^{1}H-NMR Spectroscopy Worksheet

Part I

For each of the molecular formulas shown below calculate the index of hydrogen deficiency (IHD). In addition, suggest three possible chemical structures that are consistent with the degree of unsaturation.

a) $C_7H_{14}O_2$

b) $C_4H_{10}O$

c) $C_9H_{10}O$

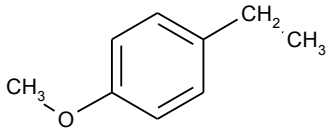
d) $C_8H_9NO_3$

e) $C_4H_6O_2$

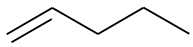
f) $C_7H_{10}Cl_2$

Part II

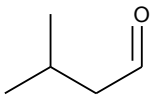
For each of the following chemical structures a ^{1}H-NMR spectrum is provided on the following 3 pages. Match each compound with its ^{1}H-NMR spectrum. Draw the structure above the corresponding spectrum and clearly assign the chemical shifts to the appropriate protons on the molecule.



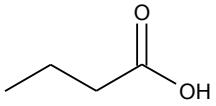
p-ethylanisole



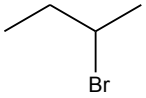
1-pentene



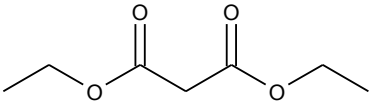
3-methylbutanal



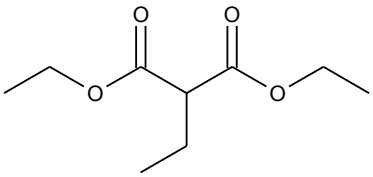
butanoic acid



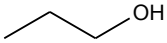
2-bromobutane



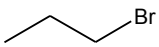
diethyl malonate



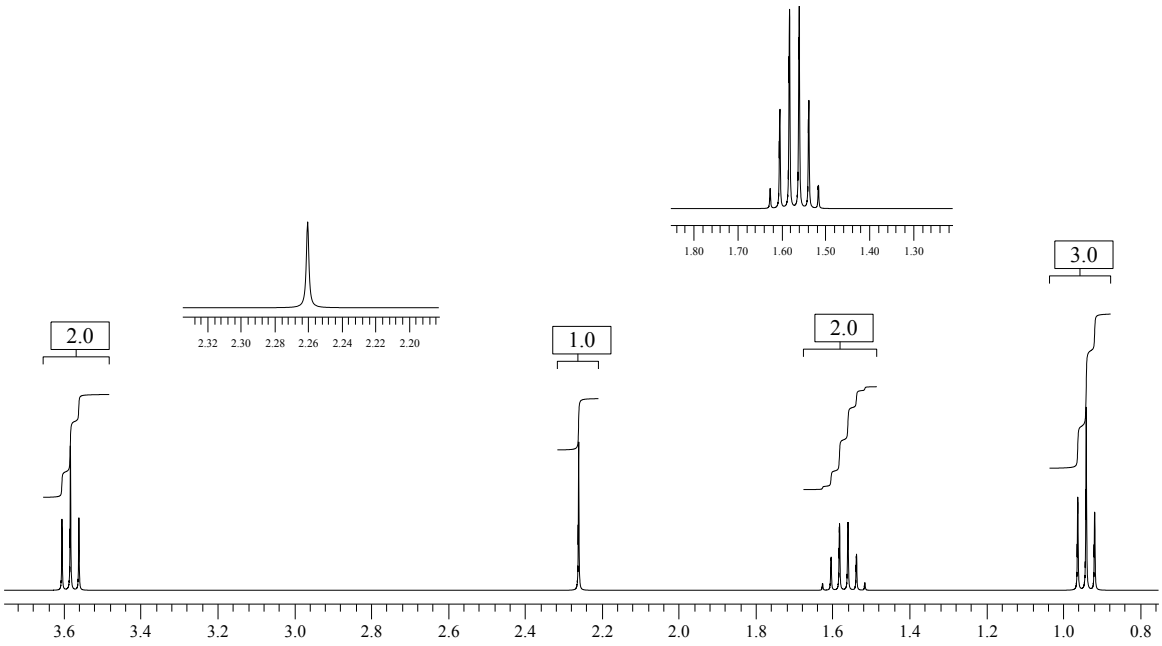
diethyl ethylmalonate



1-propanol



1-bromopropane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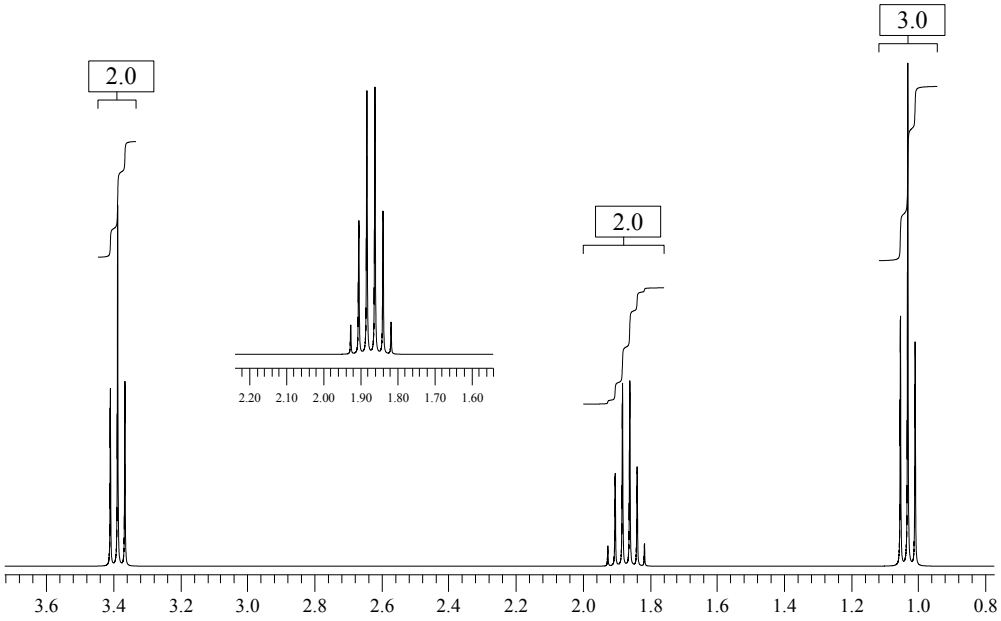
2.0
3.0
3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8
2.32 2.30 2.28 2.26 2.24 2.22 2.20
1.80 1.70 1.60 1.50 1.40 1.30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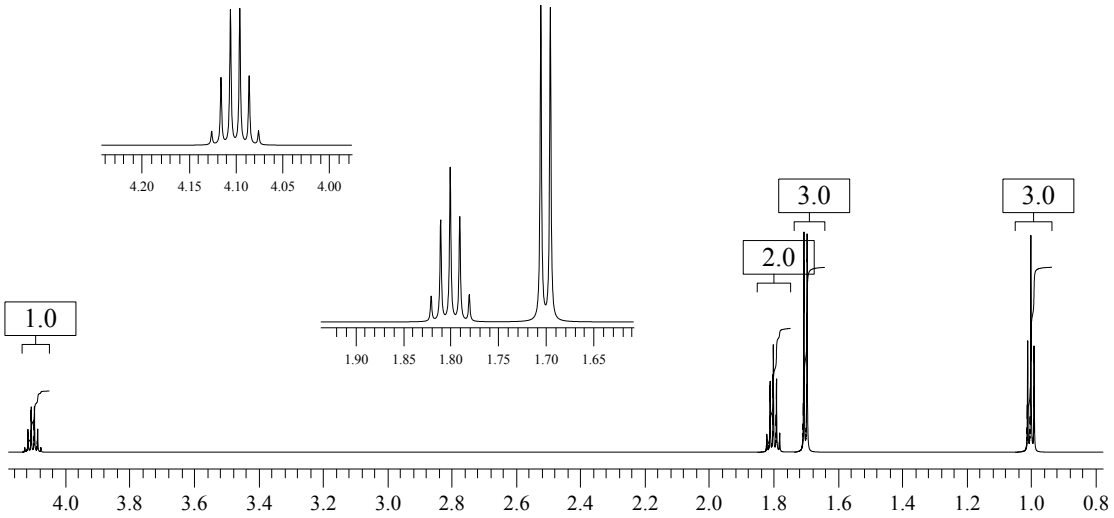
2.0
3.0
3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8
2.20 2.10 2.00 1.90 1.80 1.70 1.60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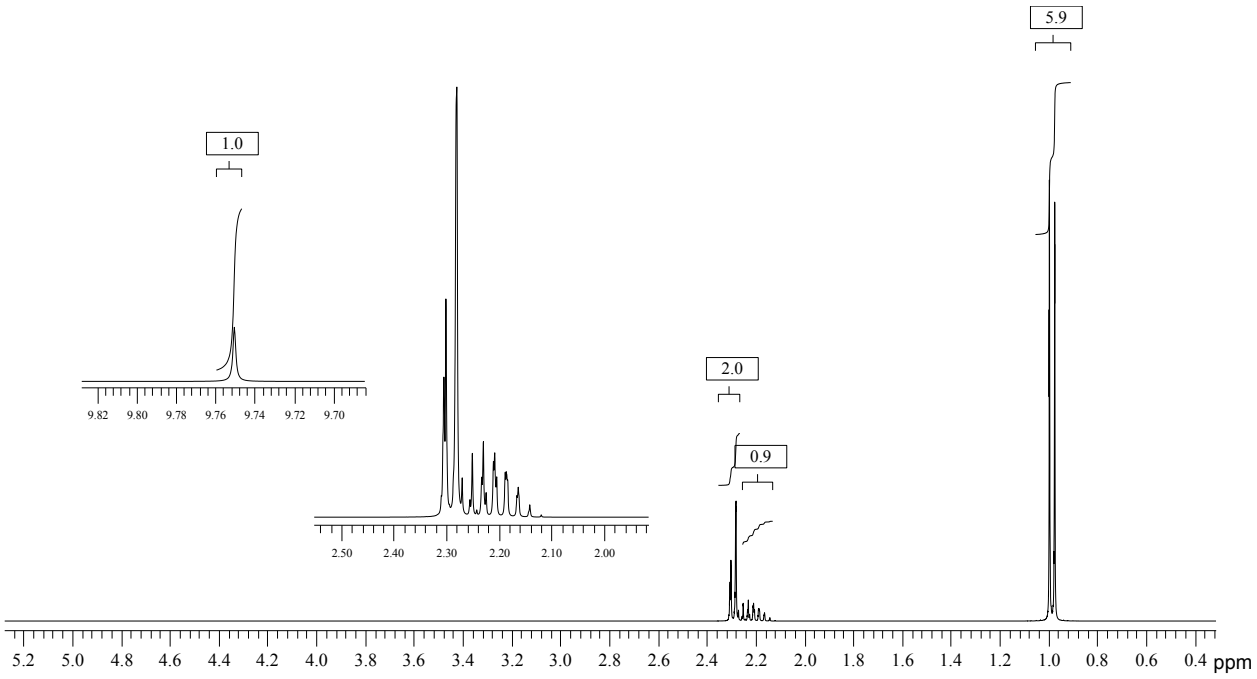
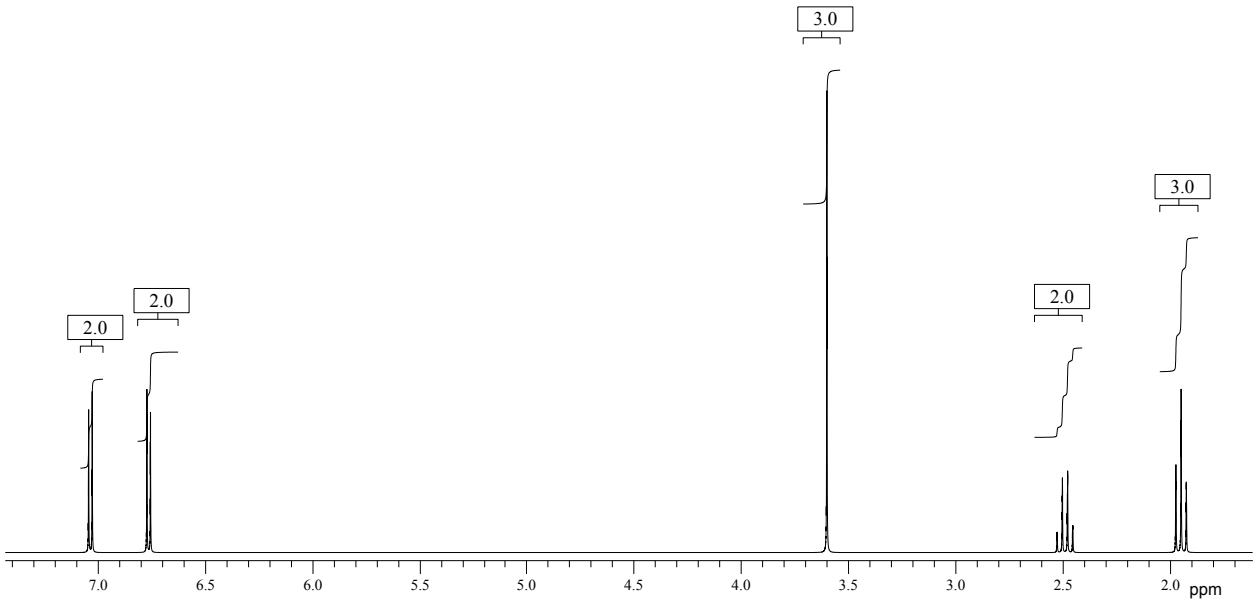
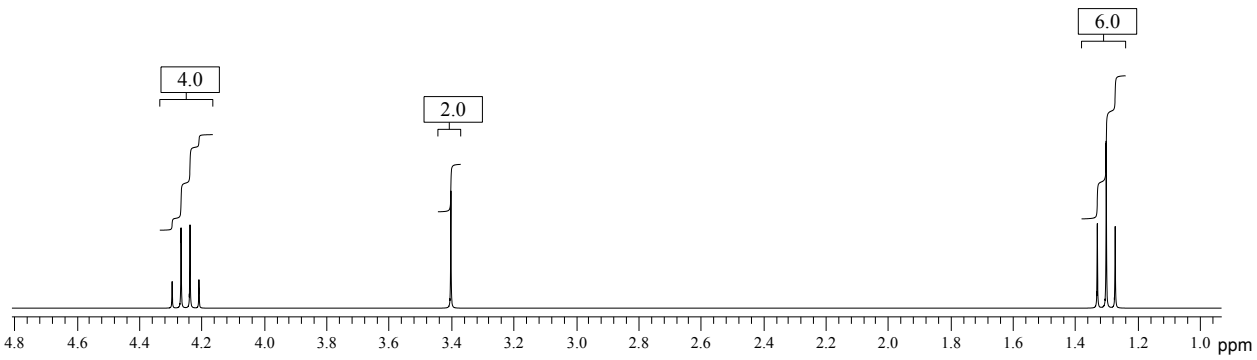
2.0
3.0
3.0
4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8
4.20 4.15 4.10 4.05 4.00
1.90 1.85 1.80 1.75 1.70 1.65


5.9
1.0
2.0
0.9
9.82 9.80 9.78 9.76 9.74 9.72 9.70
2.50 2.40 2.30 2.20 2.10 2.00
5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4 ppm


3.0
3.0
2.0
2.0
2.0
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm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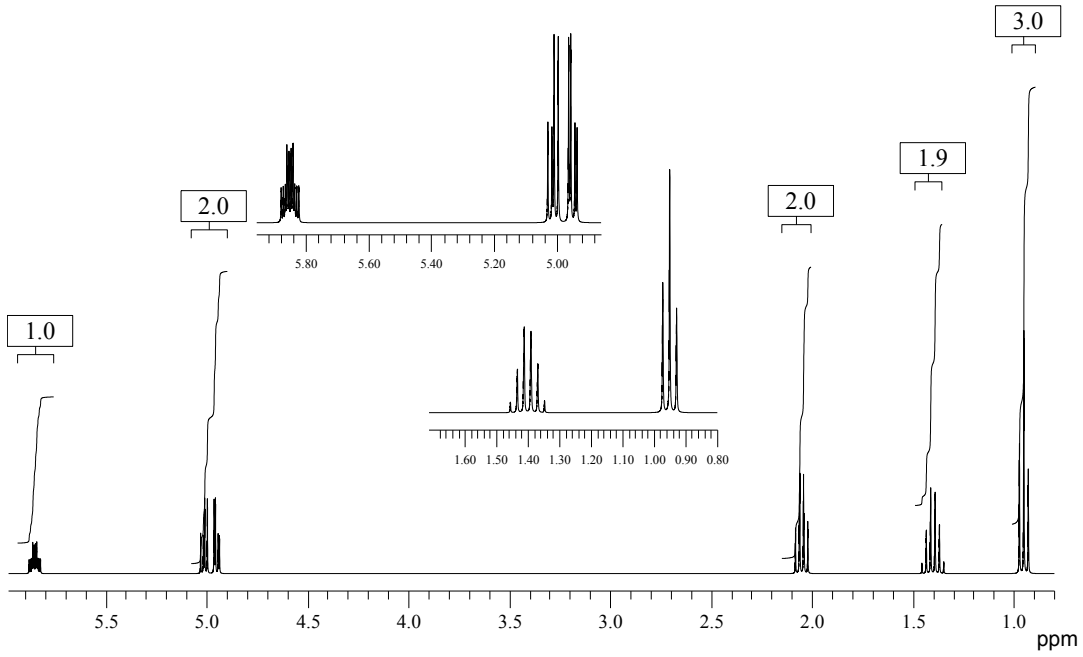
4.0
2.0
4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 ppm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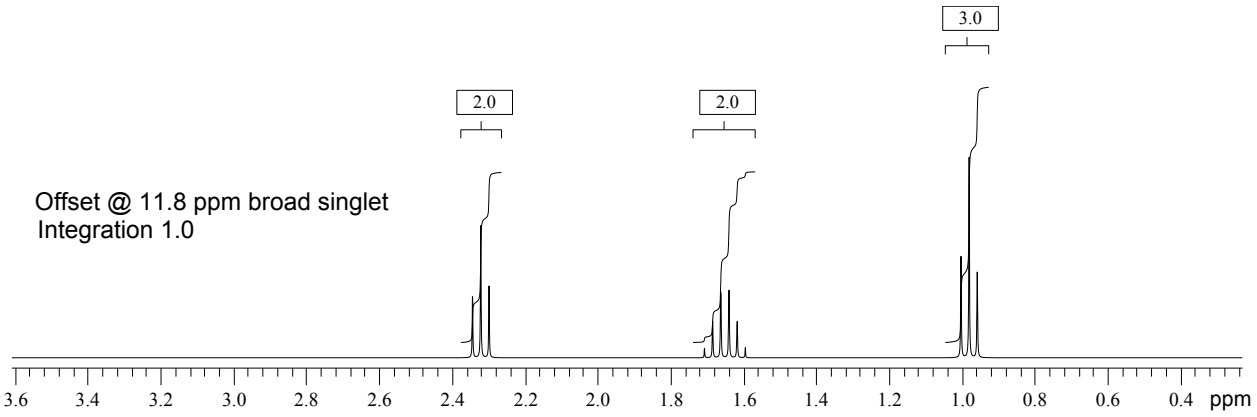
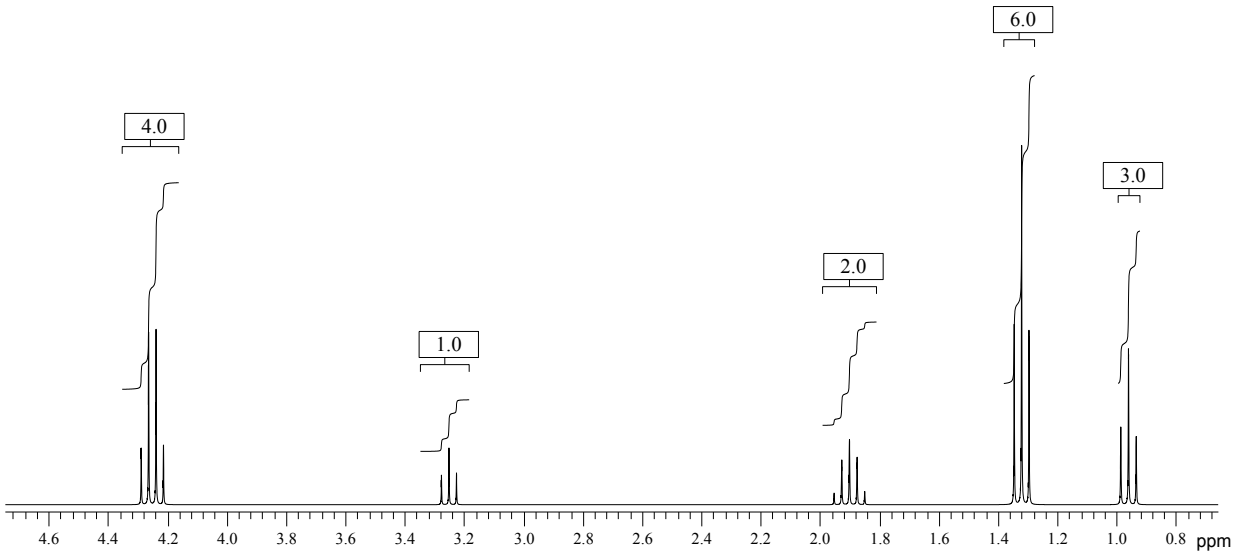
1.9
2.0
2.0
1.0
5.80 5.60 5.40 5.20 5.00
1.60 1.50 1.40 1.30 1.20 1.10 1.00 0.90 0.80
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
ppm


3.0
2.0
2.0
Offset @ 11.8 ppm broad singlet
Integration 1.0
3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4
ppm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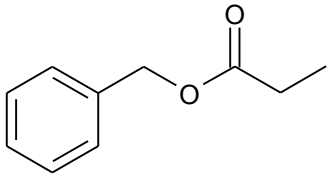
4.0
3.0
2.0
1.0
4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8
ppm

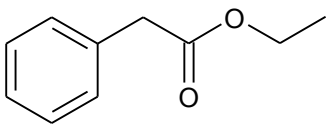
Part III

Shown below are the structures of two esters. They are isomers and the only difference between the two compounds is the orientation around the ester functional group. We have provided the ^{1}H-NMR of each ester in the next page.

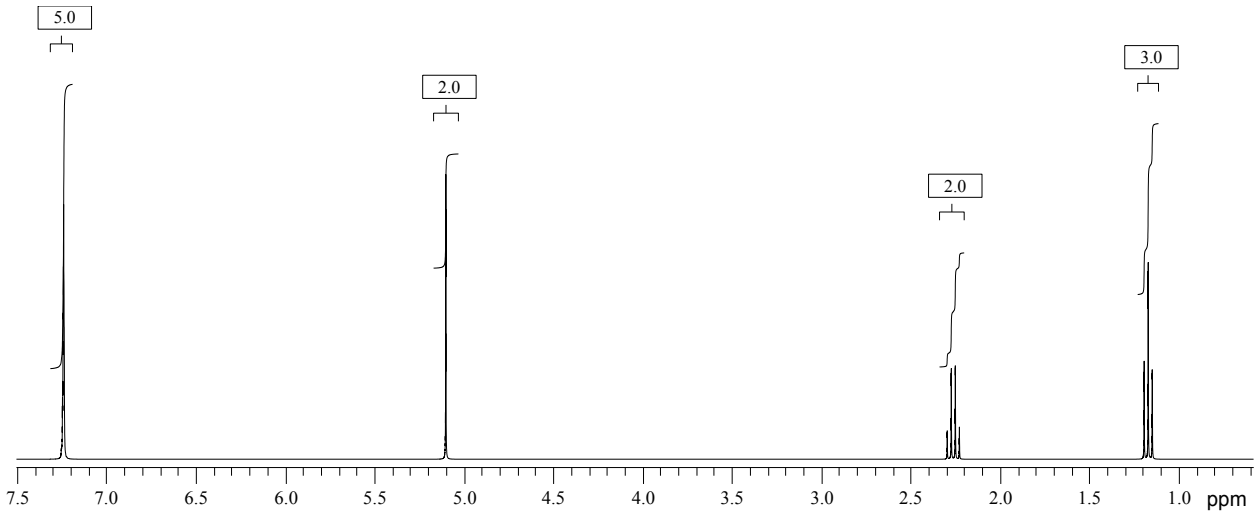
1) Match each compound with its ^{1}H-NMR.
2) Draw the structure above the spectrum and assign the protons to their appropriate chemical shifts.

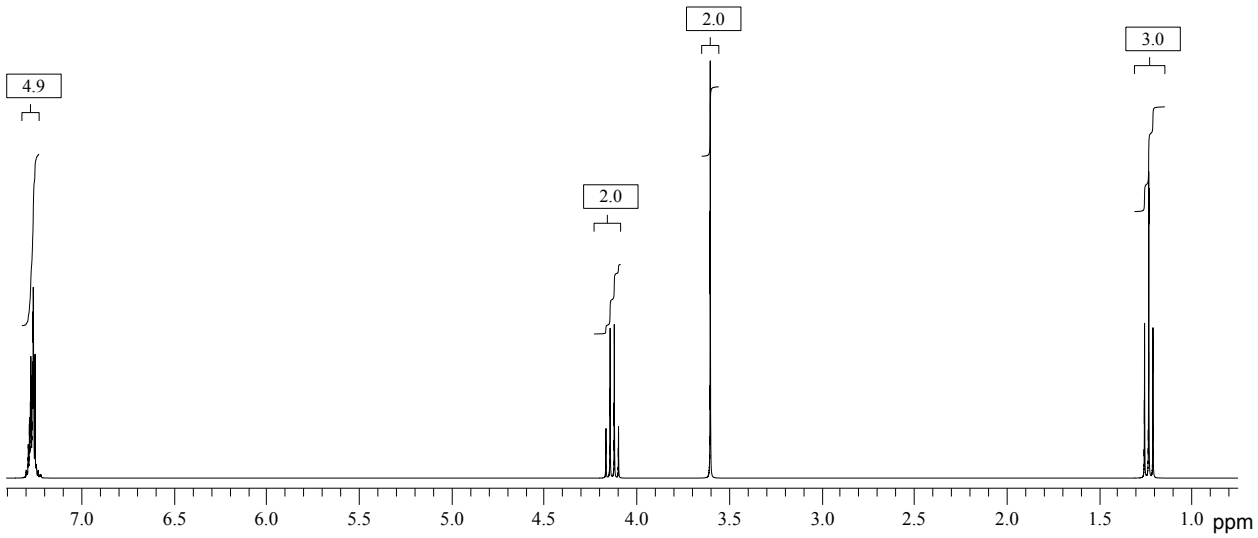


benzyl propionate



ethyl phenylacetate

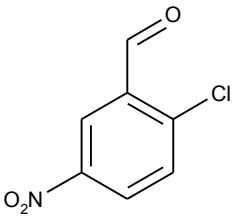

5.0
2.0
2.0
3.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm


4.9
2.0
2.0
3.0
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

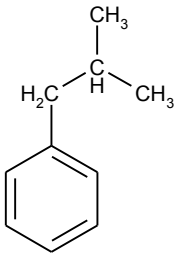
Part IV

The ^{1}H-NMR spectra of the following pages represent mono, di and trisubstituted aromatic compounds. Also included are disubstituted compounds as ortho, meta and para. The compounds representing each spectrum are shown below.

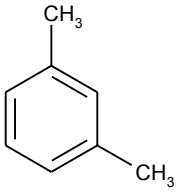
a) Match each ^{1}H-NMR spectrum to its compound.
b) Draw the chemical structure above the spectrum and indicate the protons on each chemical shift. You do not have to assign each specific peak on the aromatic region.



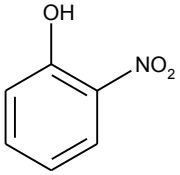
2-chloro-5-nitrobenzaldehyde



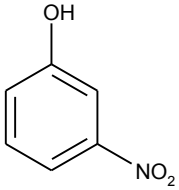
Isobutylbenzene



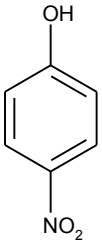
m-xylene



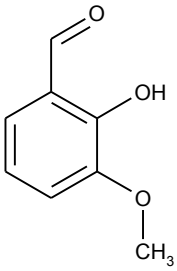
o-nitrophenol



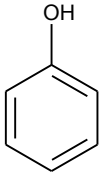
m-nitrophenol



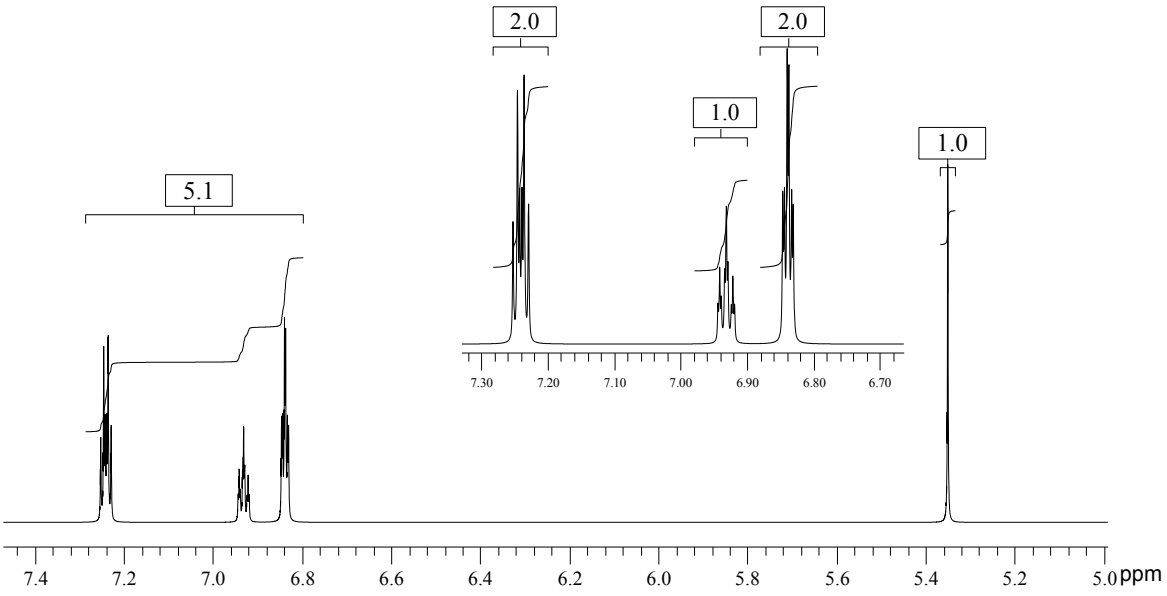
p-nitrophenol

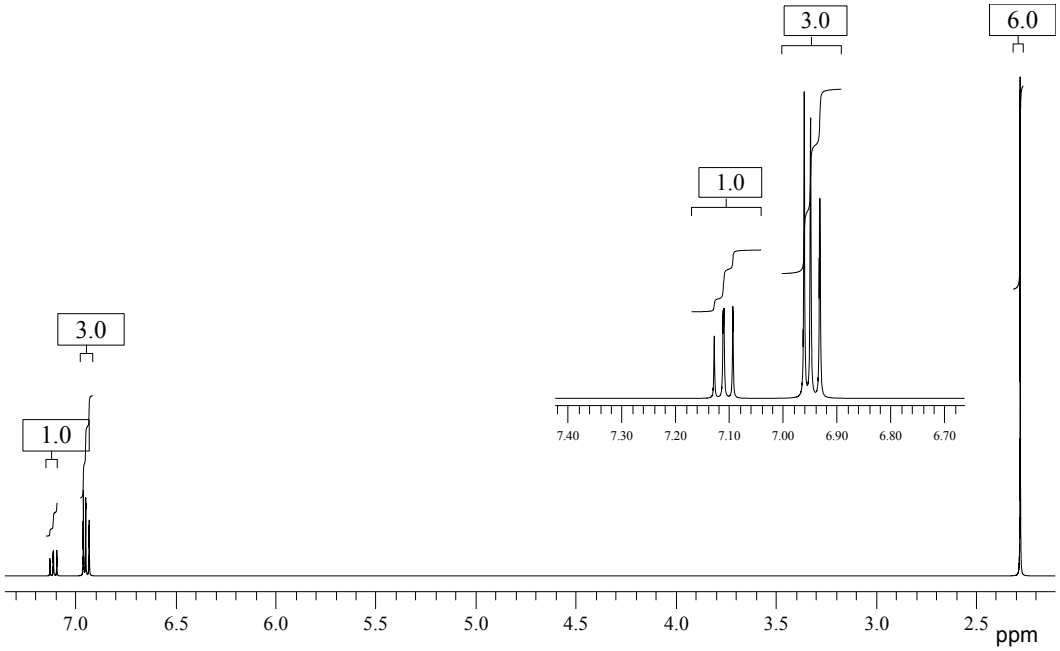


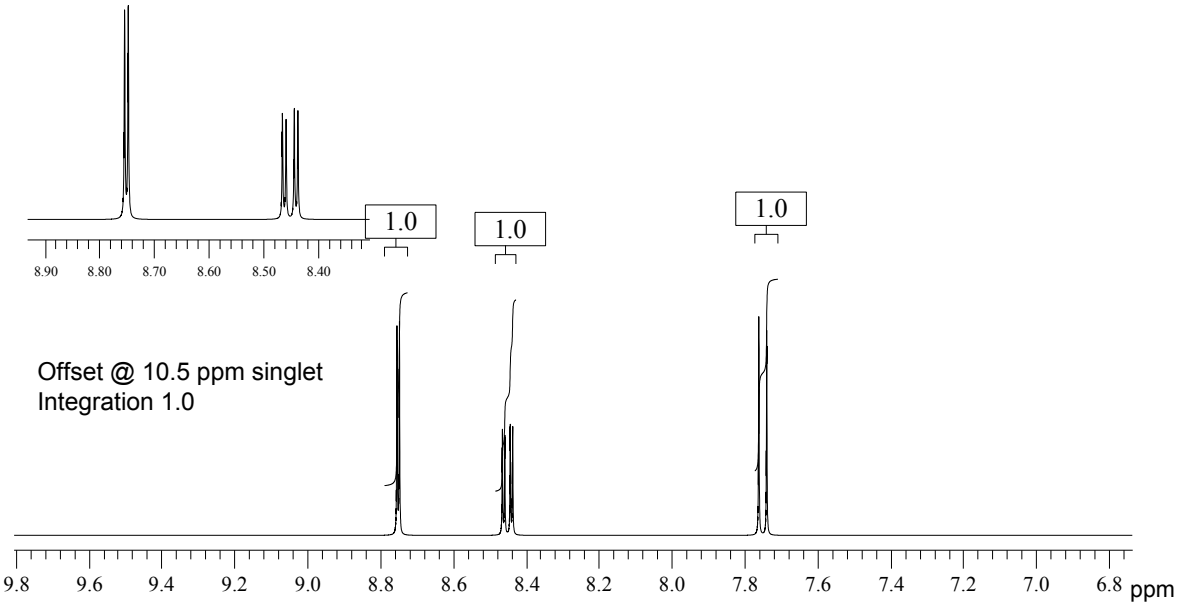
o-vanillin

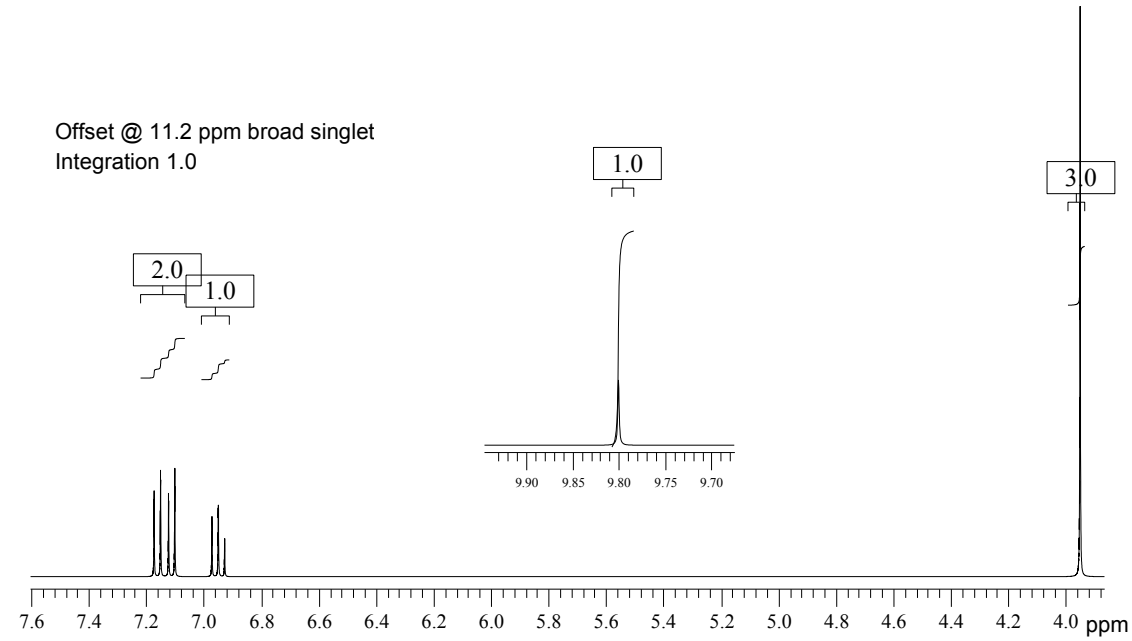


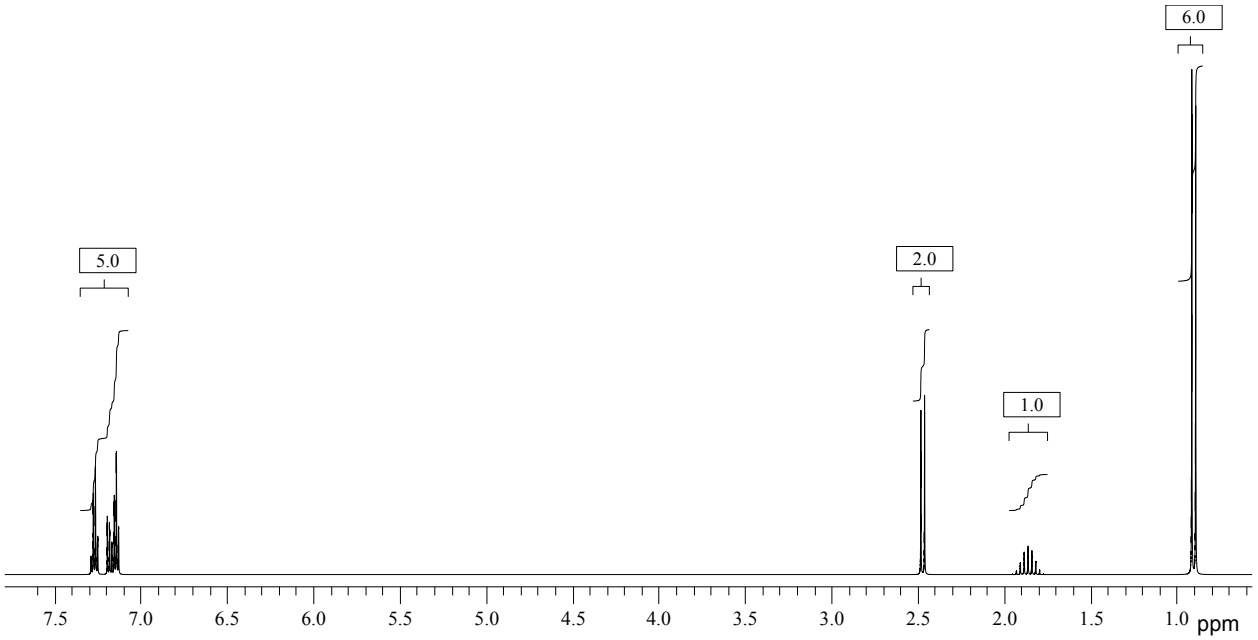
phenol

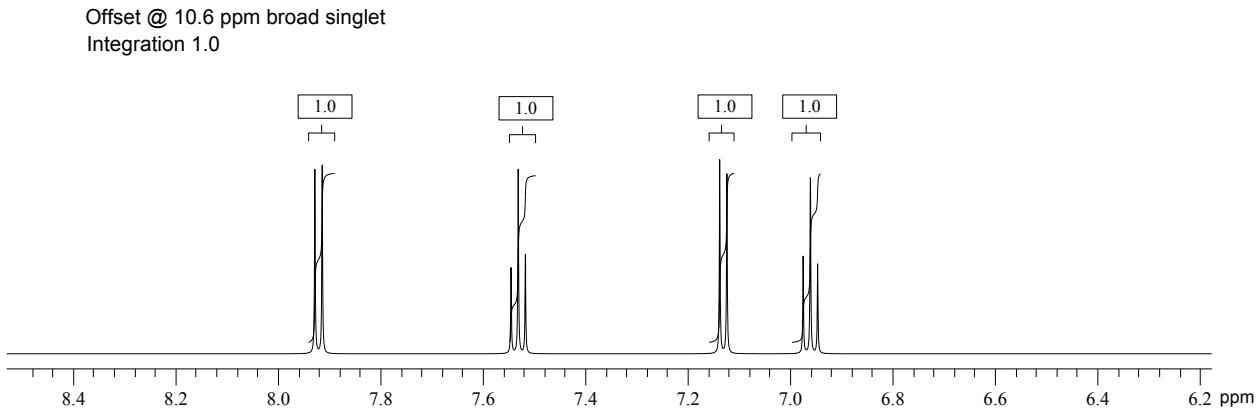

2.0
2.0
1.0
1.0
5.1
7.30 7.20 7.10 7.00 6.90 6.80 6.70
7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 ppm


3.0
6.0
1.0
3.0
1.0
7.40 7.30 7.20 7.10 7.00 6.90 6.80 6.70
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm

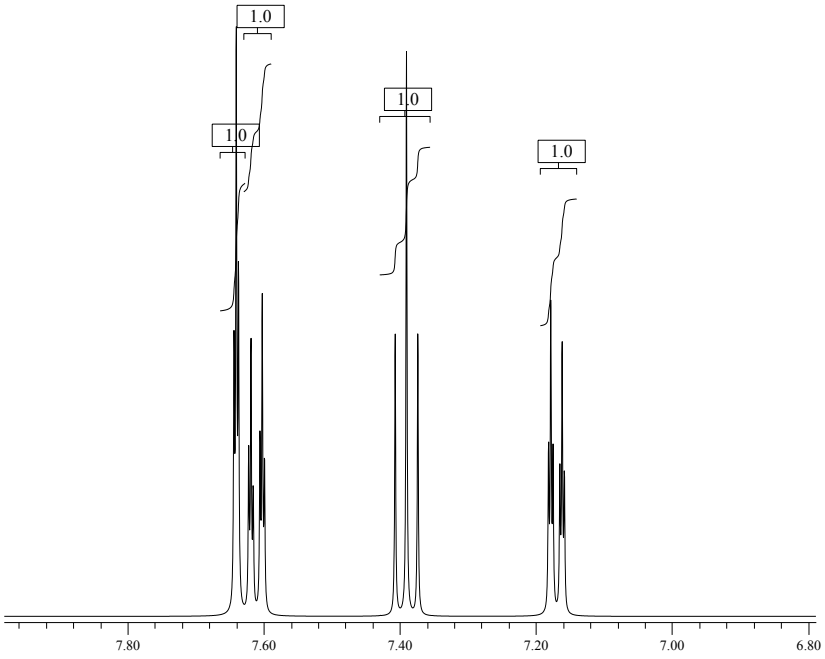

1.0
1.0
1.0
8.90 8.80 8.70 8.60 8.50 8.40
Offset @ 10.5 ppm singlet
Integration 1.0
9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 ppm


Offset @ 11.2 ppm broad singlet
Integration 1.0
1.0
3.0
2.0
1.0
9.90 9.85 9.80 9.75 9.70
7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 ppm


6.0
5.0
2.0
1.0
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


Offset @ 10.6 ppm broad singlet
Integration 1.0
1.0
1.0
1.0
1.0
8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 ppm

Offset at 10.3 ppm small broad singlet
Integration 1.0



Offset @ 10.7 ppm broad singlet
Integration 1.0