound 2 ($C_{14}H_{12}O_2$): $^{13}$C-NMR



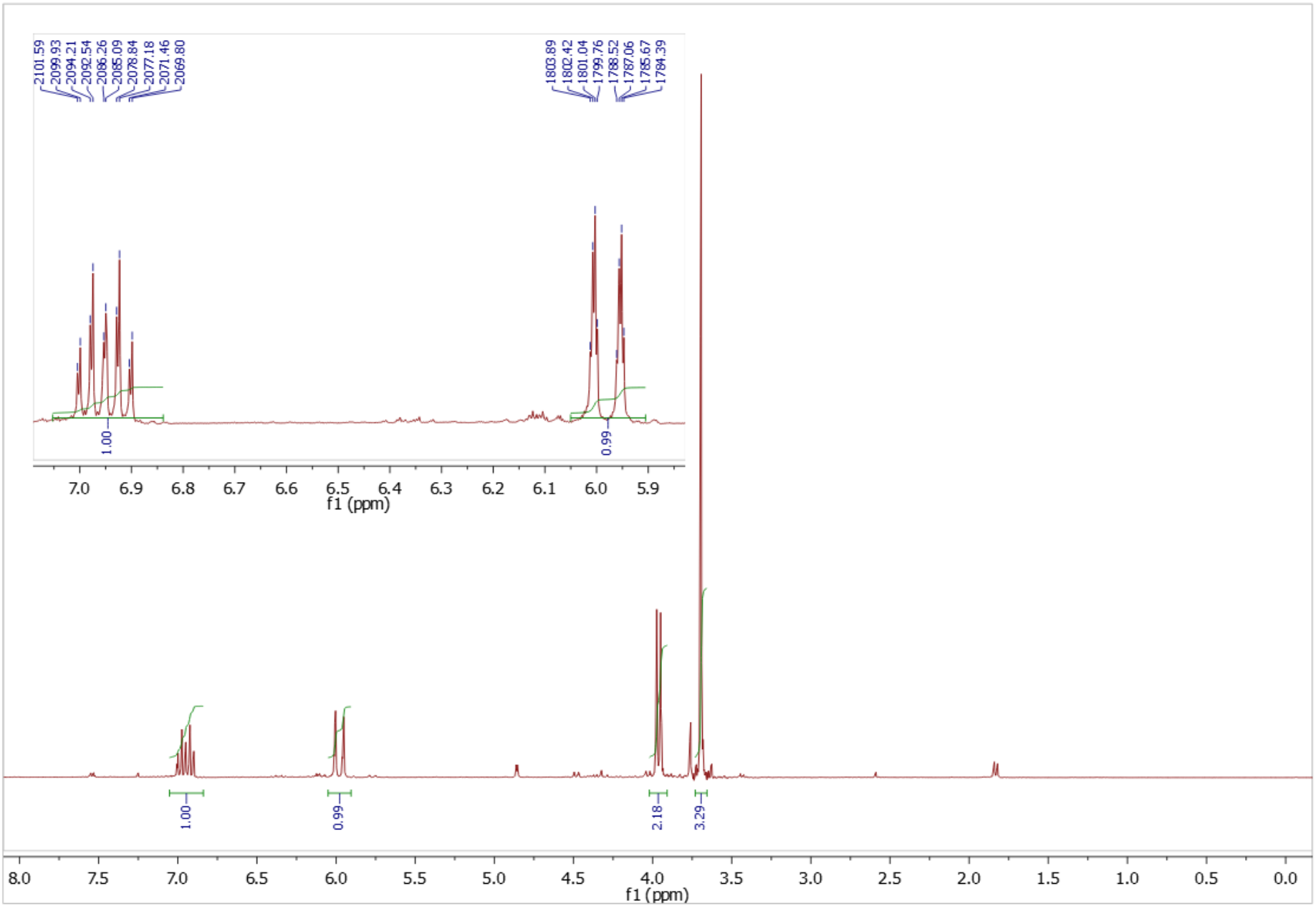
2) Compound 2 ($C_{14}H_{12}O_2$): IR



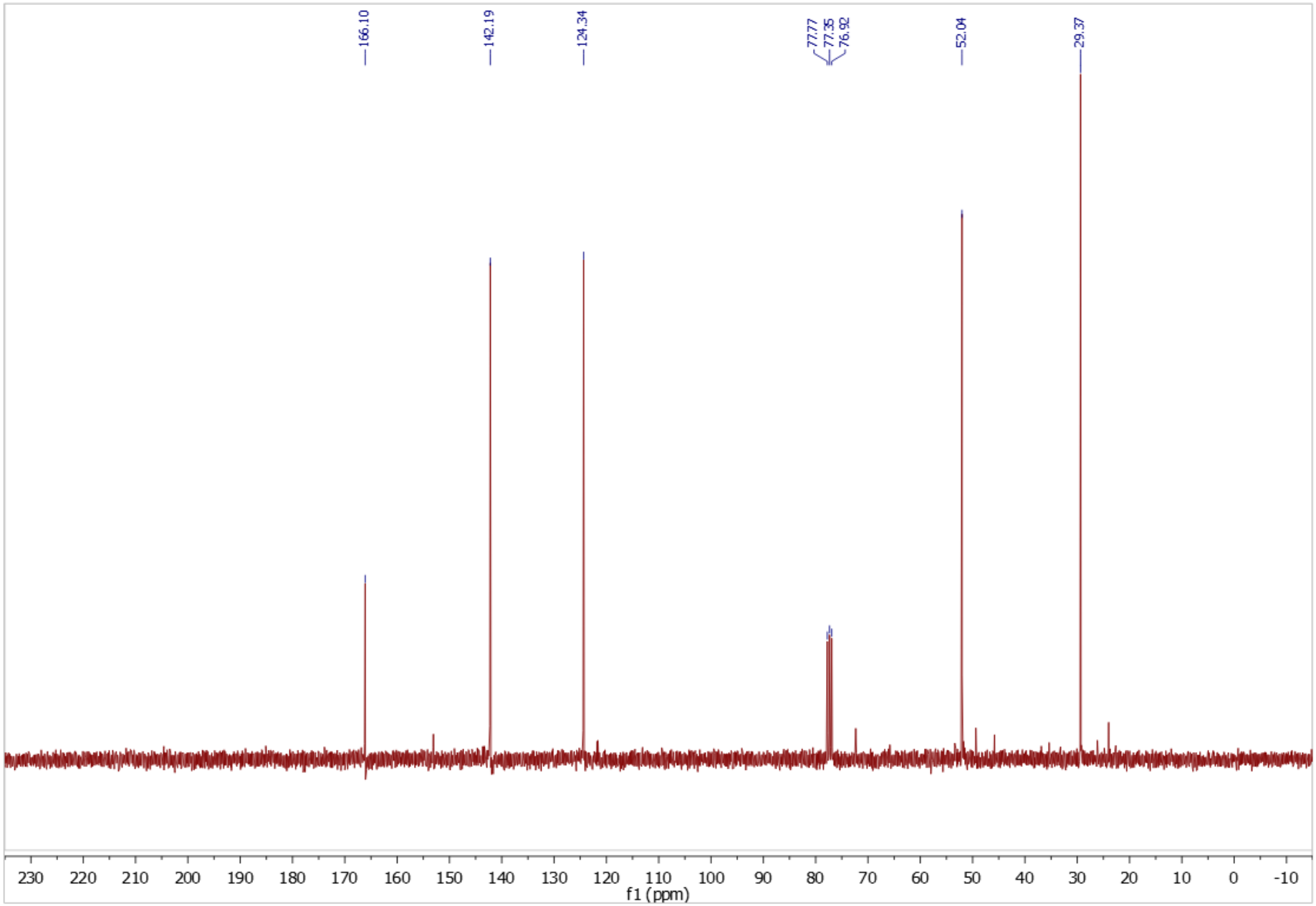
2) Compound 2 ($C_{14}H_{12}O_2$): EI-MS



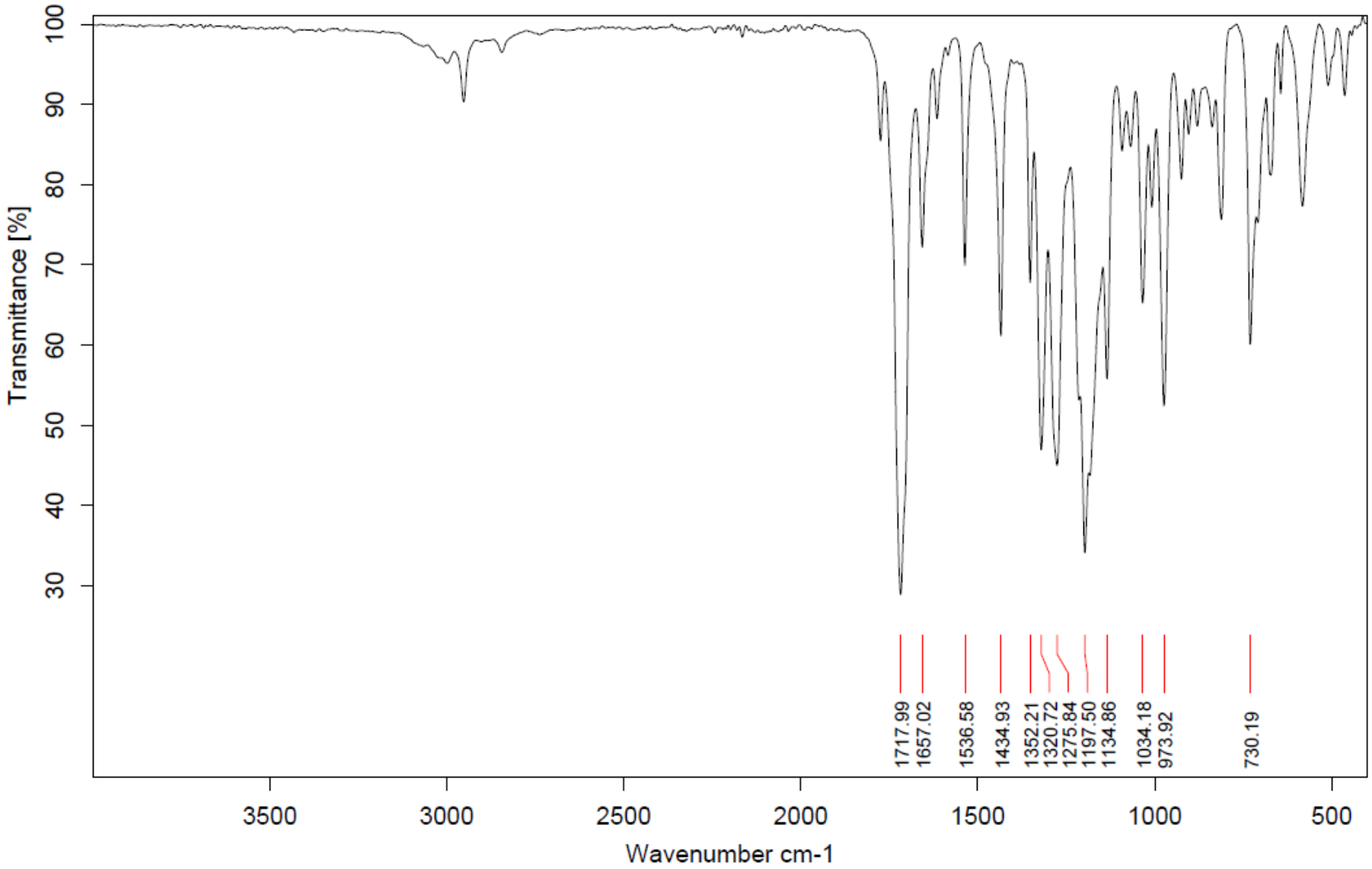
3) Compound 3 ($C_5H_7BrO_2$): $^1$H-NMR



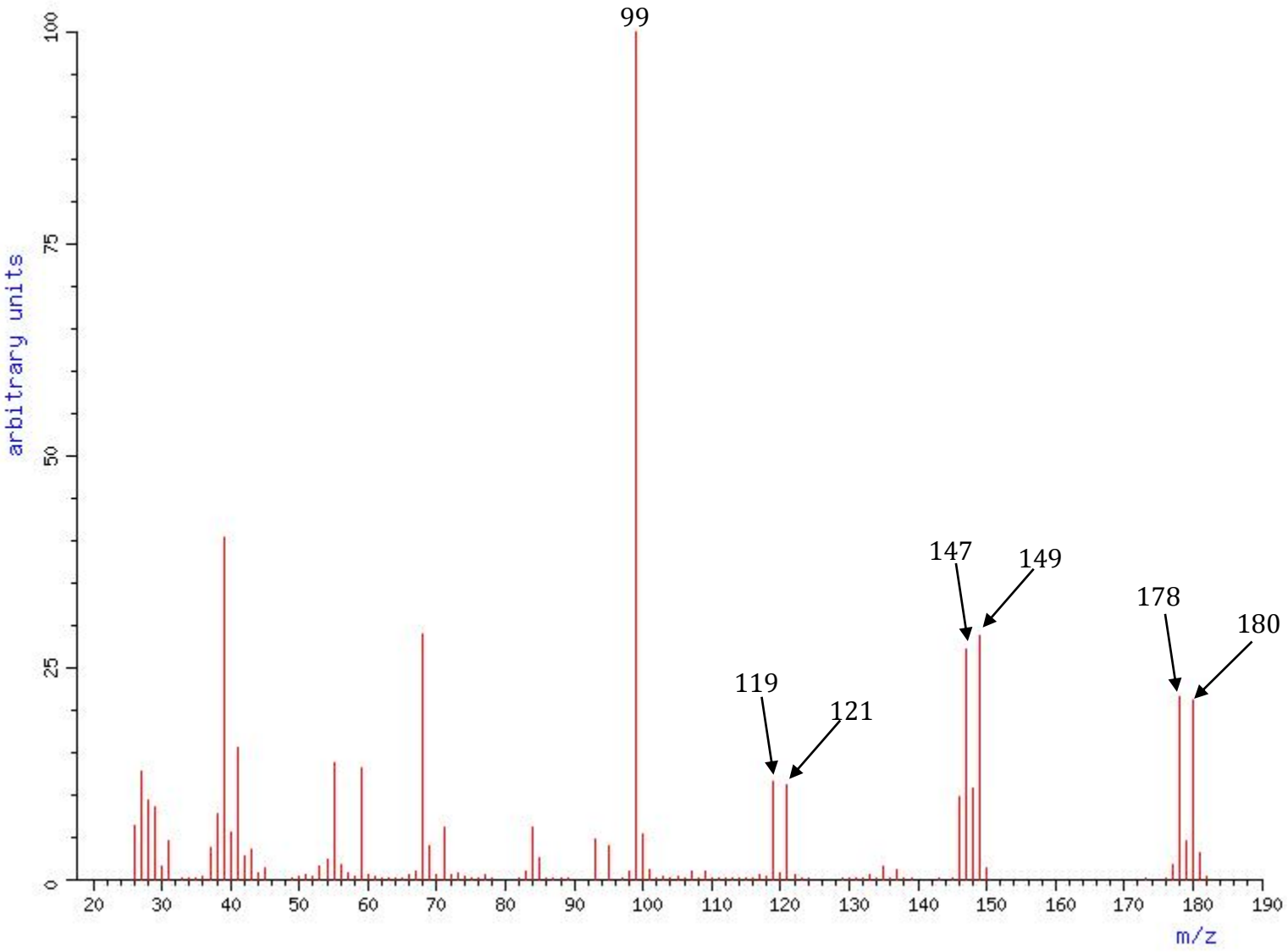
3) Compound 3 ($C_5H_7BrO_2$): $^{13}$C-NMR



3) Compound 3 ($C_5H_7BrO_2$): IR

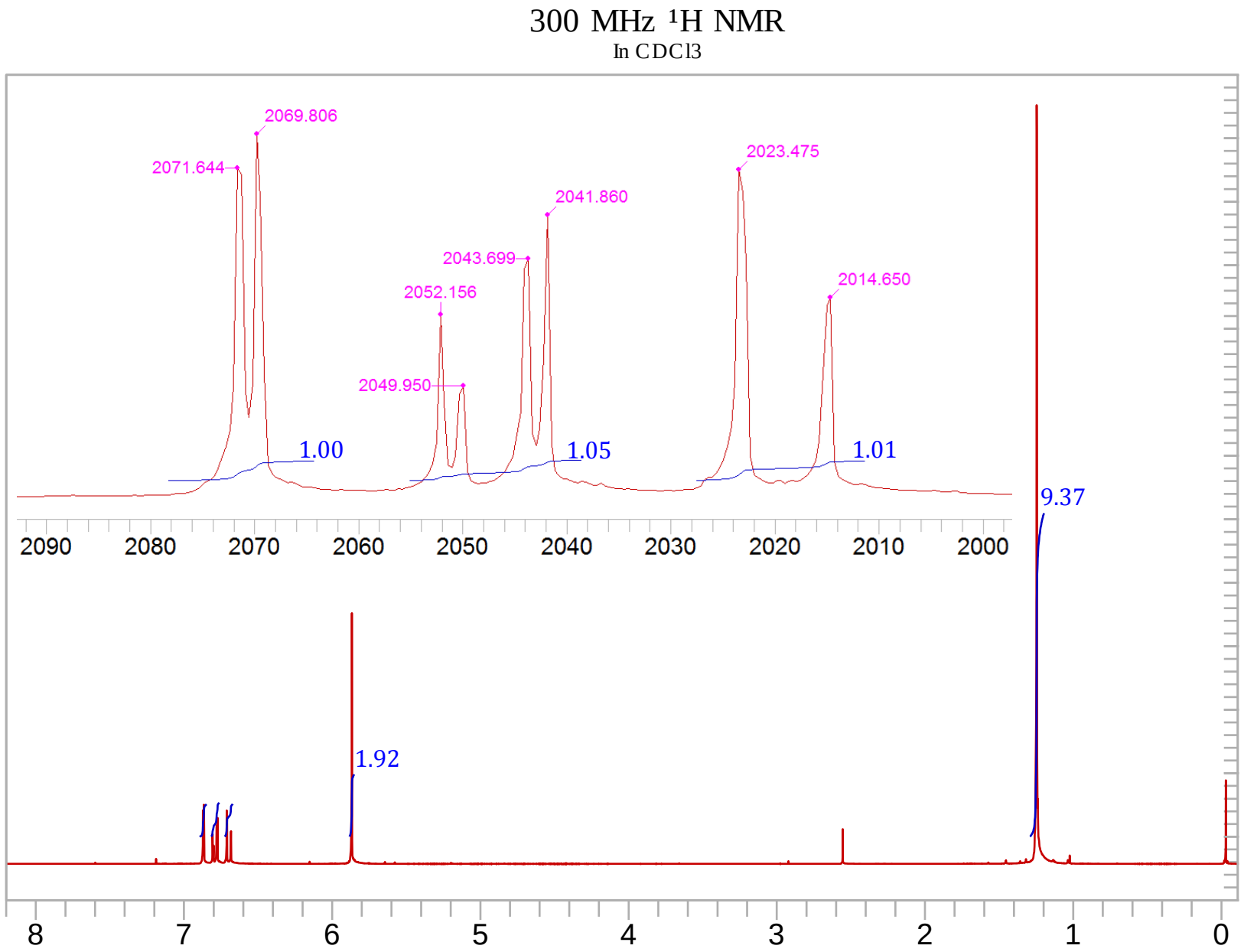


3) Compound 3 ($C_5H_7BrO_2$): EI-MS

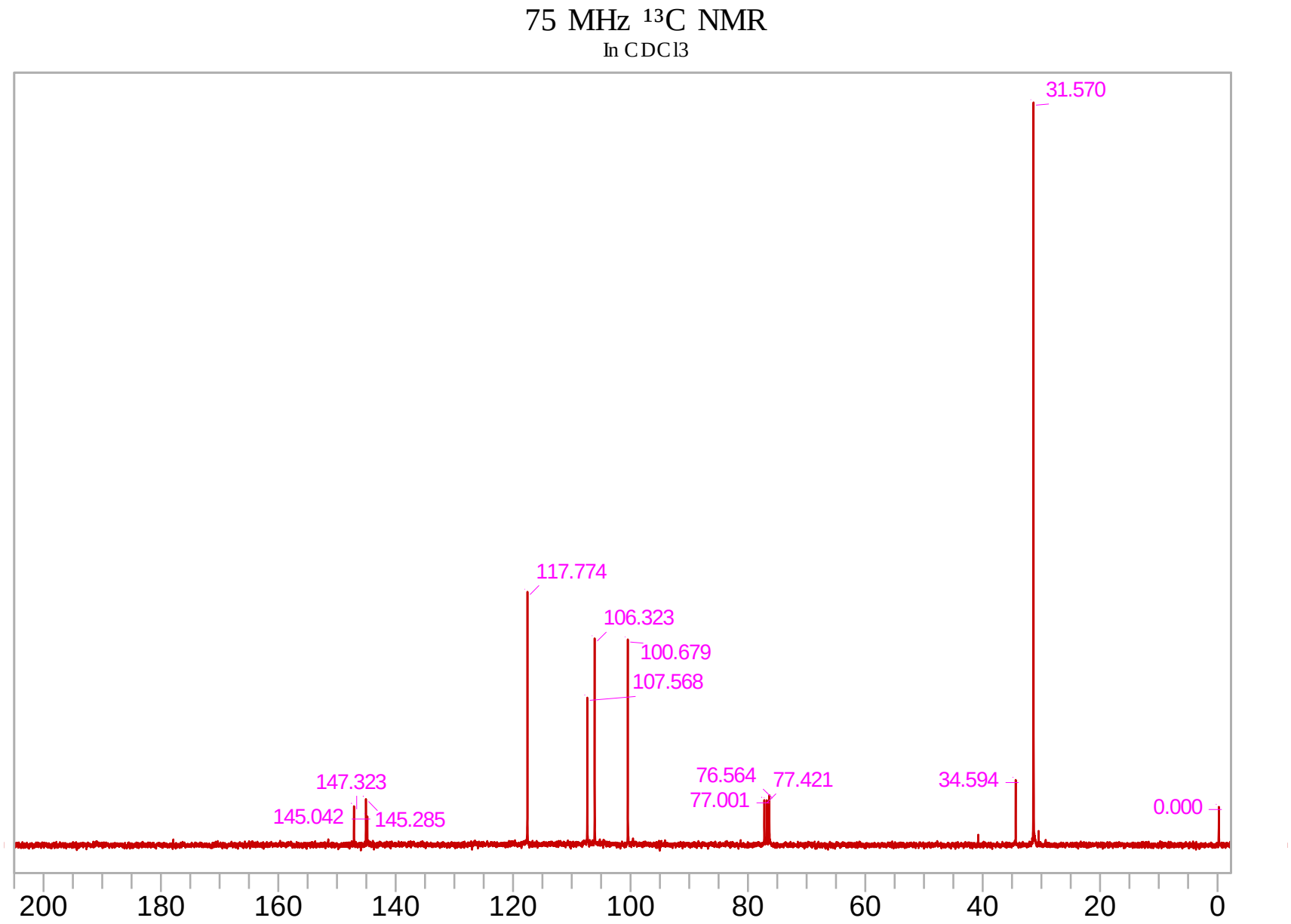



4)

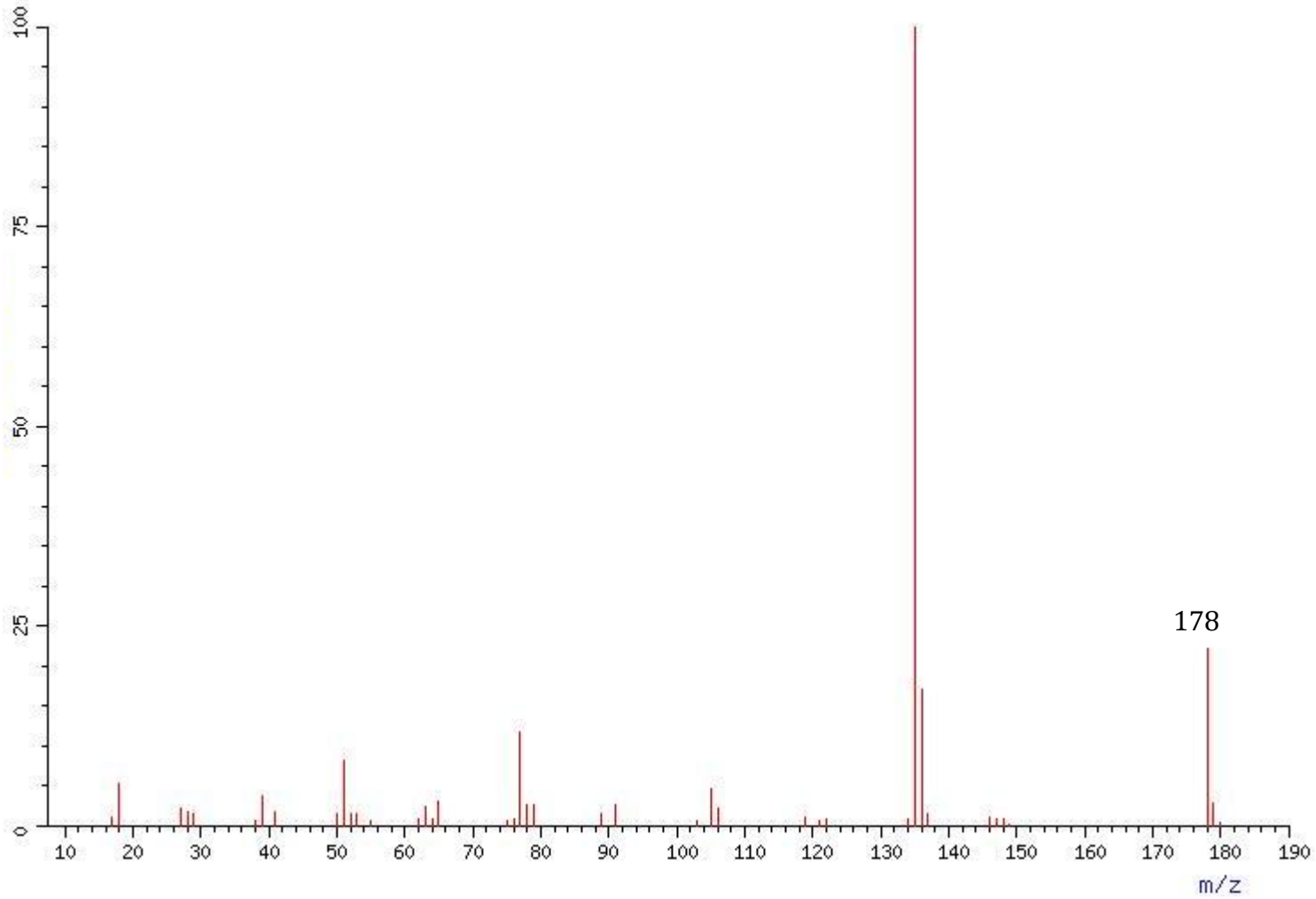
4) Compound 4 ($C_{11}H_{14}O_2$): $^1$H-NMR



4) Compound 4 ($C_{11}H_{14}O_2$): $^{13}$C-NMR



4) Compound 4 ($C_{11}H_{14}O_2$): EI-MS



**Last Name (print): _____**

**First Name (print): _____**

**TA's Name: _____**

**CHEM 344**

**Summer 2014**

**Spectroscopy Problem Set**

1) _____ **(10 pts)**

2) _____ **(14 pts)**

3) _____ **(14 pts)**

4) _____ **(12 pts)**

Total _____ **(50 pts)**

_____ **(math double-check)**