CHEM 344 Spectroscopy Problem Set Fall 2013

Due at start of discussion session Wednesday 25th/Thursday 26th September

1) Draw the ^{1}H-NMR spectrum of a 2:3:2 mixture of 1,4-dimethoxybenzene, 2-propanone, and diethyl ether.

Clearly show the multiplicity, the relative peak heights, and integration value of each signal in the ^{1}H-NMR spectrum of this mixture. You do not need to show signals from the solvent or reference compound.

1,4-Dimethoxybenzene ($CDCl_3$): δ 3.80 (CH_3), 6.80 ppm (Ph-H).

2-Propanone ($CDCl_3$): 2.10 ppm (CH_3)

Diethyl ether ($CDCl_3$): δ 1.20 ppm (CH_3), 3.40 ppm (CH_2)

10 pts total

Questions 2 - 4 require you to use a combination of molecular formula, NMR and MS data in order to identify each unknown compound. Spectroscopic data are given on the following pages.

- show clearly your calculation of the IHD value for each compound.

- show all lone pairs and charges for each structure, partial structure, or fragment.

- label each set of equivalent protons using the H_a, H_b, H_c etc. labeling system shown in the NMR lectures and practice problem sets.

- assign each ^{1}H-NMR signal to a particular set of equivalent protons and write your assignments directly onto the spectrum.

- draw the molecule directly onto the ^{1}H-NMR spectrum.

- 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).

- identify each IR absorption band as due to a specific functional group.

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

- use all data supplied and hand in all spectra for each question.

- write and sketch clearly! Your TA cannot grade what he/she cannot read.

- points will be deducted for illegible writing, unclear/ambiguous drawings, etc.

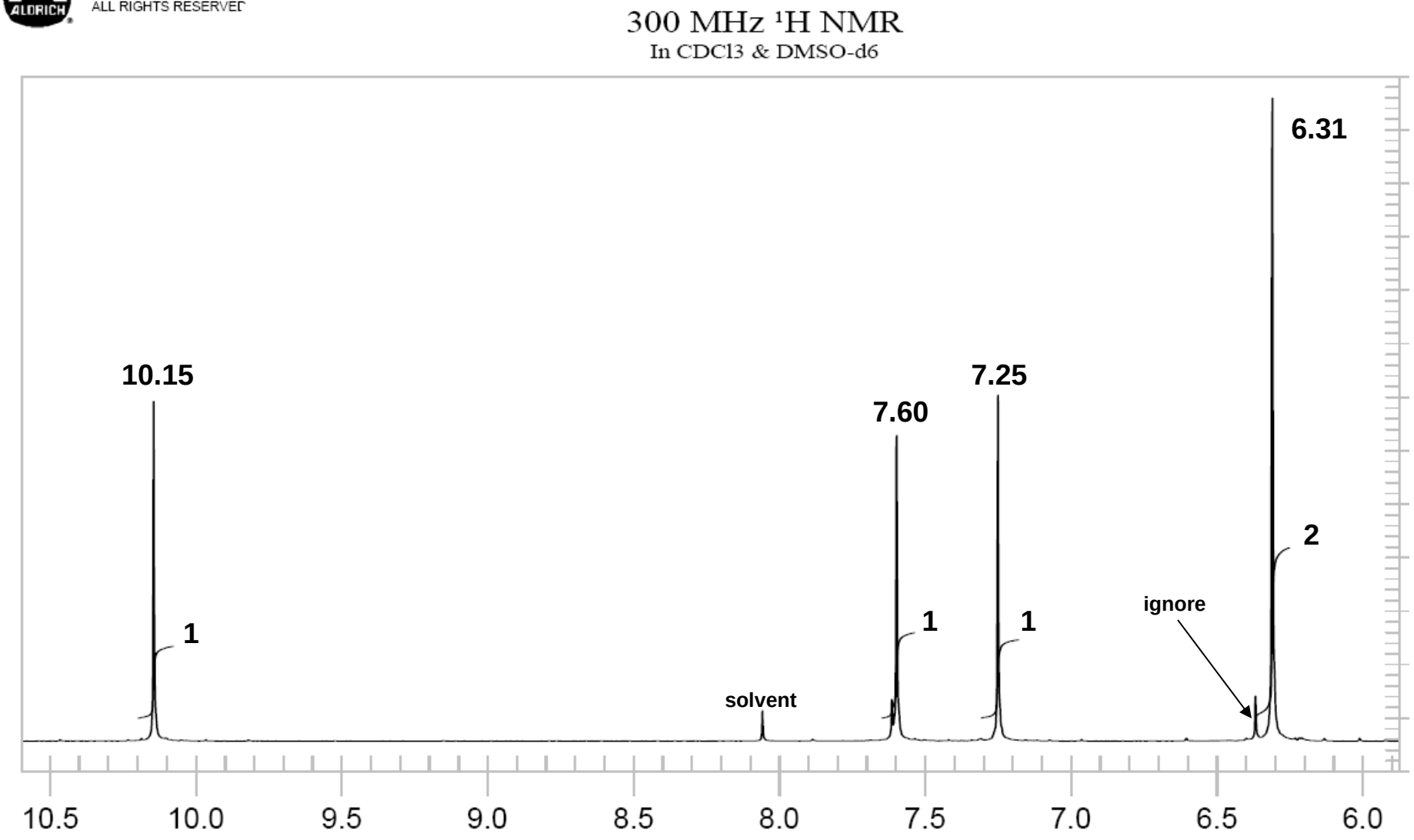
2) Use the supplied ^{1}H-NMR, ^{13}C-NMR, and IR data to identify Compound A, $C_8H_5NO_5$ (10 pts).

3) Use the supplied ^{1}H- NMR, ^{13}C-NMR, IR, and EI-MS data to identify Compound B, $C_5H_7NO_2$ (14 pts).

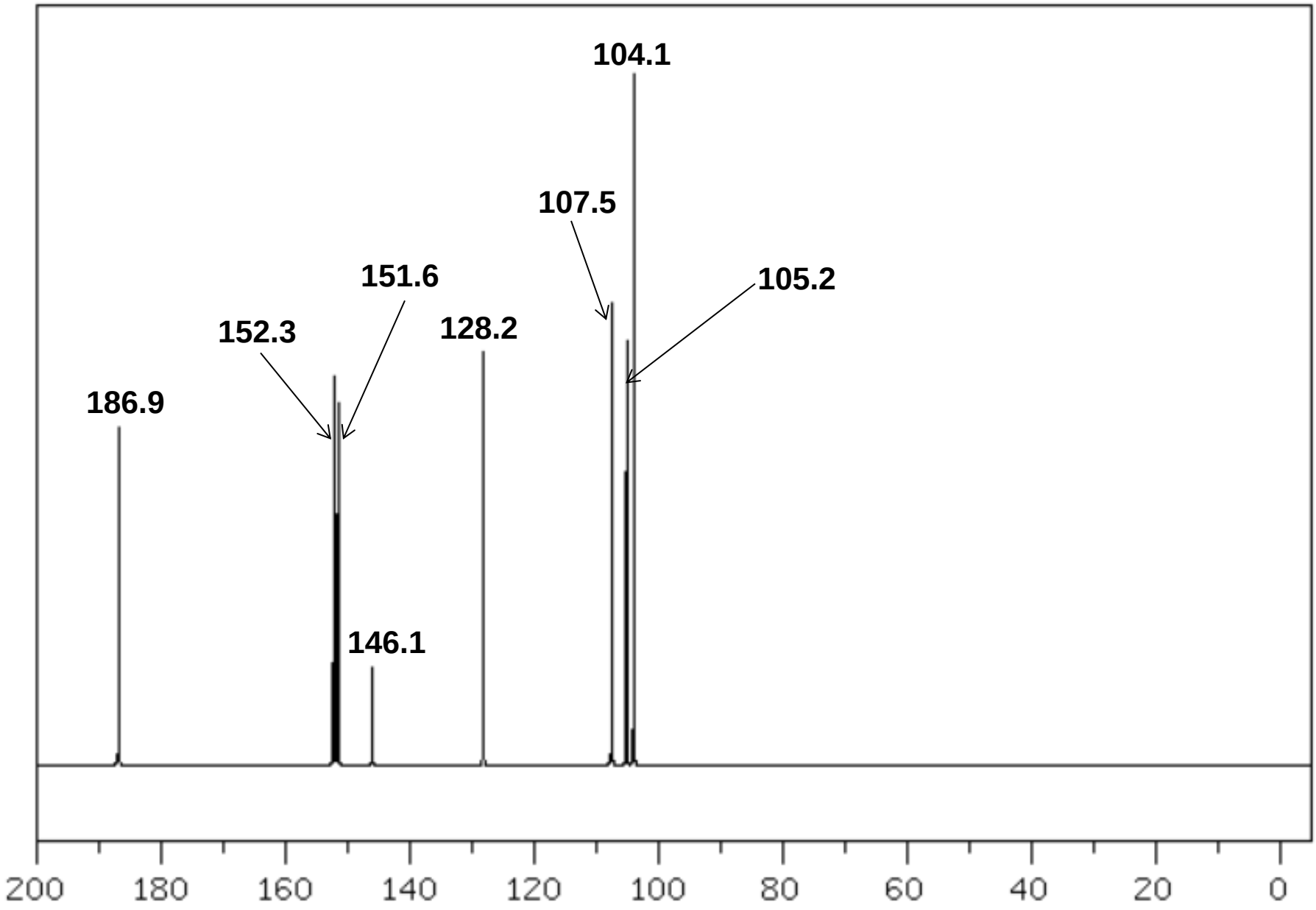
4) Use the supplied ^{1}H- NMR, ^{13}C-NMR, and EI-MS data to identify Compound C, $C_{13}H_{20}N_2O_2$ (16 pts).

Q2) Compound A $C_8H_5NO_5$

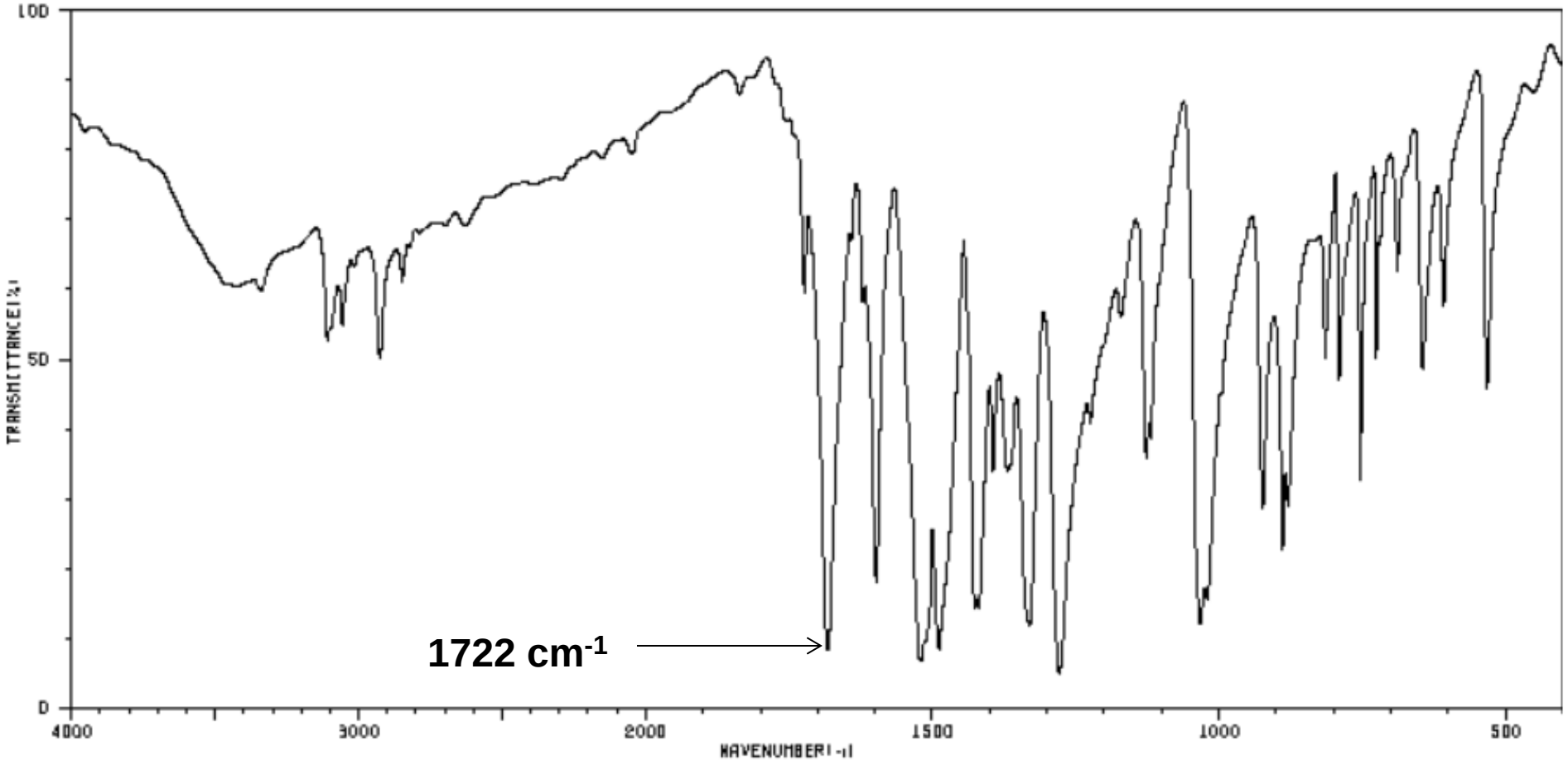
^{1}H-NMR Spectrum 6 – 10.5 ppm (no signals 0-6 ppm)



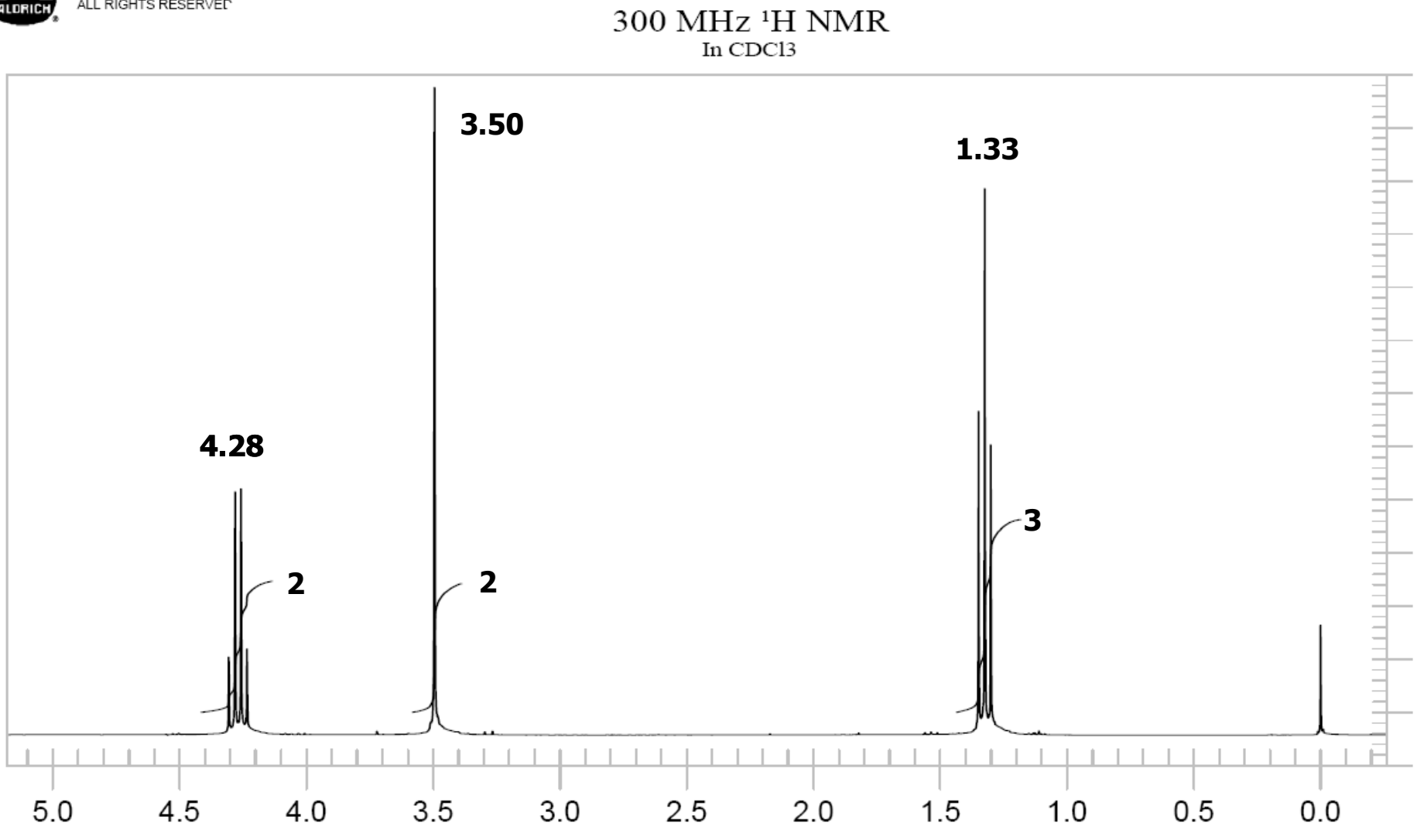
Q2) Compound A $C_8H_5NO_5$ ^{13}C-NMR Spectrum



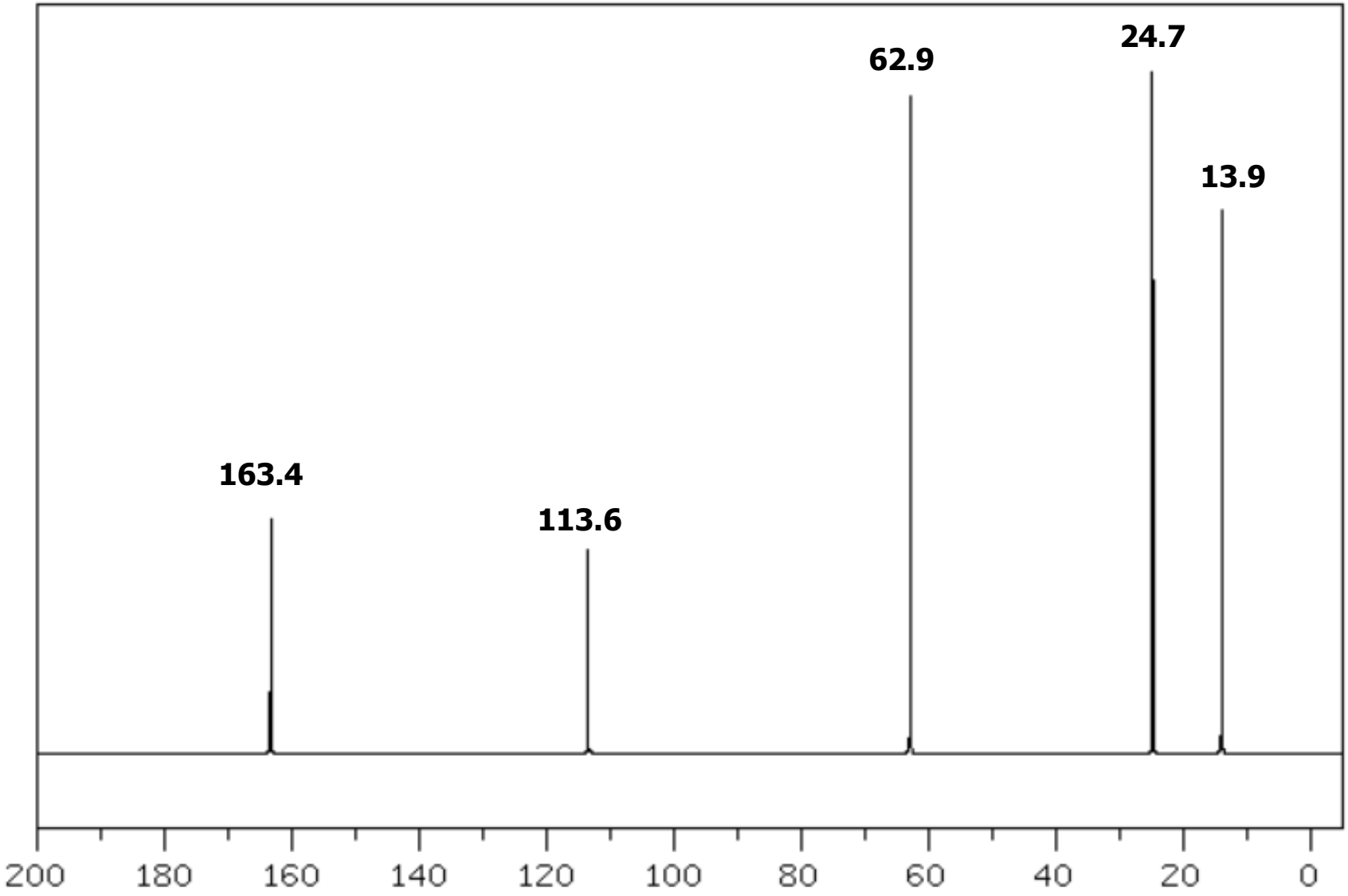
Q2) Compound A $C_8H_5NO_5$ IR Spectrum



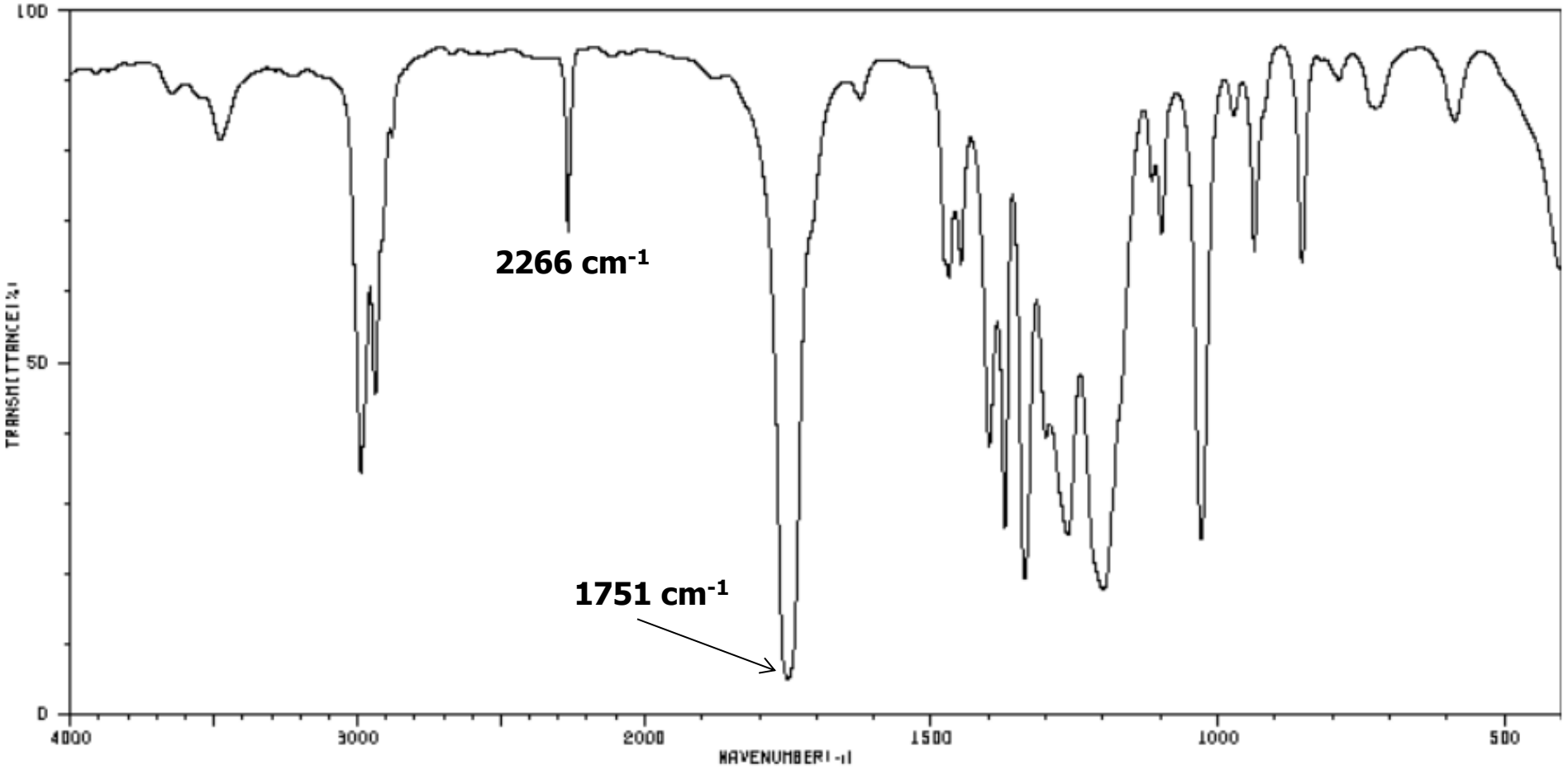
Q3) Compound B $C_5H_7NO_2$ ^{1}H-NMR Spectrum



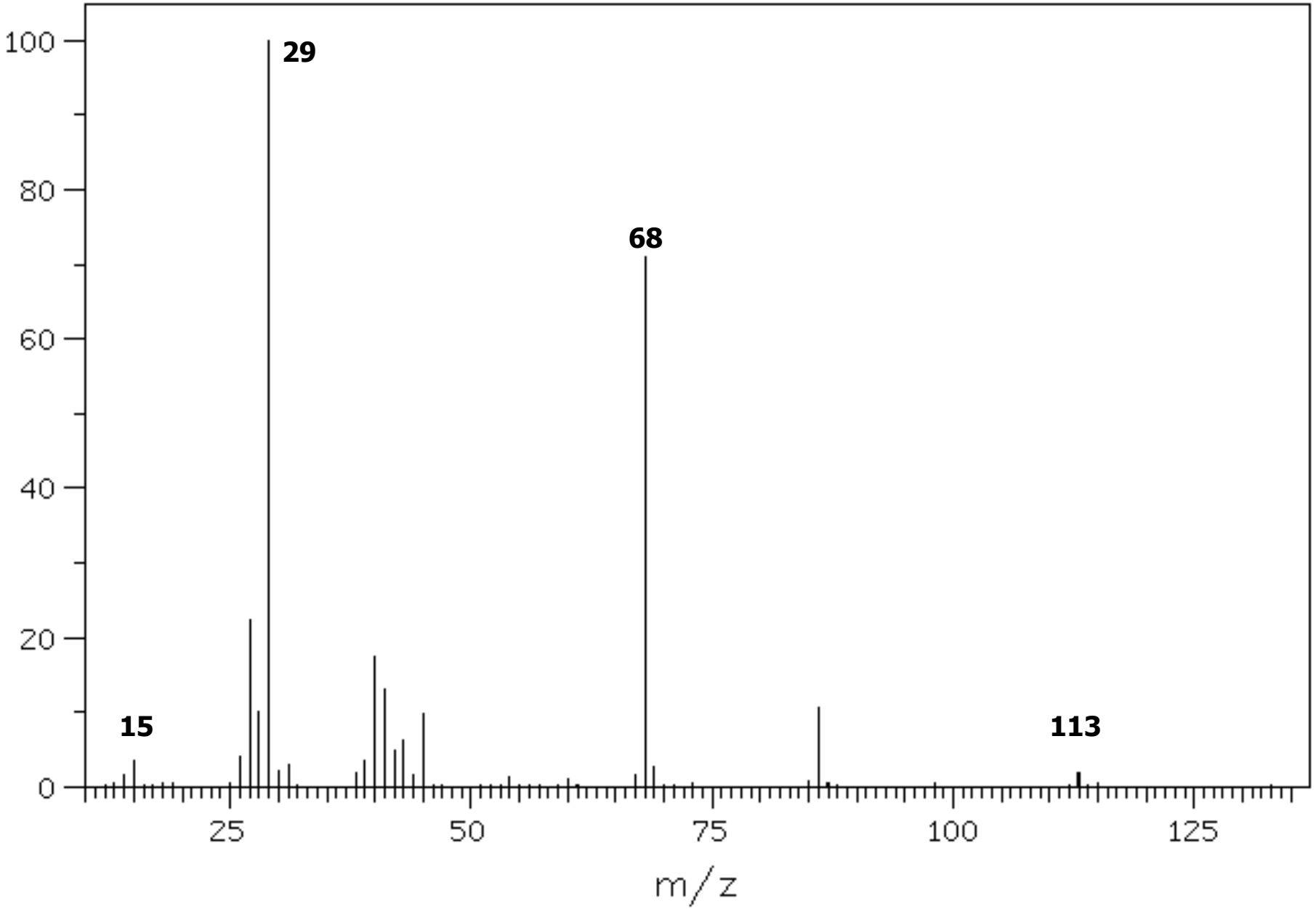
Q3) Compound B $C_5H_7NO_2$ ^{13}C-NMR Spectrum



Q3) Compound B $C_5H_7NO_2$ IR Spectrum

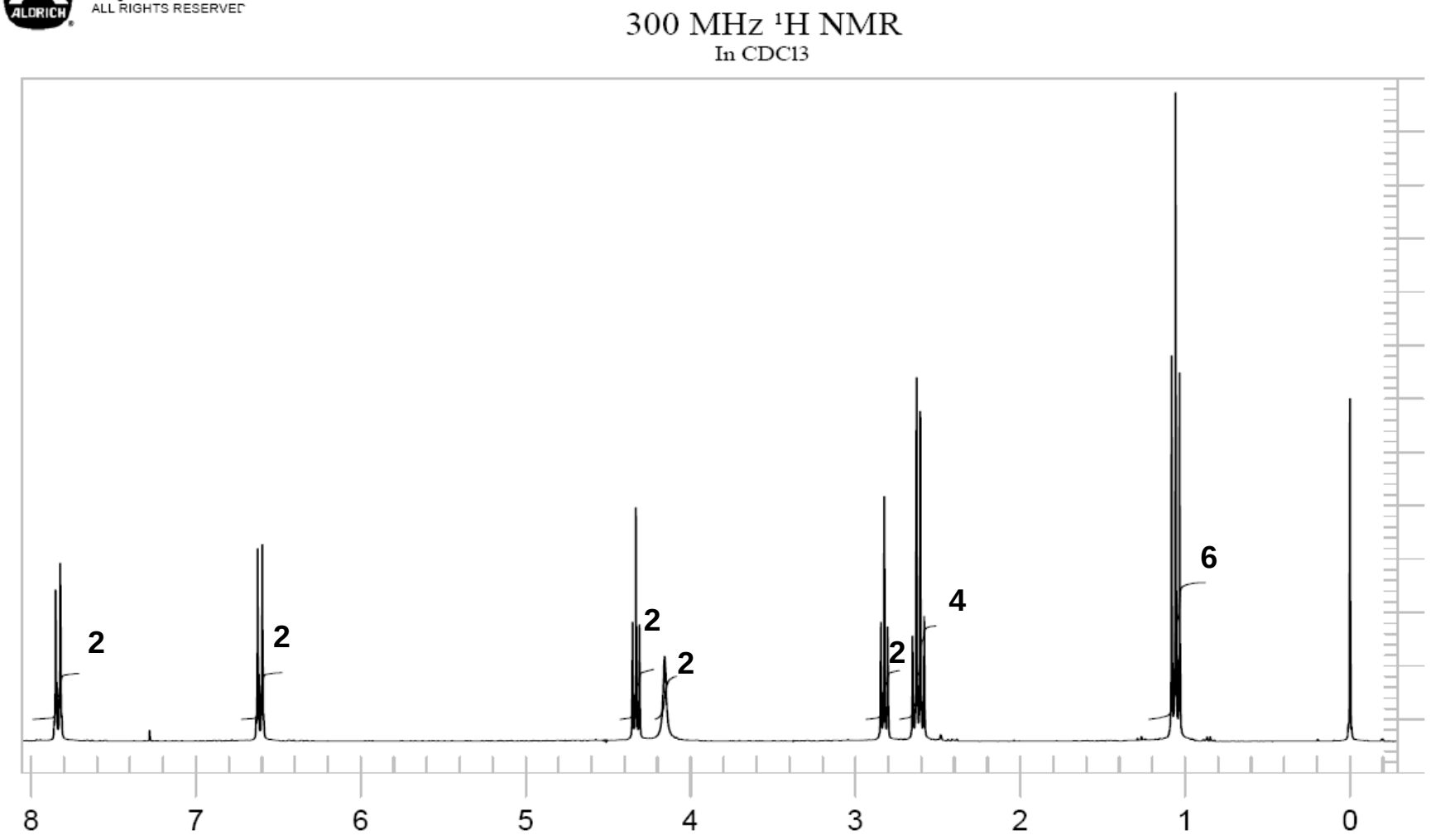


Q3) Compound B $C_5H_7NO_2$ EI-MS



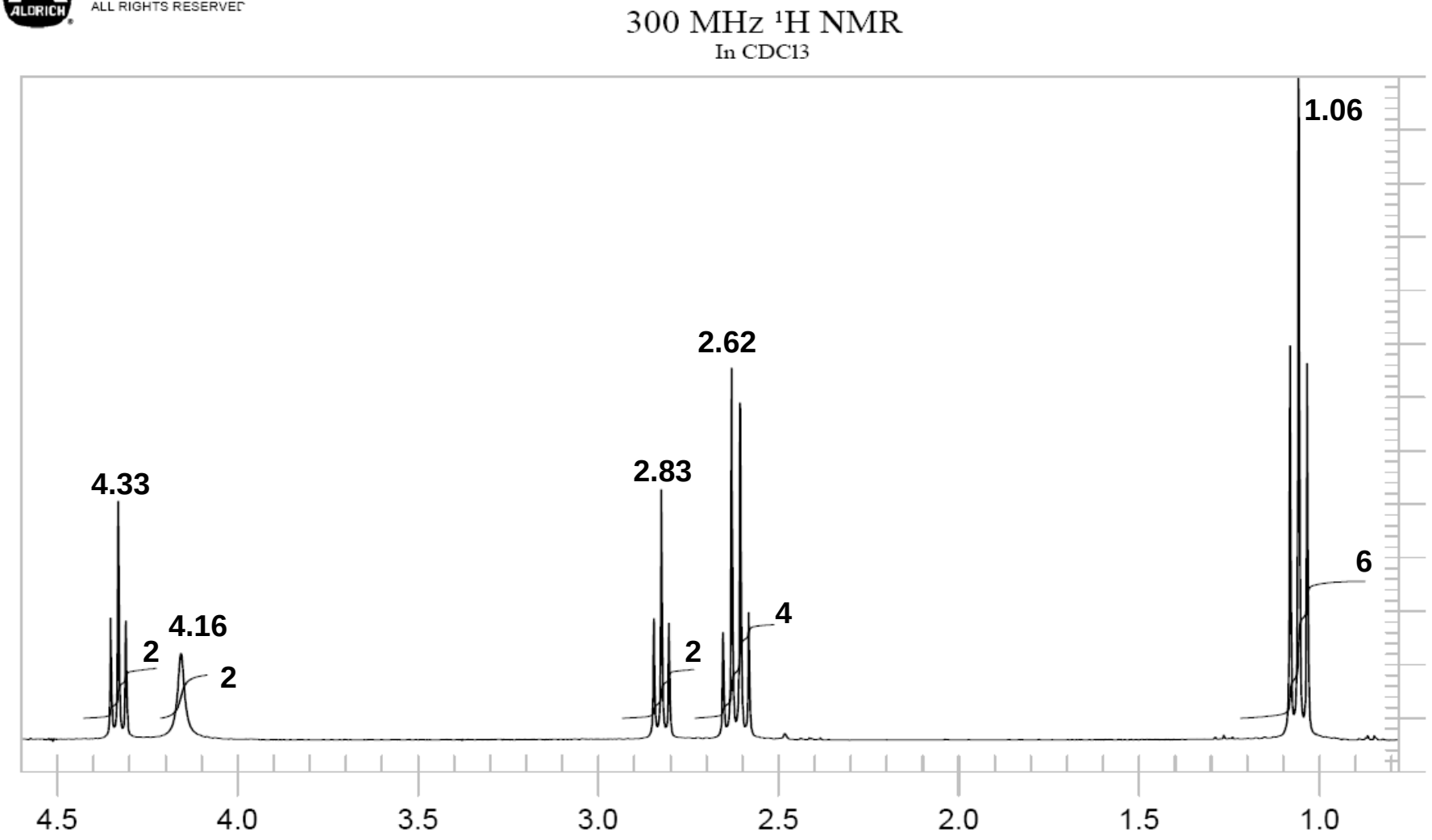
Q4) Compound C $C_{13}H_{20}N_2O_2$

^{1}H-NMR Spectrum 0- 8 ppm



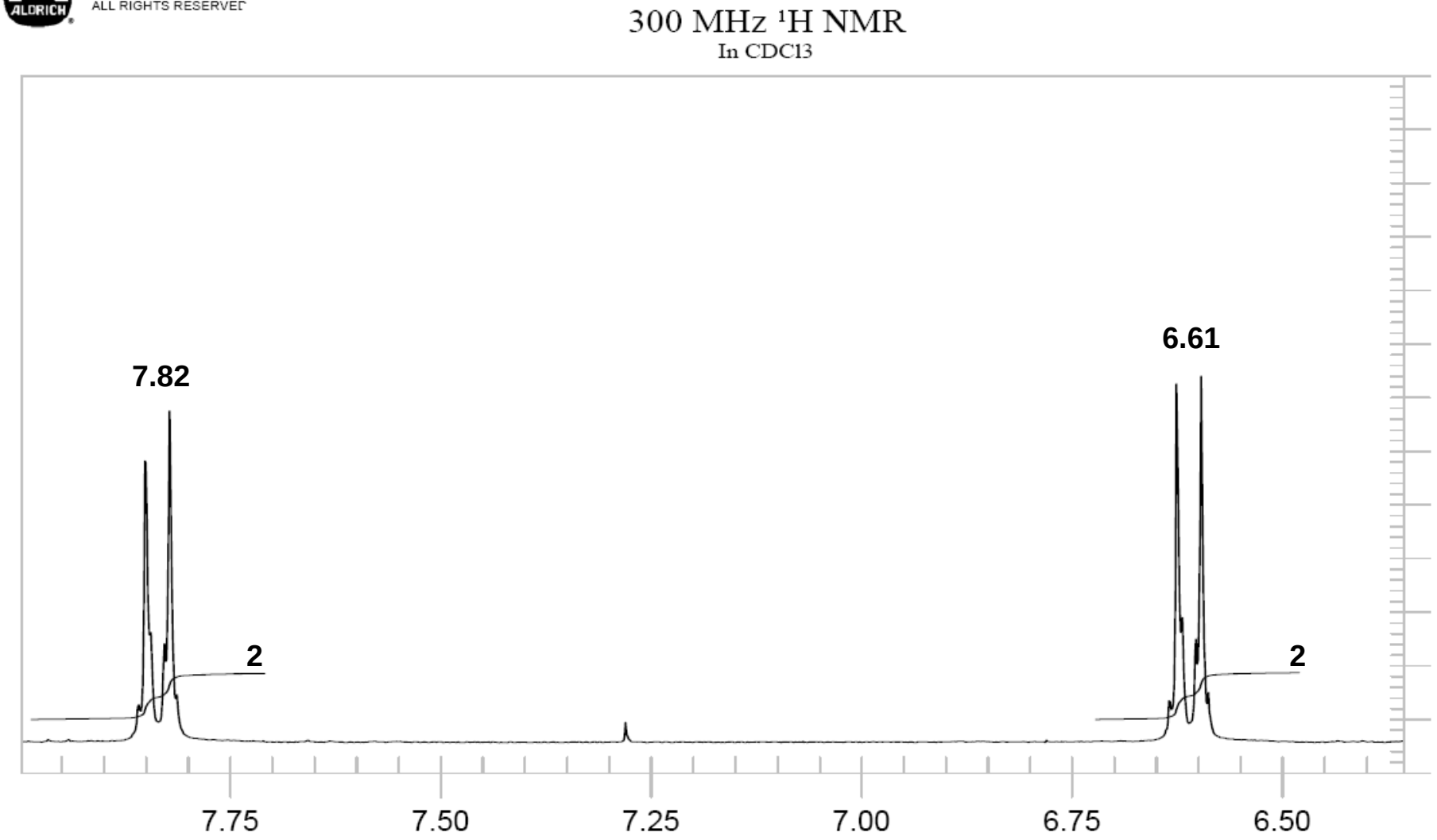
Q4) Compound C $C_{13}H_{20}N_2O_2$

^{1}H-NMR Spectrum 1.0 – 4.5 ppm

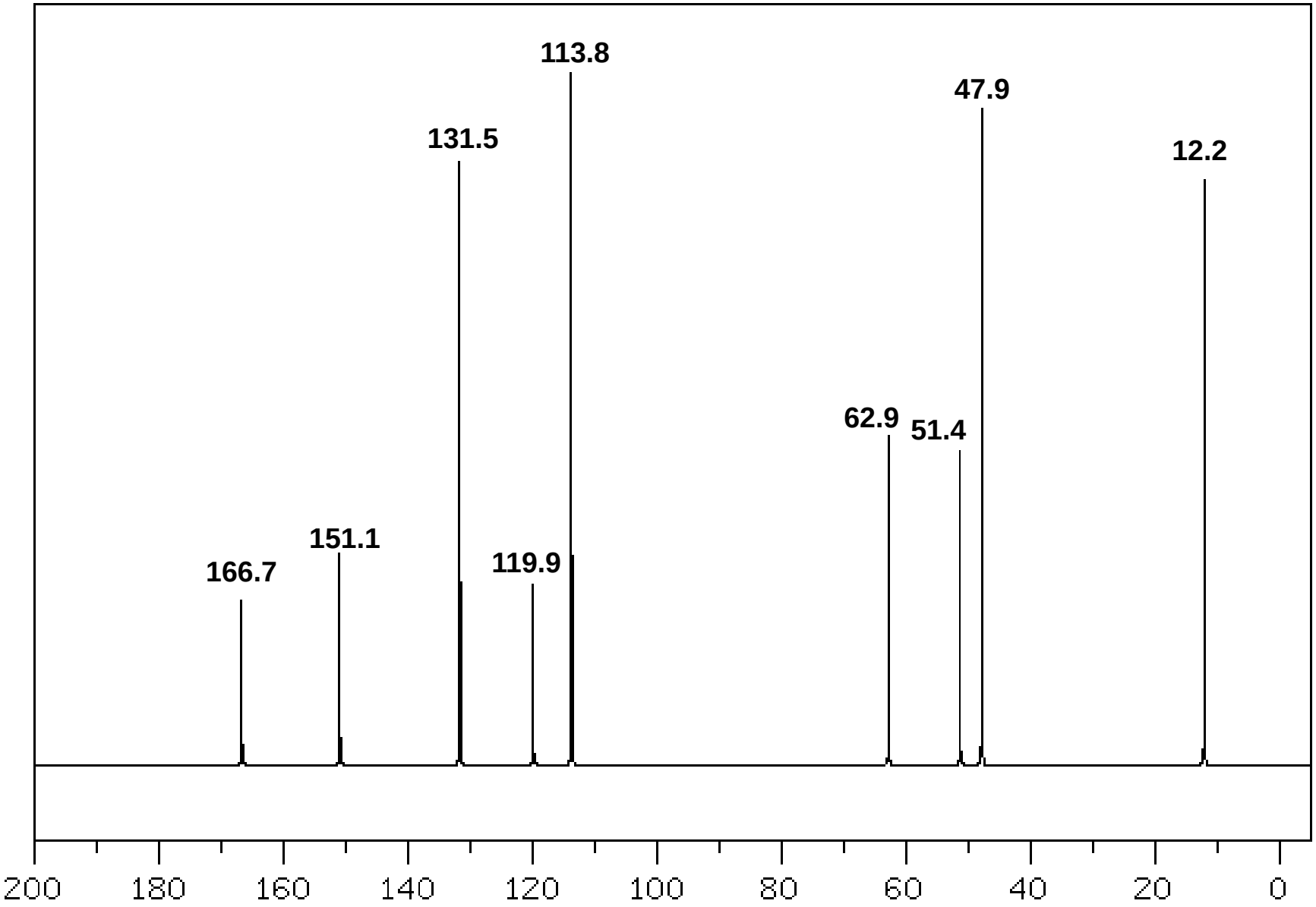


Q4) Compound C $C_{13}H_{20}N_2O_2$

^{1}H-NMR Spectrum 6.5 – 8.0 ppm



Q4) Compound C $C_{13}H_{20}N_2O_2$ ^{13}C-NMR Spectrum



Q4) Compound C $C_{13}H_{20}N_2O_2$ EI-MS