Organic spectroscopy problem set

Teacher guide

This document is intended to provide opportunities for students to apply their understanding of the spectroscopic techniques in Module 8 Inquiry Question 2 to a wide range of compounds including those with functional groups from Module 7 Inquiry Question 1. The question stem is adapted from the HSC 2019 Chemistry examination Question 26a with the attached selection of spectra provided to adapt this question to new structures for students. This resource can be used in several ways:

1. Practice HSC style exam question for Module 8 Inquiry Question 2
2. Internal assessment stimulus material
3. Teaching resource for the comparison of each spectrum across the range of techniques covered in Module 8 Inquiry Question 2

Each spectrum provided for use as an unknown is identified in the table below along with a link to the original source (National Institute of Advanced Industrial Science and Technology, Japan, 2018). A complete worked example for each compound is provided as a **video resource** to guide students on how to extract data from each spectrum and identify the unknown compound.

Each unknown may be printed on a single double-sided sheet and allocated to students. An answer key is provided on page 5.

This project has been a joint collaboration between the NSW Department of Education, the Royal Australia Chemical Institute NSW Chemistry Education Group and Chemistry Education Division, the University of Sydney, and the University of New South Wales.

Contents

Syllabus reference

HSC Chemistry Module 7

Outcomes

- **CH11/12-5** - analyses and evaluates primary and secondary data and information
- **CH11/12-6** - solves scientific problems using primary and secondary data, critical thinking skills and scientific processes
- **CH11/12-7** - communicates scientific understanding using suitable language and terminology for a specific audience or purpose
- **CH12-14** - analyses the structure of, and predicts reactions involving, carbon compounds

Content

Inquiry question - How do we systematically name organic chemical compounds?

Investigate the nomenclature of organic chemicals, up to C8, using IUPAC conventions, including simple methyl and ethyl branched chains, including: (ACSCH127)

- alkanes
- alkenes
- alkynes
- alcohols (primary, secondary and tertiary)
- aldehydes and ketones
- carboxylic acids
- amines and amides
- halogenated organic compounds

Explore and distinguish the different types of structural isomers, including saturated and unsaturated hydrocarbons, including: (ACSCH035)

- chain isomers
- position isomers
- functional group isomers

HSC Chemistry Module 8

Outcomes

- **CH11/12-1** - develops and evaluates questions and hypotheses for scientific investigation
- **CH11/12-2** - designs and evaluates investigations in order to obtain primary and secondary data and information
- **CH11/12-3** - conducts investigations to collect valid and reliable primary and secondary data and information
- **CH11/12-4** - selects and processes appropriate qualitative and quantitative data and information using a range of appropriate media
- **CH11/12-7** - communicates scientific understanding using suitable language and terminology for a specific audience or purpose
- **CH12-15 -** describes and evaluates chemical systems used to design and analyse chemical processes

Content

Inquiry question: How is information about the reactivity and structure of organic compounds obtained?

Conduct qualitative investigations to test for the presence in organic molecules of the following functional groups:

- carbon–carbon double bonds
- hydroxyl groups
- carboxylic acids (ACSCH130)

Investigate the processes used to analyse the structure of simple organic compounds addressed in the course, including but not limited to:

- proton and carbon-13 NMR
- mass spectrometry
- infrared spectroscopy (ACSCH130)

Answer key

Table 1: Answer key for sample compounds A-Z

Sample spectra	Compound
A	Pentane
B	Hexane
C	Pent-1-ene
D	Hex-1-ene
E	Methanol
F	Ethanol
G	Ethanoic acid
H	Propan-1-ol
I	Propanal
J	Propan-2-ol
K	Propan-2-one
L	Butan-1-ol
M	Butan-2-ol
N	Ethyl acetate
O	2-methylpropan-2-ol
P	Methyl propanoate
Q	Pentanal
R	Pentanoic acid
S	Pentan-2-ol
T	Pentan-2-one
U	Propan-1-amine
V	Butan-1-amine
W	Butanamide
X	Pentanamide
Y	2-chloropropane
Z	1-bromopropane

Student activity: example

What is the structural formula of this compound? Justify your answer with reference to the information given on its reactivity and to at least three of the provided spectra. (5 marks)

Infrared absorption data

Bond	Wavenumber/cm^{-1}
N—H (amines)	3300–3500
O—H (alcohols)	3230–3550 (broad)
C—H	2850–3300
O—H (acids)	2500–3000 (very broad)
C≡N	2220–2260
C=O	1680–1750
C=C	1620–1680
C—O	1000–1300
C—C	750–1100

^{13}C NMR chemical shift data

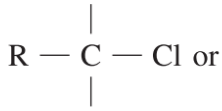
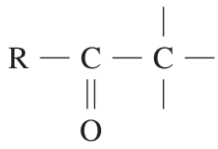
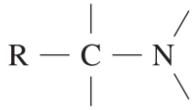
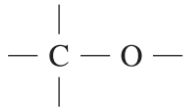
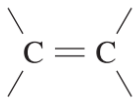
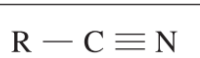
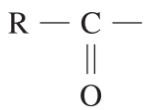
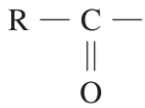
Type of carbon		δ/ppm
		5–40
		10–70
		20–50
		25–60
	alcohols, ethers or esters	50–90
		90–150
		110–125
		110–160
	esters or acids	160–185
	aldehydes or ketones	190–220

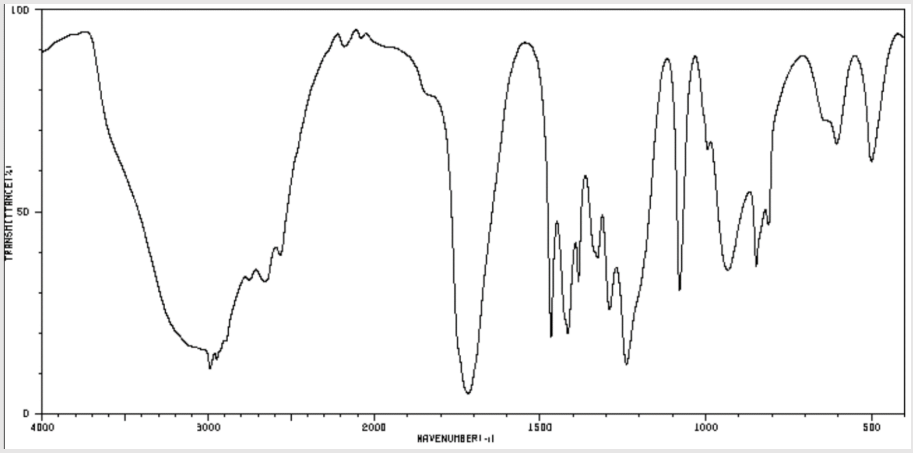
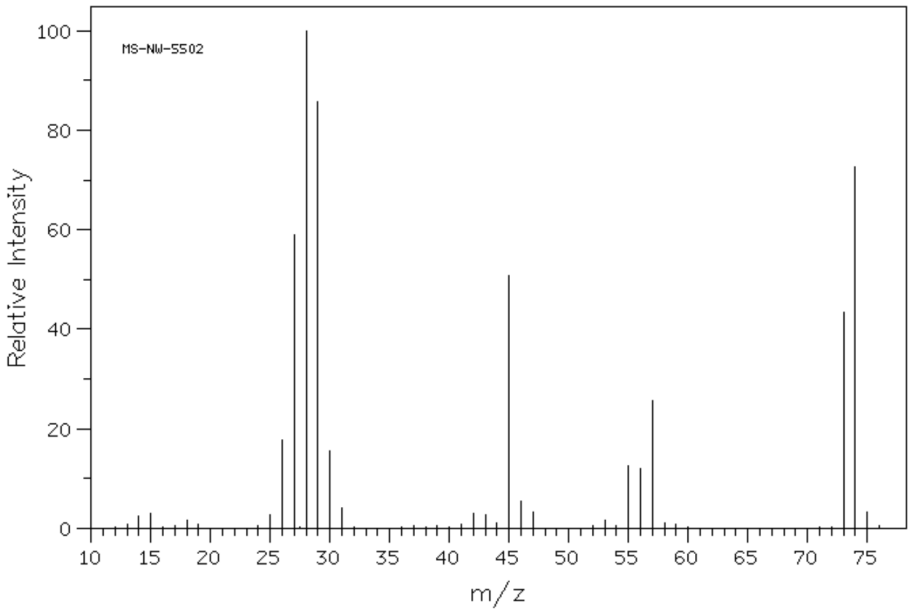
Figure 1: extract from Chemistry HSC Data Sheet © 2019 NSW Education Standards Authority (NESA) for and behalf of the Crown in right of the State of New South Wales

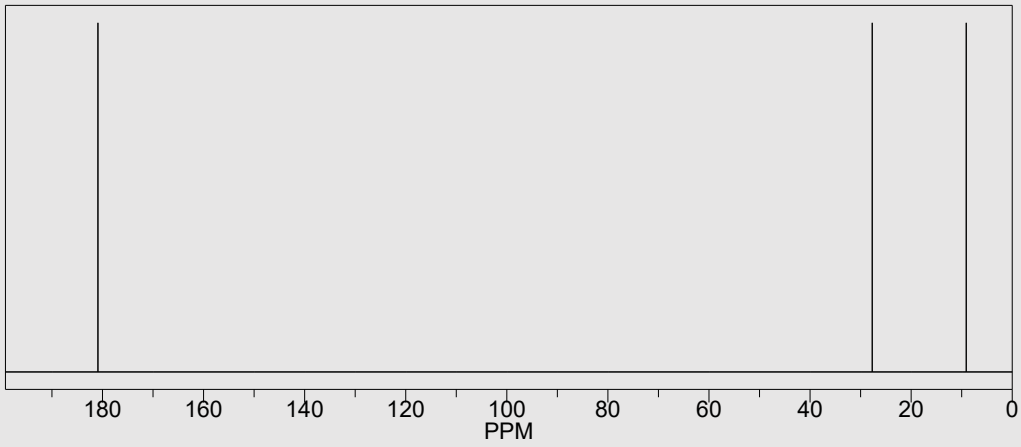
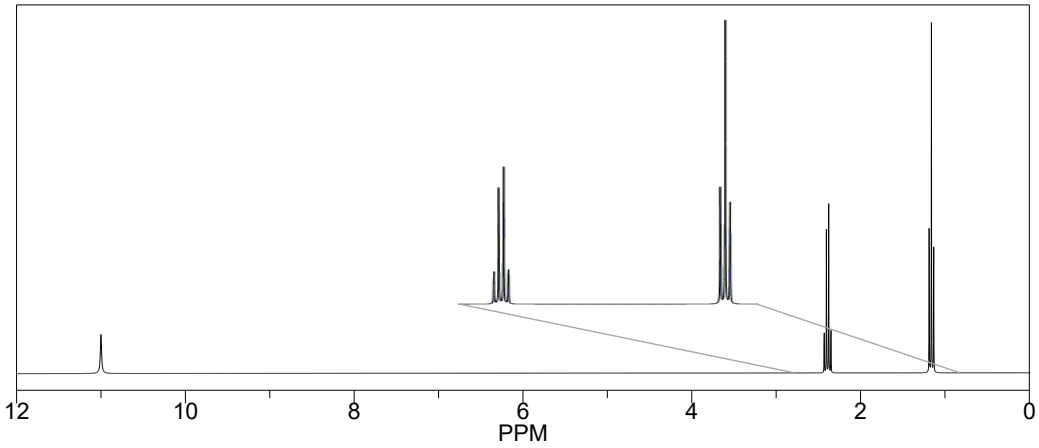
Marking scheme

Table 2: Marking scheme from the 2019 HSC Chemistry examination pack Question 26a

Criteria	Marks
• Gives correct structure and justifies using reactivity and at least three spectra	5
• Gives substantially correct structure and justifies using reactivity and at least two spectra **or** • Gives a correct structure and justifies using at least three spectra	4
• Gives substantially correct structure and some correct analyses **or** • Gives substantially correct analyses with incorrect structure	2-3
• Provides some relevant information	1

Example data analysis

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	Bubbles of carbon dioxide
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 74**	

Test	Result
Carbon-13 NMR	
Proton NMR	

Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
11.00	1	1
2.38	4	2
1.16	3	3

Observations and inferences

This question requires the use of a minimum of three (all four are discussed here) of these spectra and the other chemical reactivity information given in the table to propose the identity of this unknown organic compound. It is important to have a structure which agrees with all the information obtained to justify the compound you have proposed. The solution provided here is highly detailed and intended to fully explain the justification above the requirement of the justification needed in the marking scheme.

Chemical tests

- The orange colour remaining in the unsaturation test is a negative result indicating this compound does not contain a double or triple carbon-carbon bonds.
- The orange colour remaining in the oxidation test is a negative result indicating this compound does not contain a primary/secondary alcohol or aldehyde functional group which are oxidisable.
- The bubbles of carbon dioxide in the sodium carbonate test is a positive result indicating a carboxylic acid functional group is present. This result also eliminates the possibility of any other functional group.

Infrared spectroscopy

Major observations from the IR spectrum are a broad peak at ~3000cm^{-1} which indicates the presence of a hydroxyl (OH) group and a narrow peak at ~1700cm^{-1} which indicates the presence of a carbonyl (C=O) bond. This combination is only possible with a carboxylic acid functional group being present on the structure.

Using the reference table provided, several of the peaks can be identified as the bonds in propanoic acid but does not allow confirmation of the compound's identity. The absence of peaks corresponding to the other functional groups listed in the data sheet also helps to eliminate alternative possible functional groups in this compound. Due to the common nature of C-C and C-H bonds in organic compounds, these peaks are observed in the IR spectrum of all organic compounds and are not particularly useful for determining the unknown structure.

Mass spectrometry

The mass spectrum gives the molecular ion (m+) peak at m/z = 74 (a very small m+1 peak at m/z = 75 is also present) so it can be determined that the compound has a molecular weight of 74$gmol^{-1}$. It is at this point we can first propose a structure, the only carboxylic acid which has a molecular weight of 74$gmol^{-1}$ is propanoic acid, $C_3H_6O_2$:

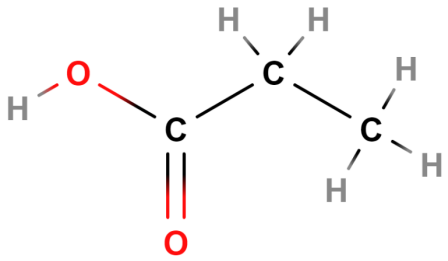


Figure 3: A molecular structure for propanoic acid (Bergwerf, 2015)

Using the proposed structure of propanoic acid the molecular weights of fragments can be more easily matched to the peaks present. When the other spectra (IR/NMR) are available, there is little benefit from analysing the fragmentation pattern in MS. For the completeness of this analysis, other prominent fragment ion peaks are:

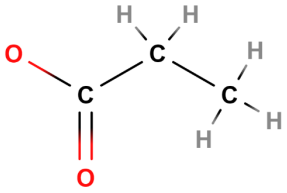
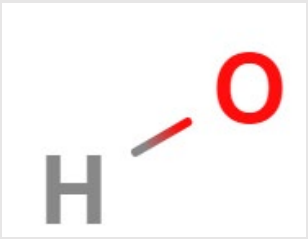
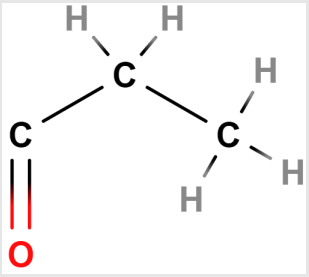
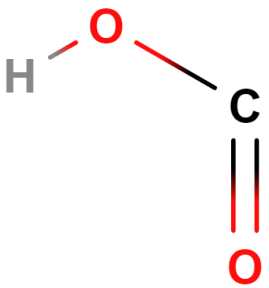
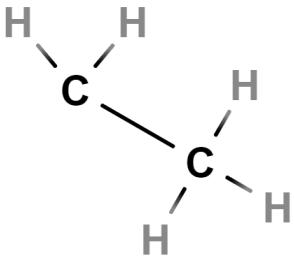
Fragment A mass (m/z)	Fragment A	Fragment B	Fragment B mass (m/z)
1			73
17			57
45			29

Table 4: Fragments for spectrometry of propanoic acid

Carbon-13 NMR

The carbon-13 NMR contains three peaks, this requires a minimum of three carbons in the compound. This excludes methanoic acid (only 1 carbon) and ethanoic acid (only 2 carbons). Continuing with the hypothesis this compound is propanoic acid allows the use of the reference table provided, these peaks can be identified as specific carbon environments:

- The peak at ~10ppm corresponds to a hydrocarbon chain and is normally a very low shift for a terminal CH_3 group
- The peak at ~27ppm corresponds to a hydrocarbon chain also and the slightly higher shift gives the indication this carbon is non-terminal as a CH_2 group
- The peak at ~180ppm corresponds to a carbonyl (C=O) group as a component of a carboxylic acid.

Proton NMR

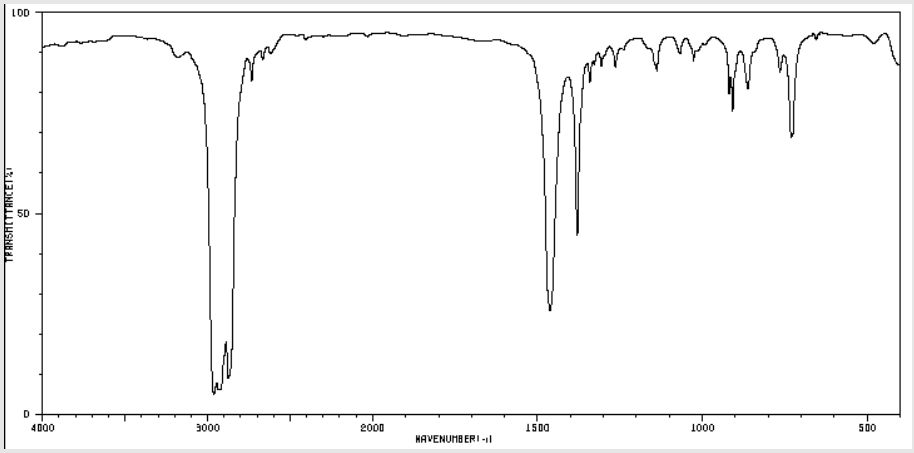
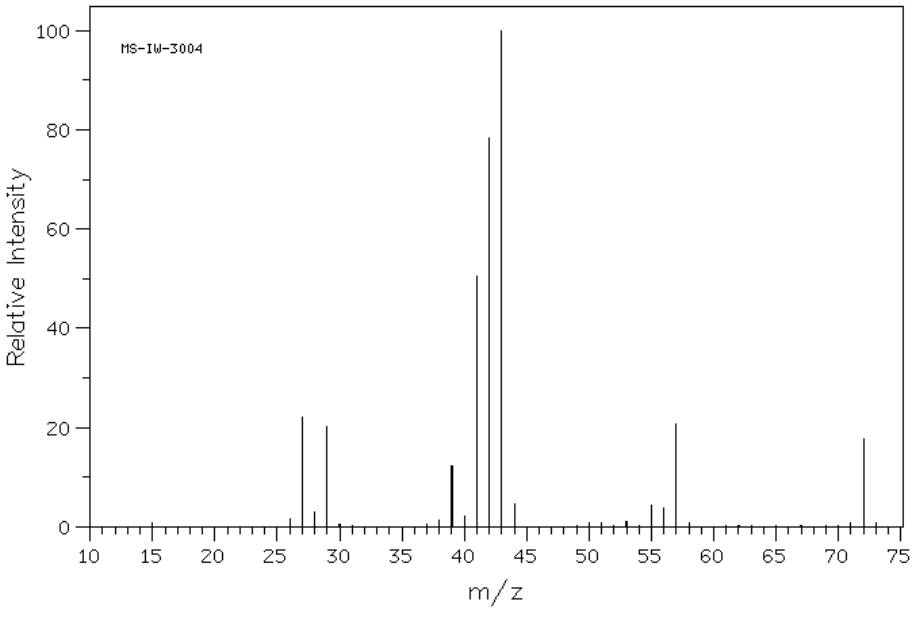
The Proton NMR contains three peaks which indicates the existence of three unique hydrogen environments where each are split according to the arrangement of adjacent hydrogen nuclei. Using the carbon-13 NMR and IR peaks it can be observed the presence of a CH_3, CH_2 and OH groups which create the hydrogen environments in propanoic acid. Continuing with the hypothesis this compound is propanoic acid allows the peaks to be identified as specific hydrogen environments:

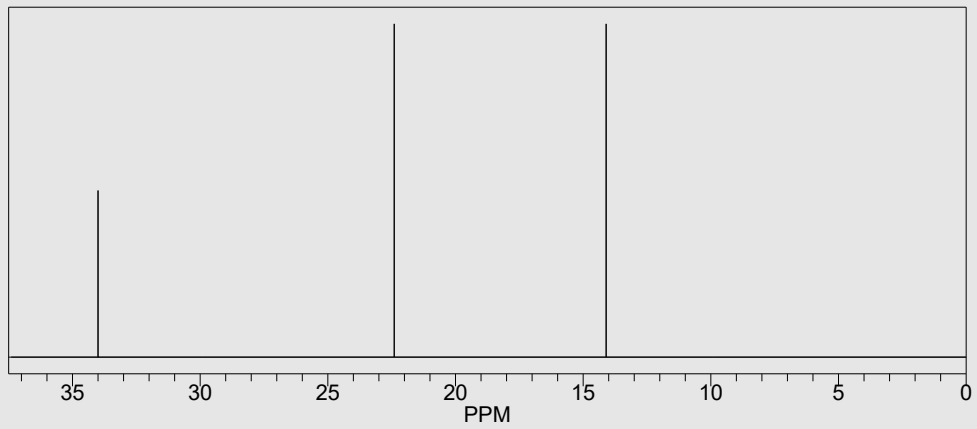
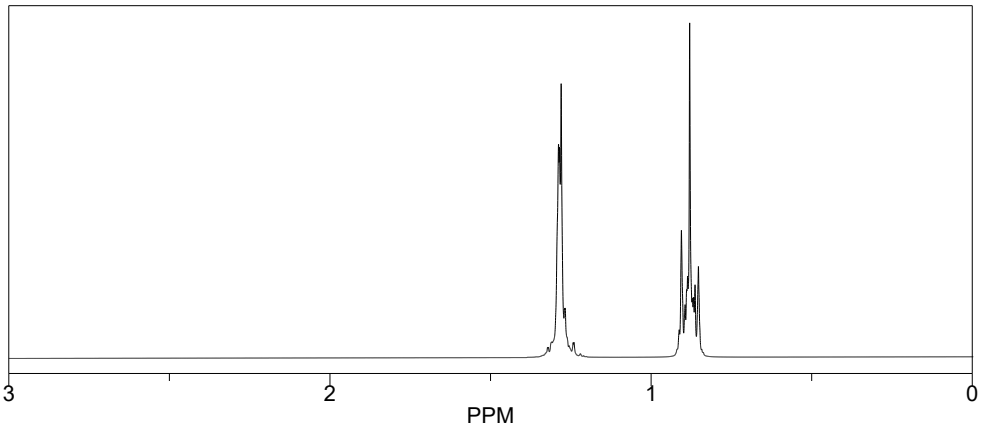
- The peak at ~1ppm is split into a triplet (3 peaks), indicating this hydrogen environment is adjacent to two hydrogens, the terminal CH_3 group is adjacent to the CH_2 group capable of this triplet peak and is normally a very low shift for a terminal hydrogen environment
- The peak at ~2.2ppm is split into a quartet (4 peaks), indicating this hydrogen environment is adjacent to three hydrogens, the CH_2 group is adjacent to the terminal CH_3 group capable of this quartet peak and the slightly higher shift gives the indication this is a non-terminal hydrogen environment
- The peak at ~11.7ppm is a singlet (not split), indicating this hydrogen environment is not adjacent to any other hydrogens, only the hydroxyl (OH) hydrogen is capable of this peak due to the separation of this hydrogen environment from the others by the oxygen.

Student activity: unknowns

What is the structural formula of the allocated compound (A-Z)? Justify your answer with reference to the information given on its reactivity and to at least three of the provided spectra for the allocated unknown (A-Z). (5 marks – using the marking scheme from 2019 Chemistry HSC question 26a)

Sample A

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 72**	

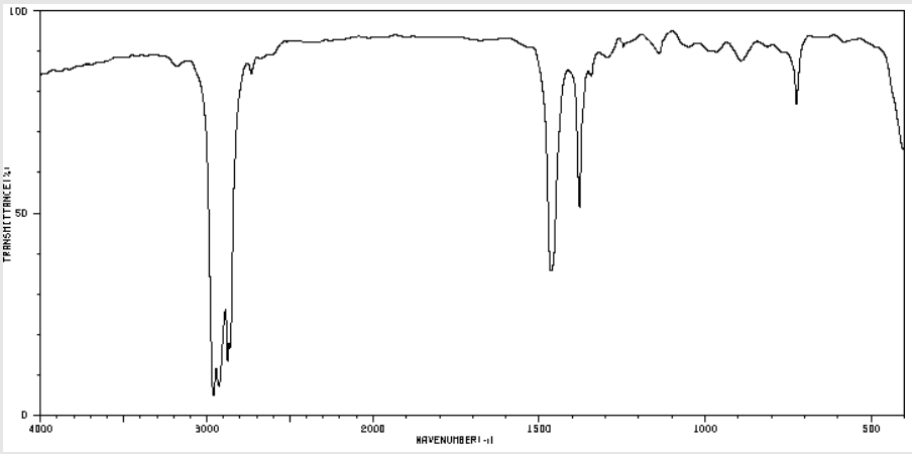
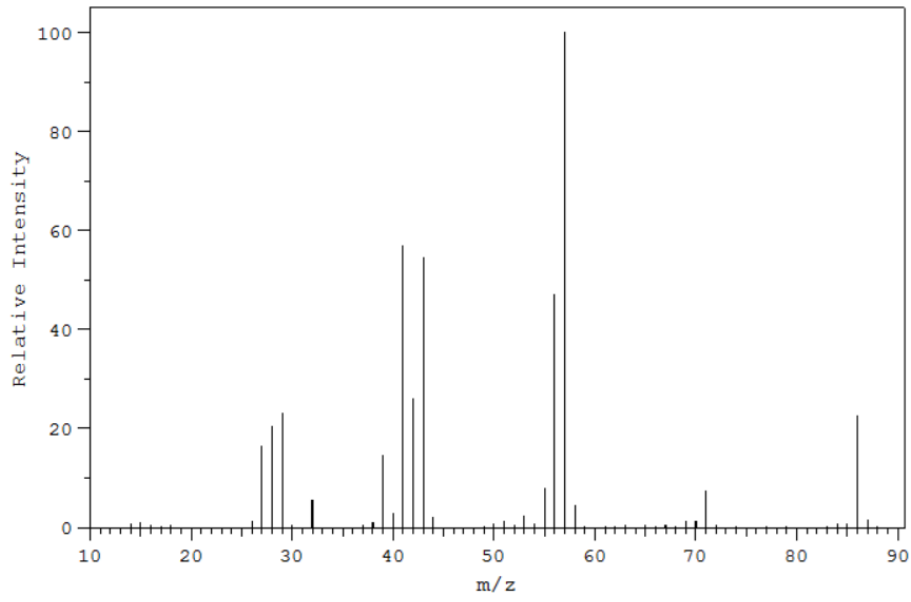
Test	Result
Carbon-13 NMR	
Proton NMR	

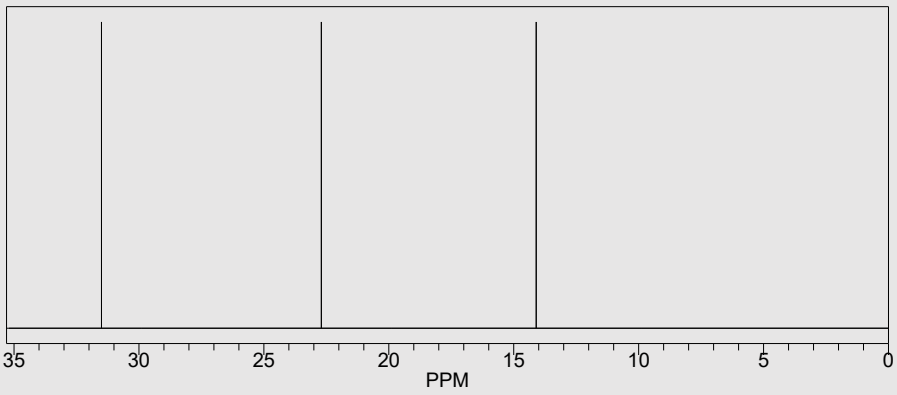
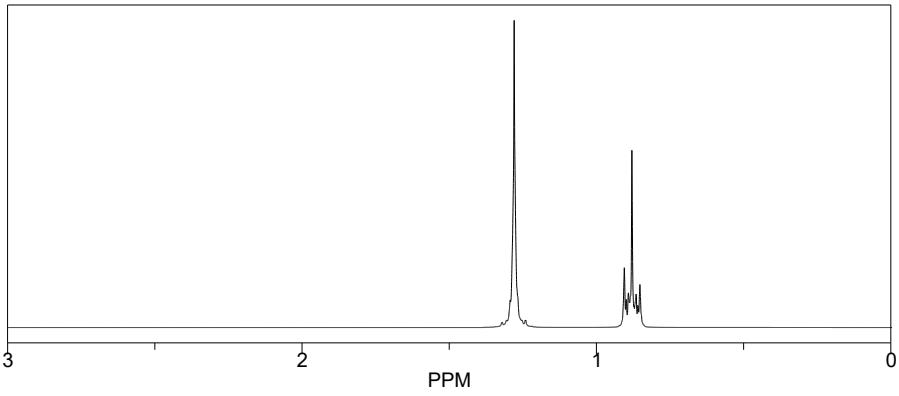
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
1.30	6	4
1.26	5	2
0.884	3	6

Check the solution to Sample A and see a work-through of the problem in this video on YouTube.

Sample B

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 86**	

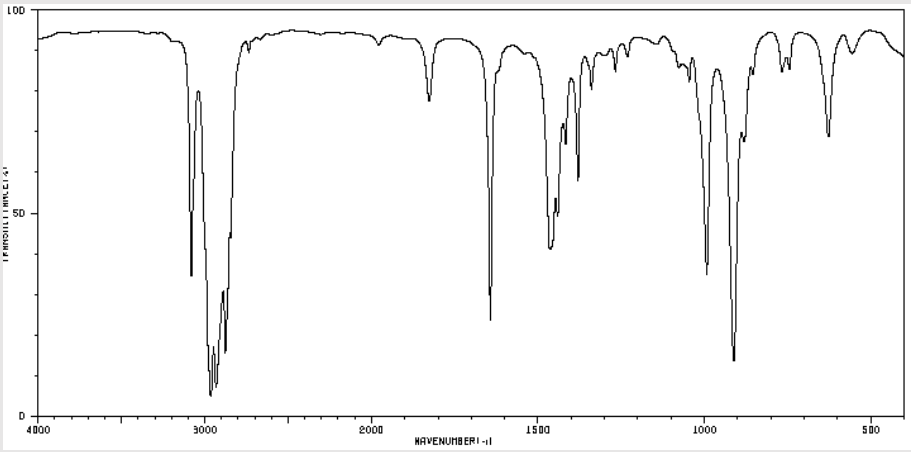
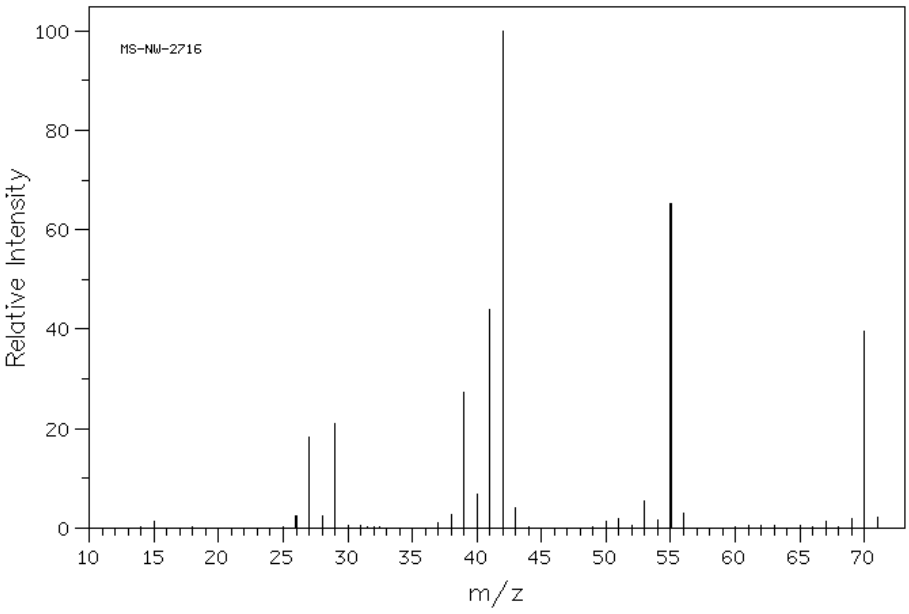
Test	Result
Carbon-13 NMR	
Proton NMR	

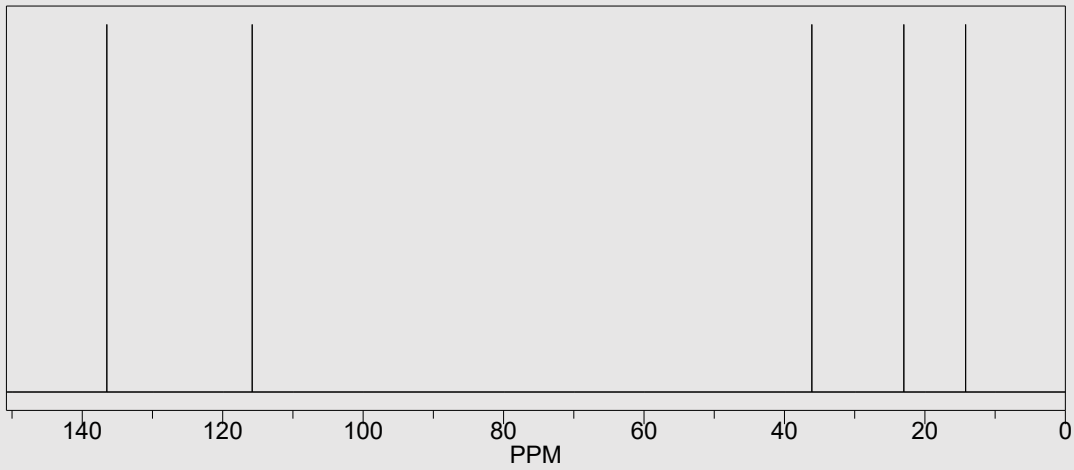
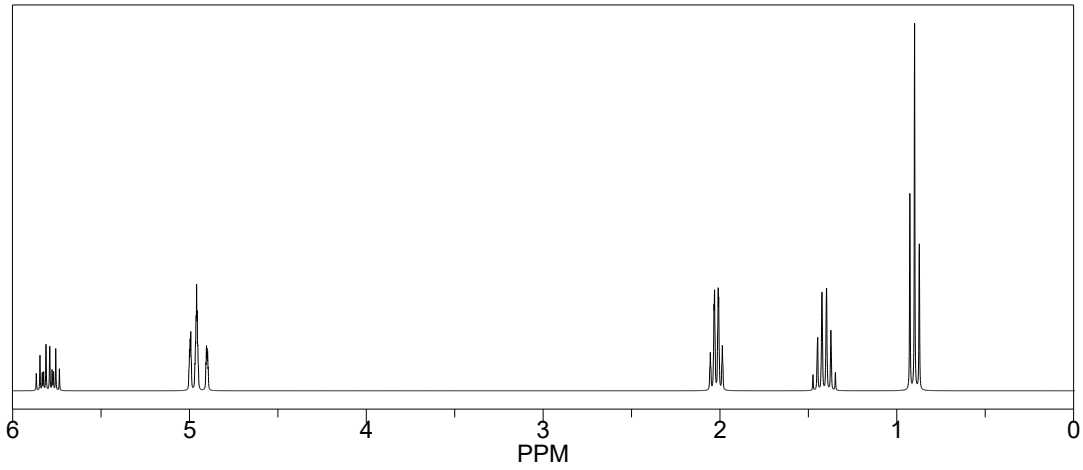
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
1.30	6	4
1.28	5	4
0.90	3	6

Check the solution to Sample B and see a work-through of the problem in this video on YouTube.

Sample C

Test	Result
Unsaturation test using bromine water	Solution turns colourless
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 70**	

Test	Result
Carbon-13 NMR	
Proton NMR	

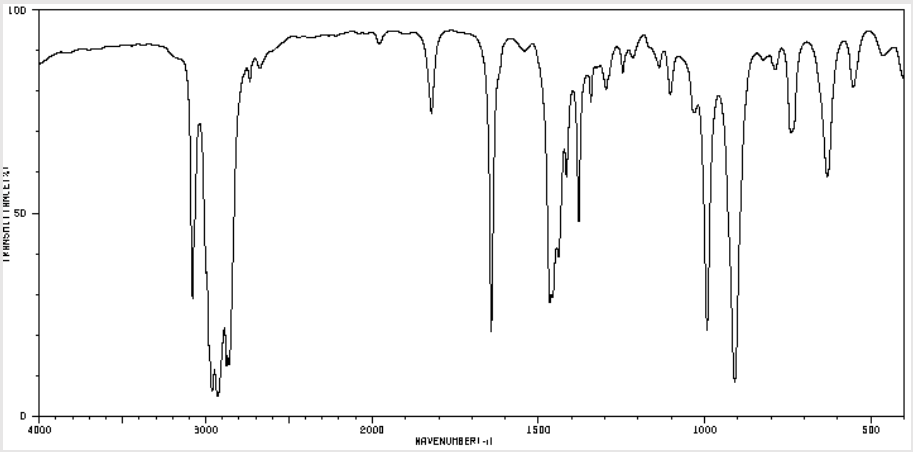
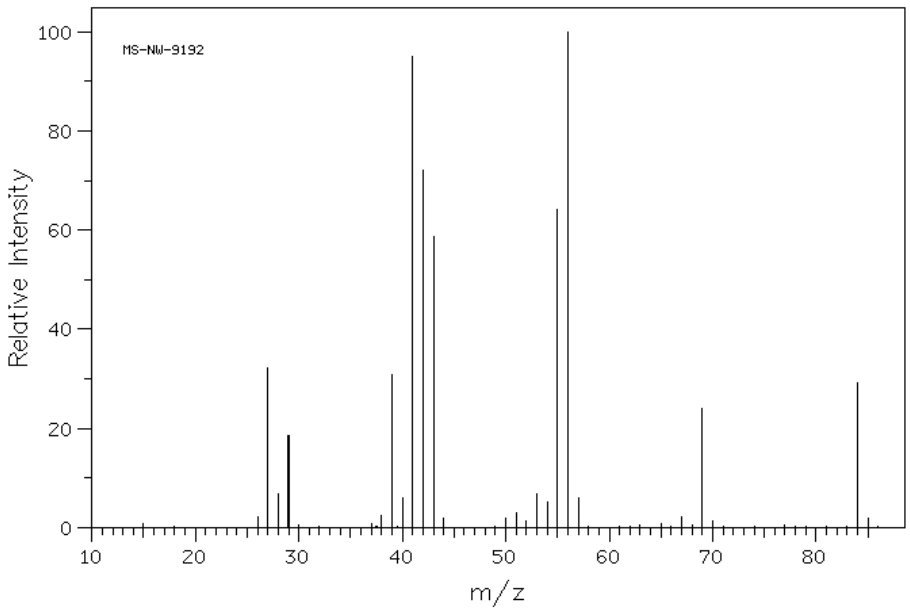
Proton NMR peak data

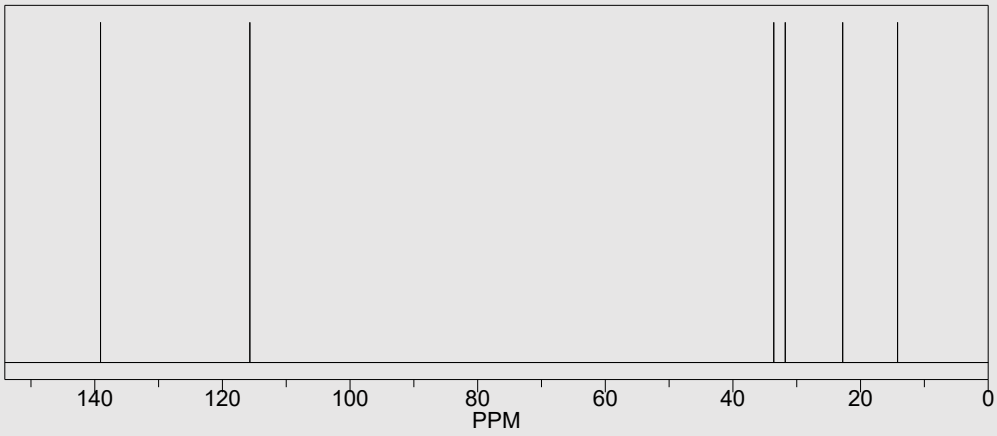
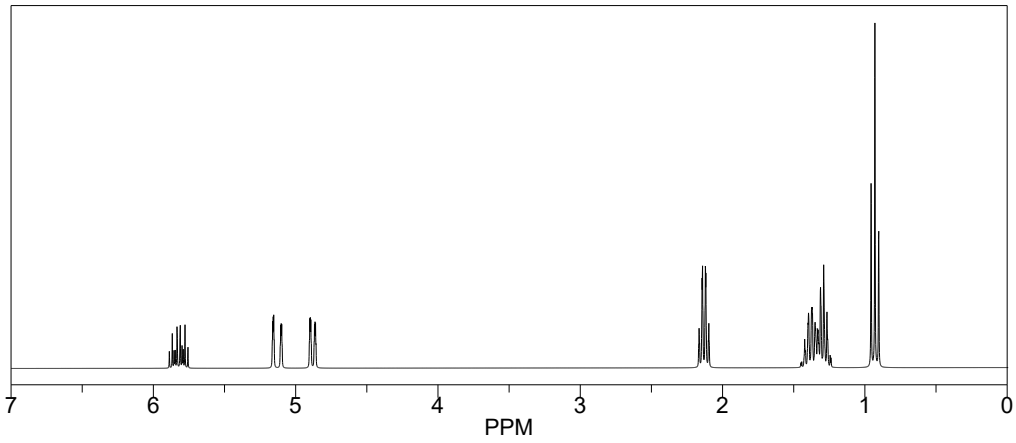
Shift (ppm)	Number of peaks	Peak area ratio
5.81	5	1
4.97	3	1
4.93	3	1

Shift (ppm)	Number of peaks	Peak area ratio
2.02	4	2
1.43	6	2
0.91	3	3

Check the solution to Sample C and see a work-through of the problem in this video on YouTube.

Sample D

Test	Result
Unsaturation test using bromine water	Solution turns colourless
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 84**	

Test	Result
Carbon-13 NMR	
Proton NMR	

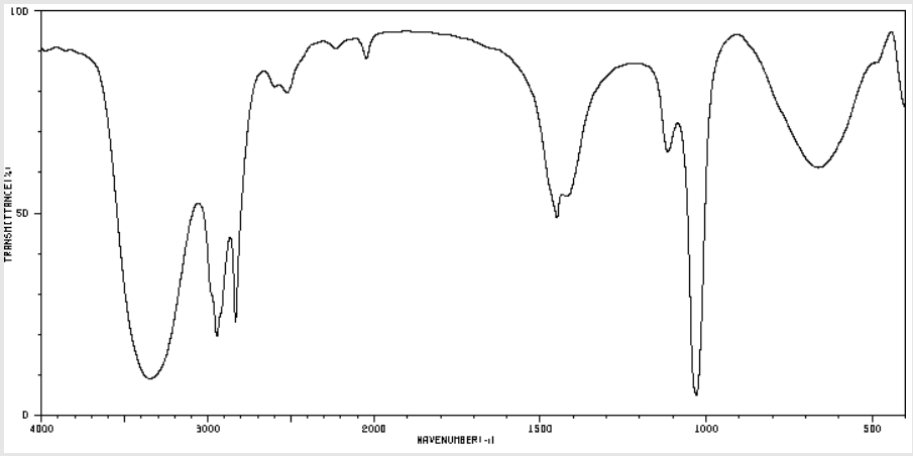
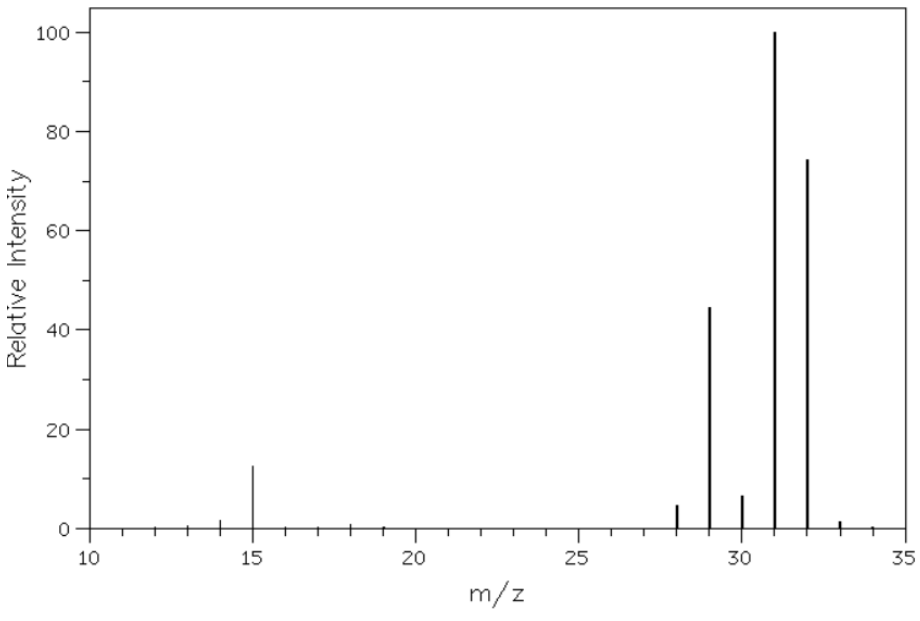
Proton NMR peak data

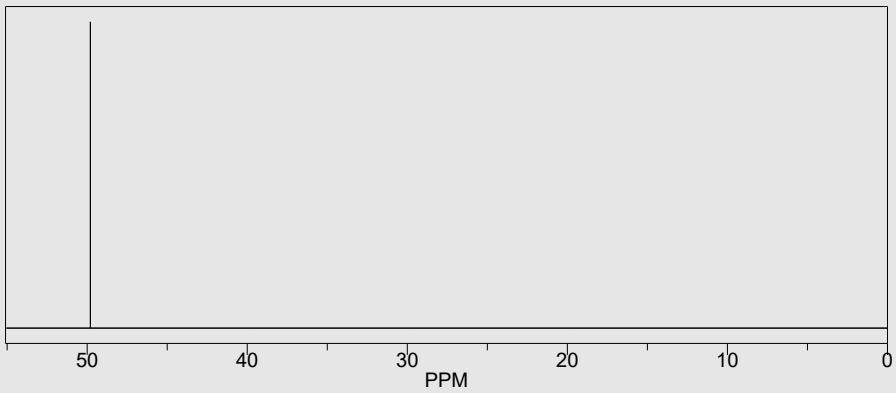
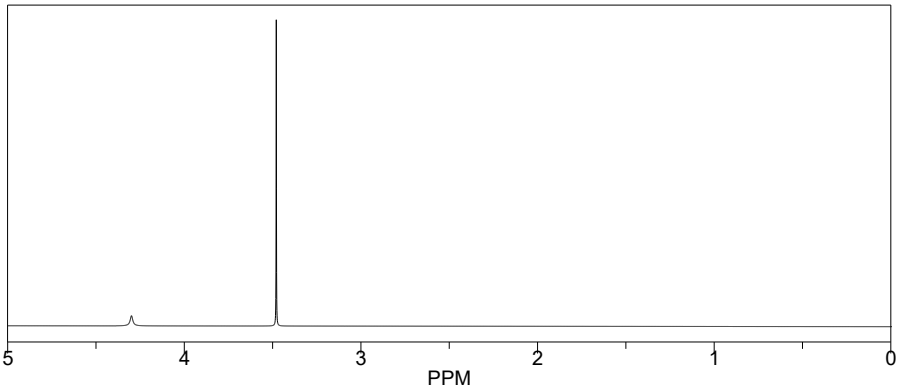
Shift (ppm)	Number of peaks	Peak area ratio
5.82	5	1
5.13	3	1
4.88	3	1
2.06	4	2

Shift (ppm)	Number of peaks	Peak area ratio
1.38	6	2
1.29	5	2
0.90	3	3

Check the solution to Sample D and see a work-through of the problem in this video on YouTube.

Sample E

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Solution turns green
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 32**	

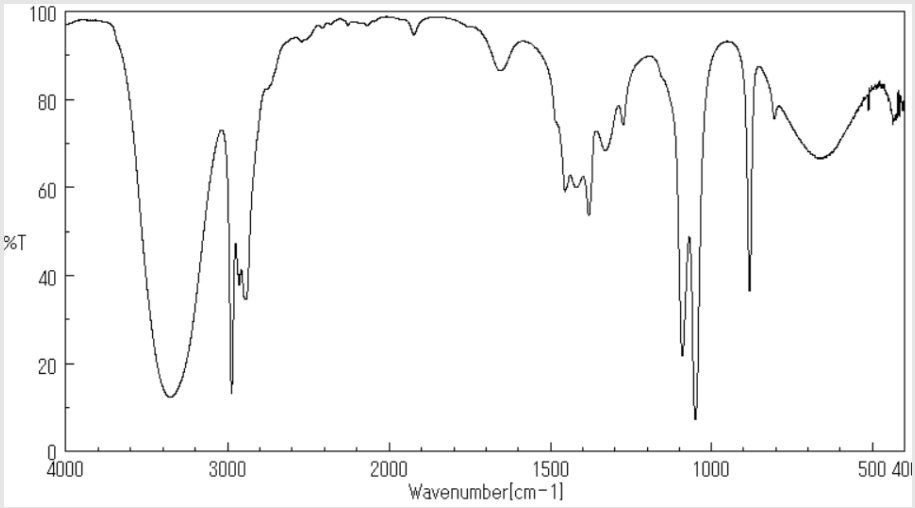
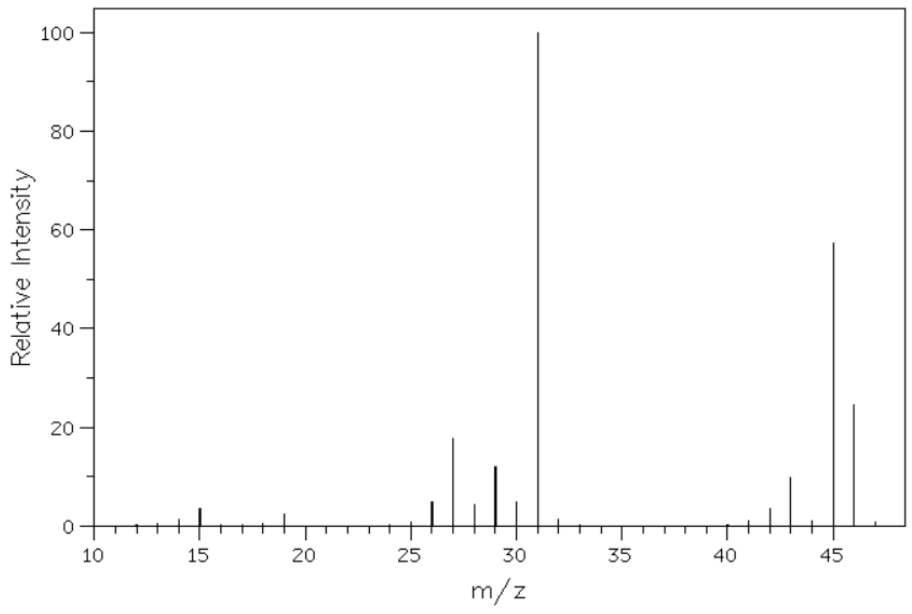
Test	Result
Carbon-13 NMR	
Proton NMR	

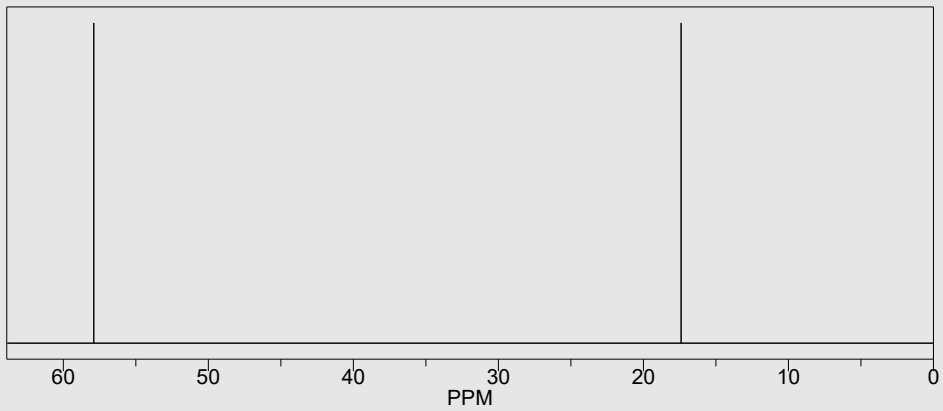
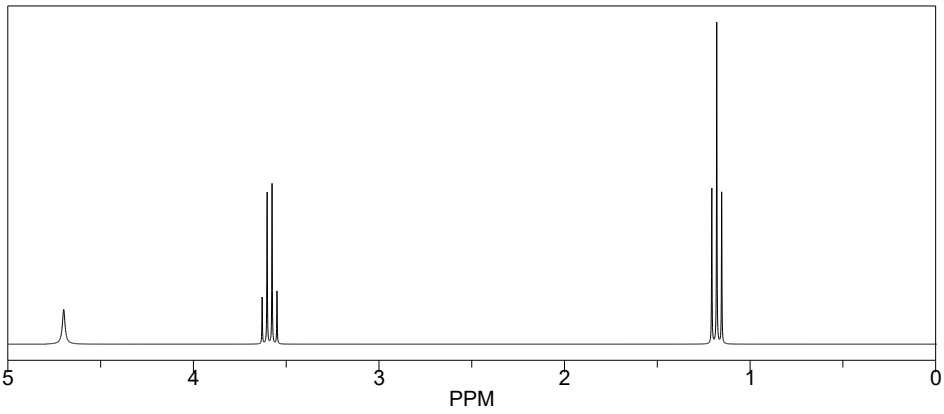
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
4.30	1	1
3.48	1	3

Check the solution to Sample E and see a work-through of the problem in this video on YouTube.

Sample F

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Solution turns green
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 46**	

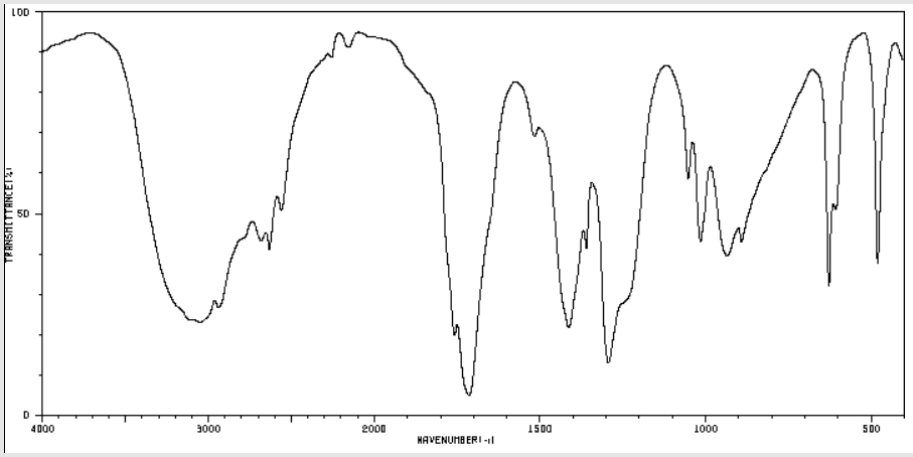
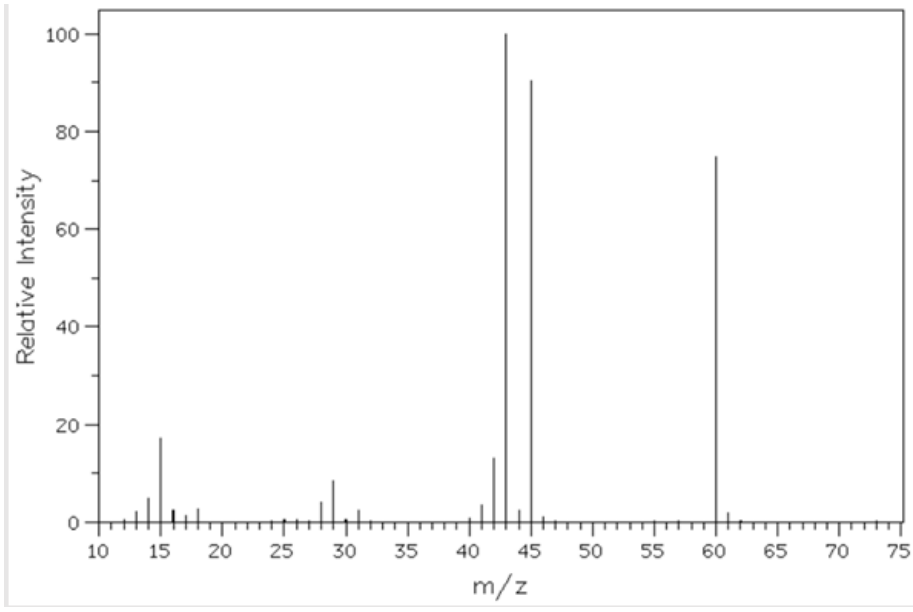
Test	Result
Carbon-13 NMR	
Proton NMR	

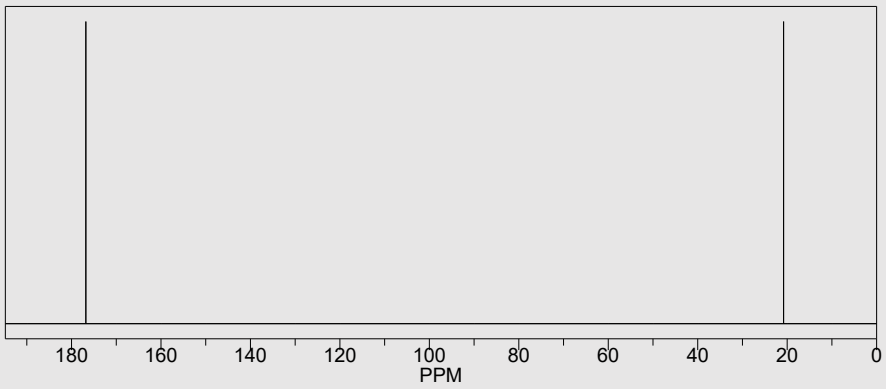
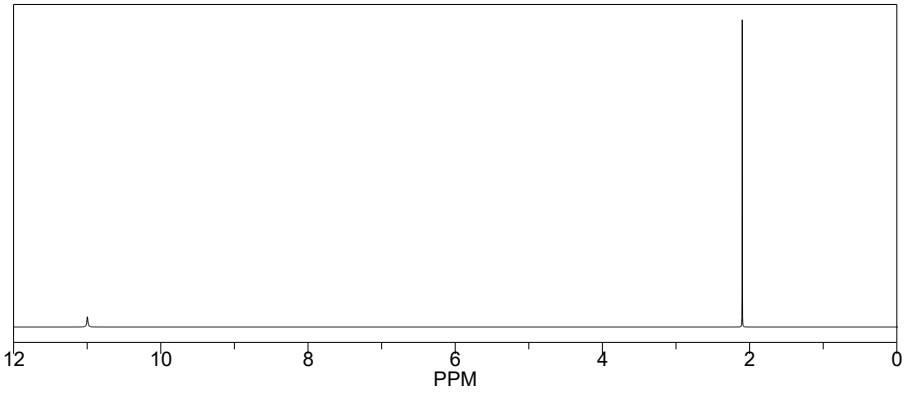
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
4.70	1	1
3.59	4	2
1.18	3	3

Check the solution to Sample F and see a work-through of the problem in this video on YouTube.

Sample G

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	Bubbles of carbon dioxide
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 60**	

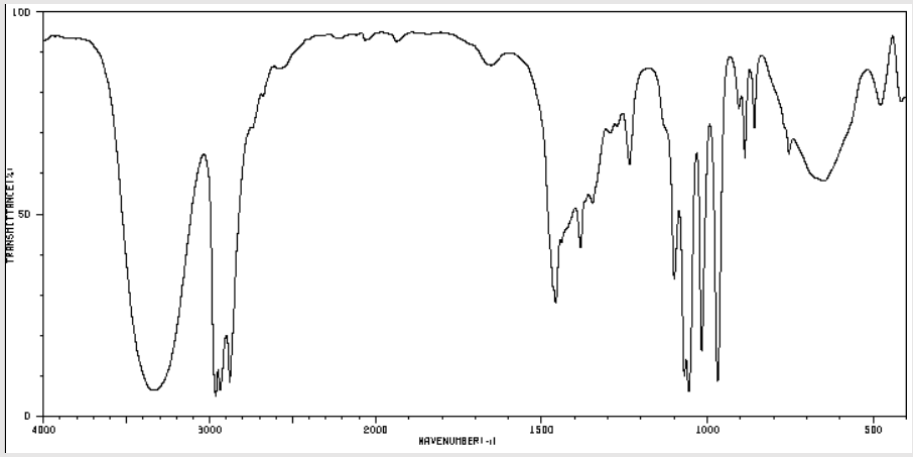
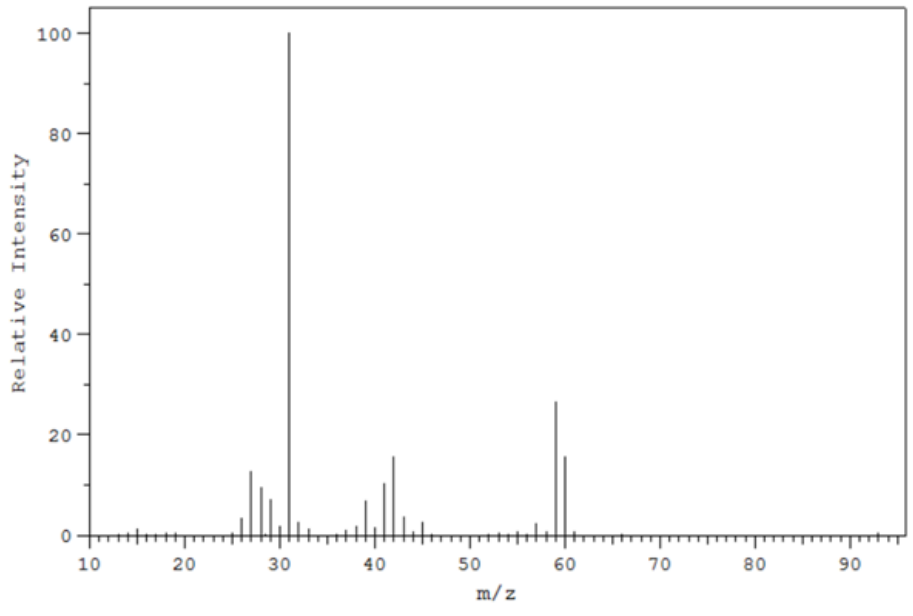
Test	Result
Carbon-13 NMR	
Proton NMR	

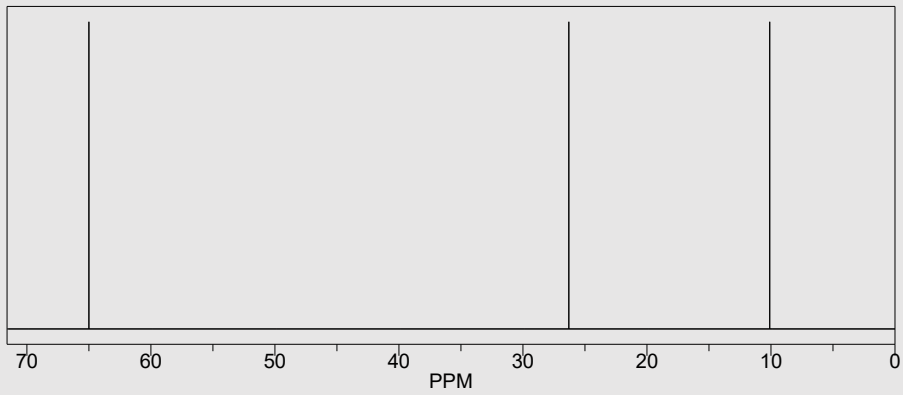
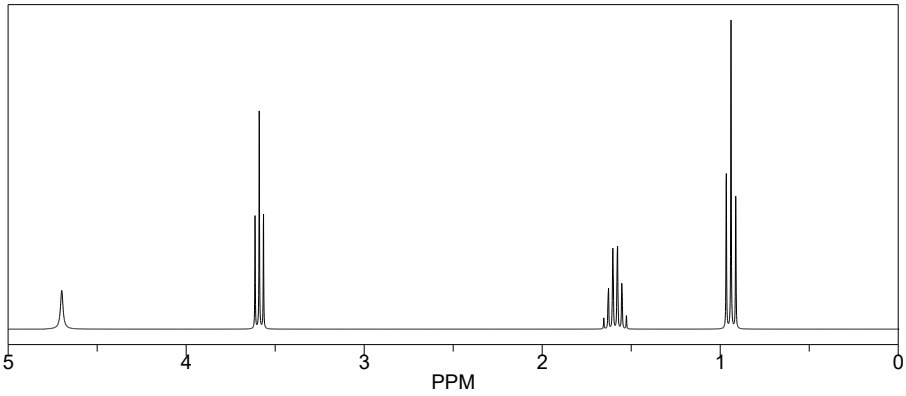
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
11.00	1	1
2.10	1	3

Check the solution to Sample G and see a work-through of the problem in this video on YouTube.

Sample H

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Solution turns green
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 60**	

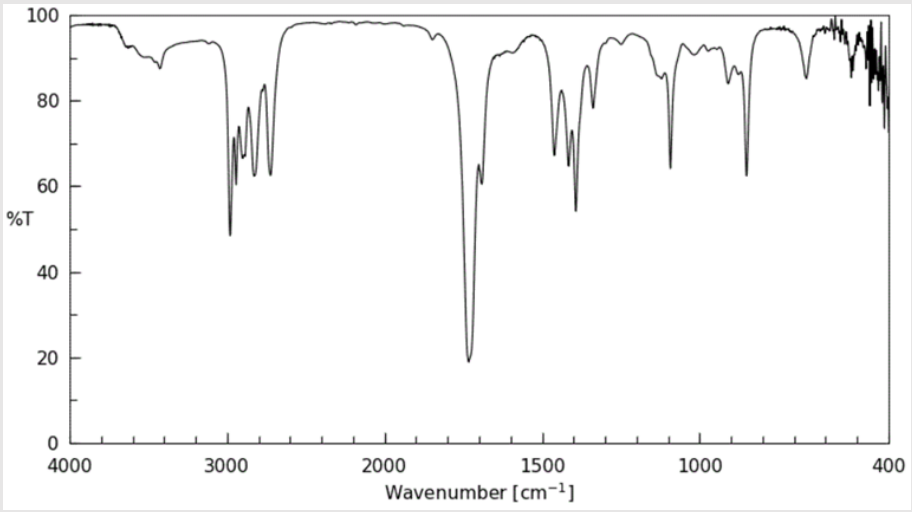
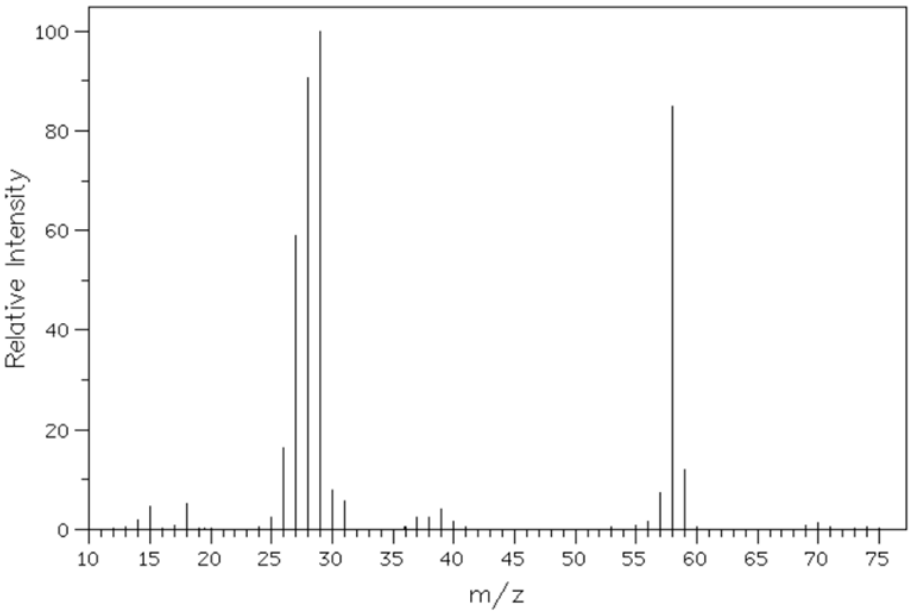
Test	Result
Carbon-13 NMR	
Proton NMR	

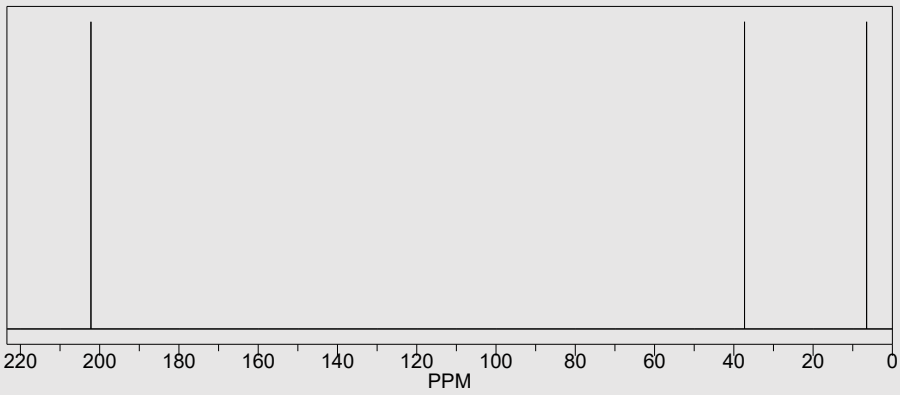
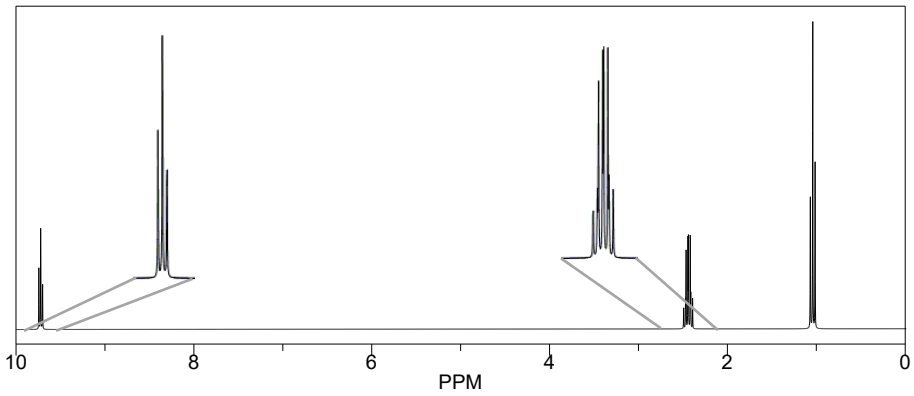
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
4.70	1	1
3.59	3	2
1.59	6	2
0.94	3	3

Check the solution to Sample H and see a work-through of the problem in this video on YouTube.

Sample I

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Solution turns green
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 58**	

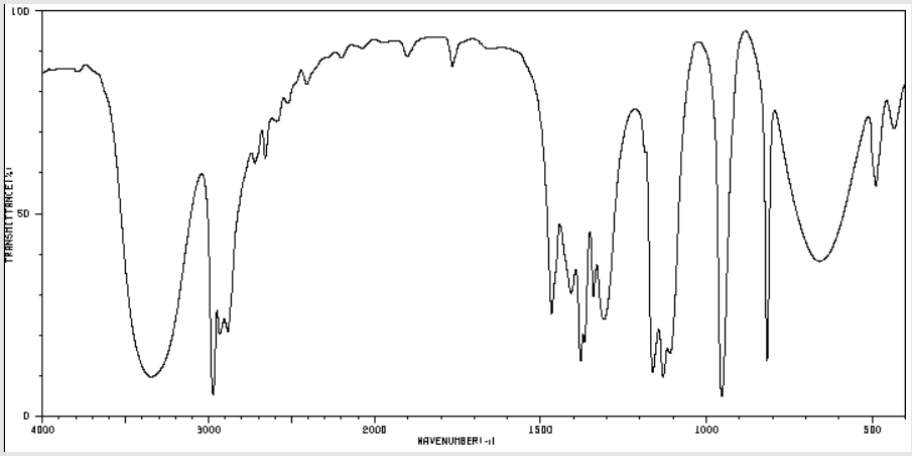
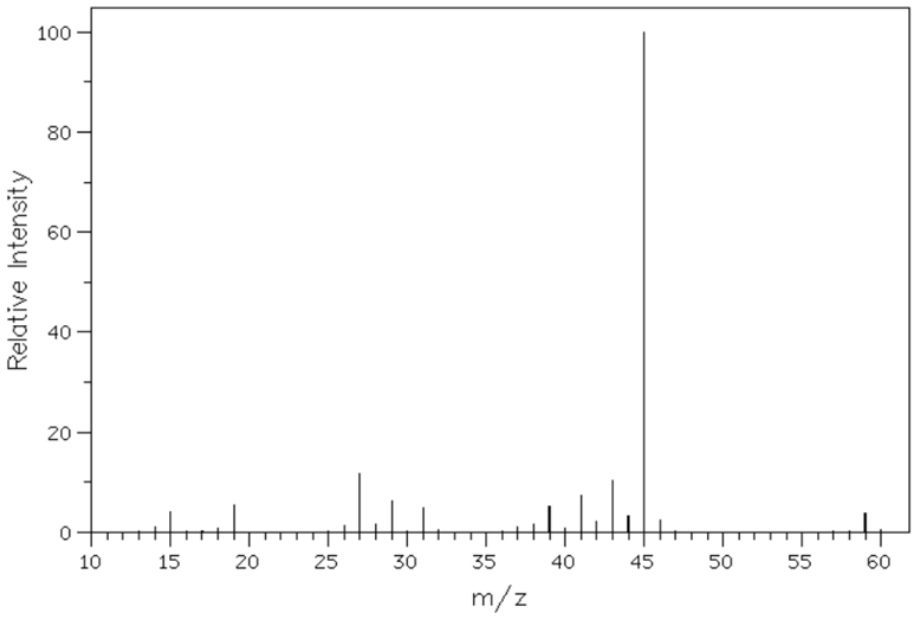
Test	Result
Carbon-13 NMR	
Proton NMR	

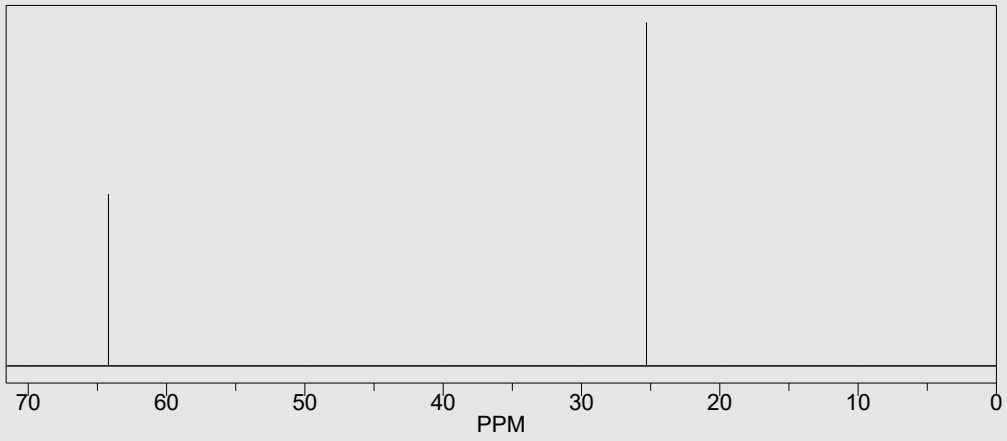
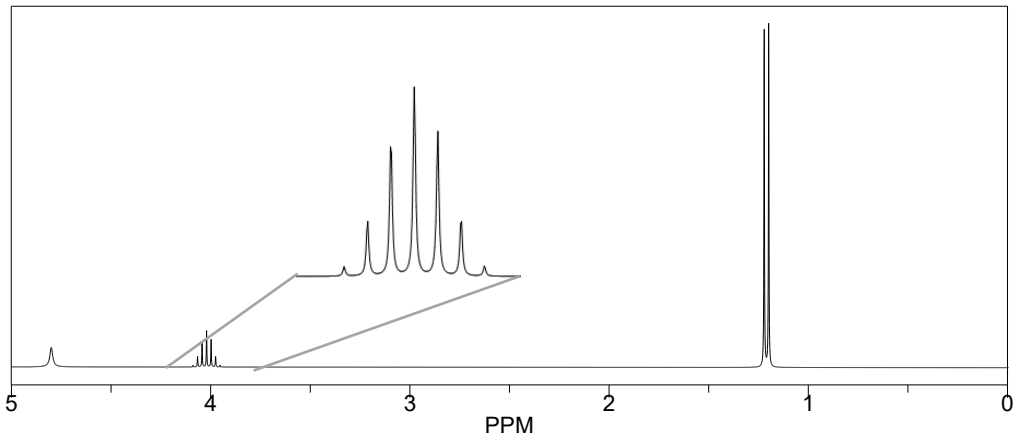
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
9.80	3	1
2.44	5	2
1.11	3	3

Check the solution to Sample I and see a work-through of the problem in this video on YouTube.

Sample J

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Solution turns green
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 60**	

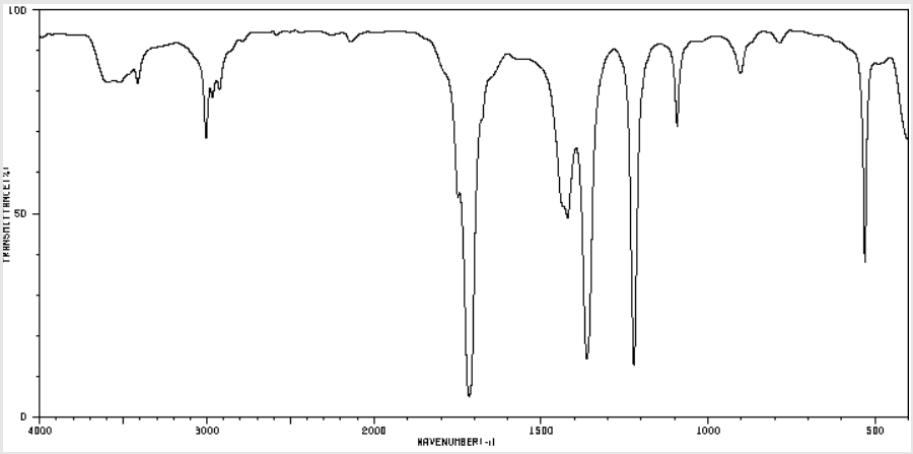
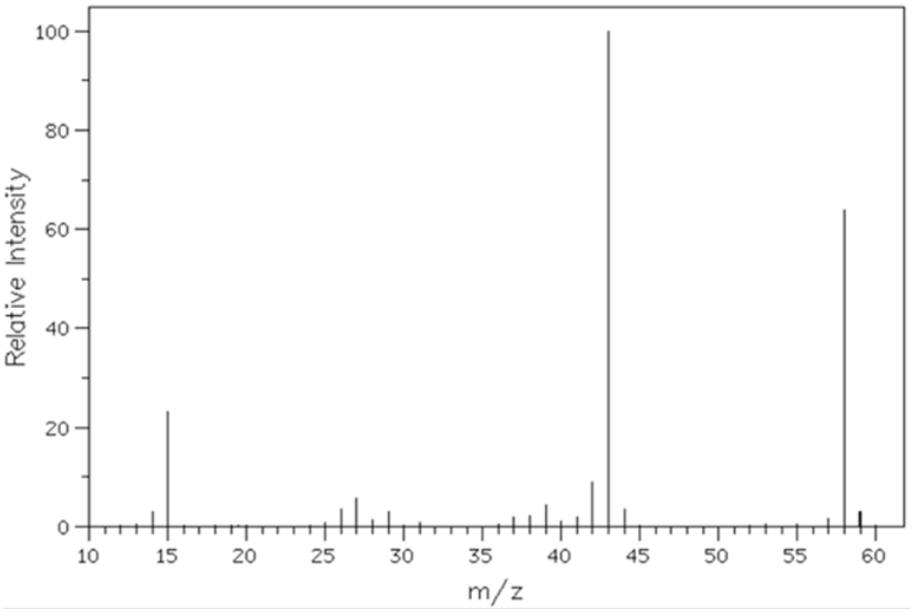
Test	Result
Carbon-13 NMR	
Proton NMR	

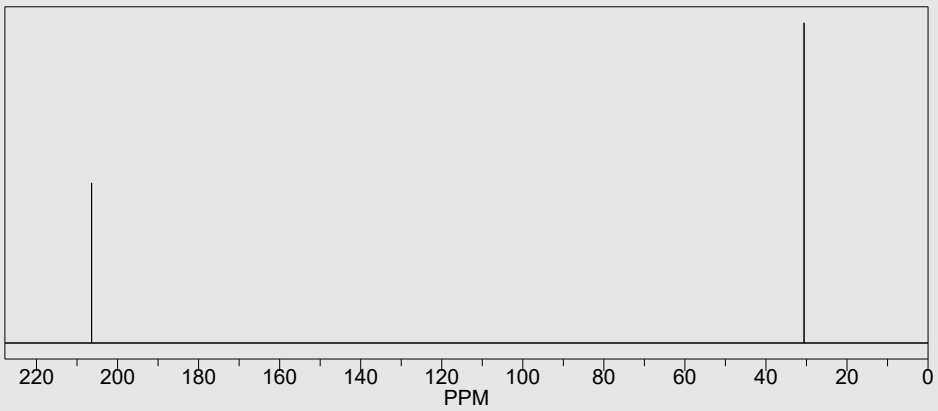
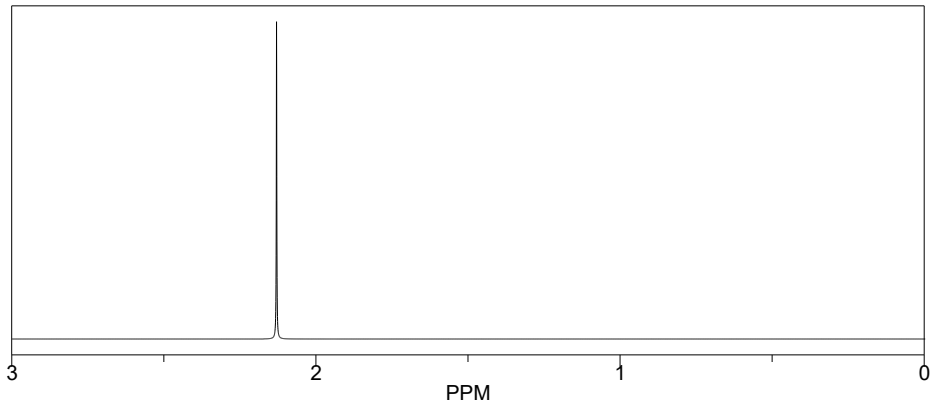
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
4.80	1	1
4.02	7	1
1.21	2	6

Check the solution to Sample J and see a work-through of the problem in this video on YouTube.

Sample K

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 58**	

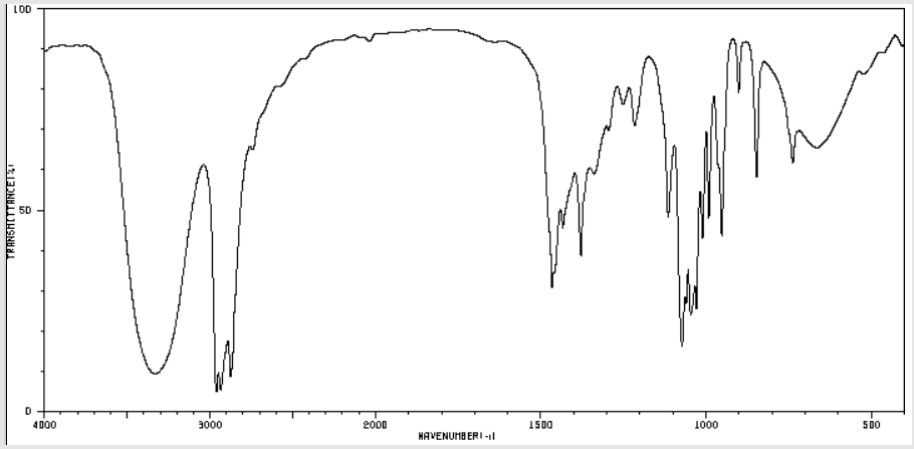
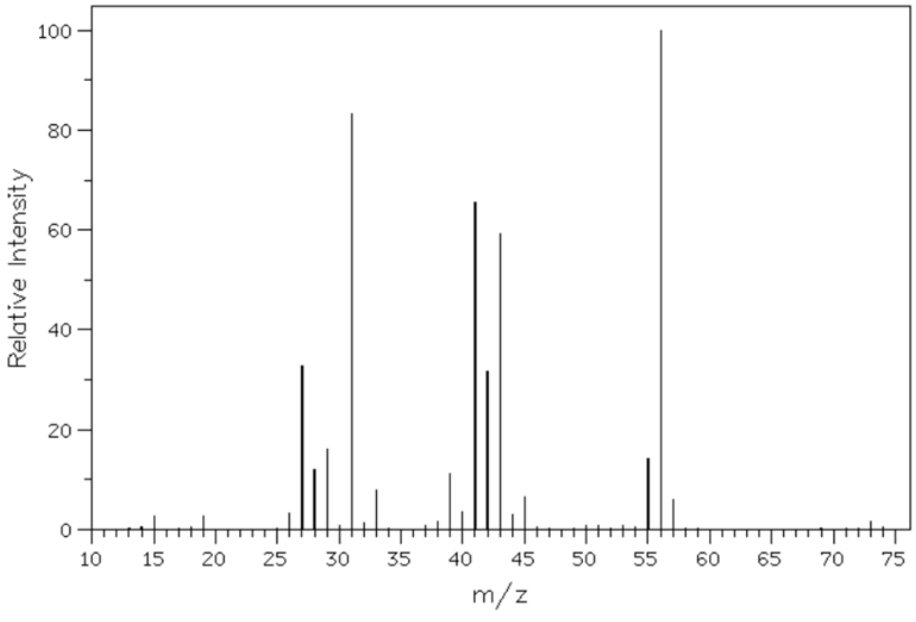
Test	Result
Carbon-13 NMR	
Proton NMR	

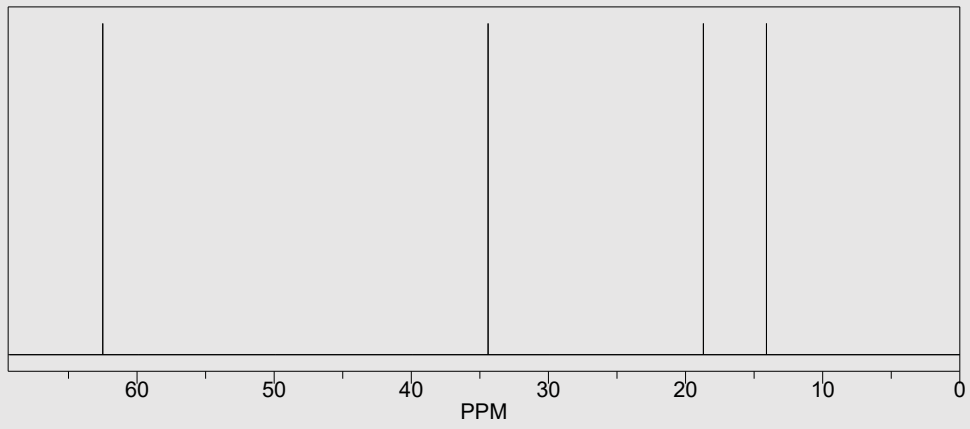
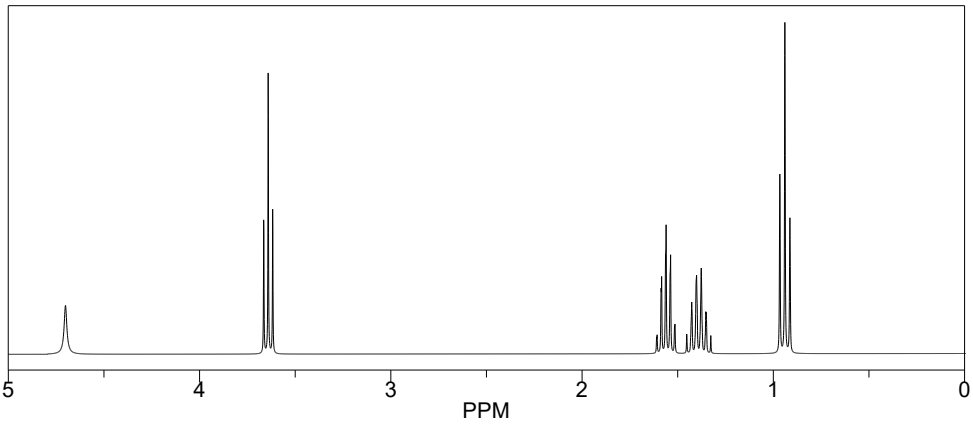
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
2.16	1	6

Check the solution to Sample K and see a work-through of the problem in this video on YouTube.

Sample L

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Solution turns green
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 74**	

Test	Result
Carbon-13 NMR	
Proton NMR	

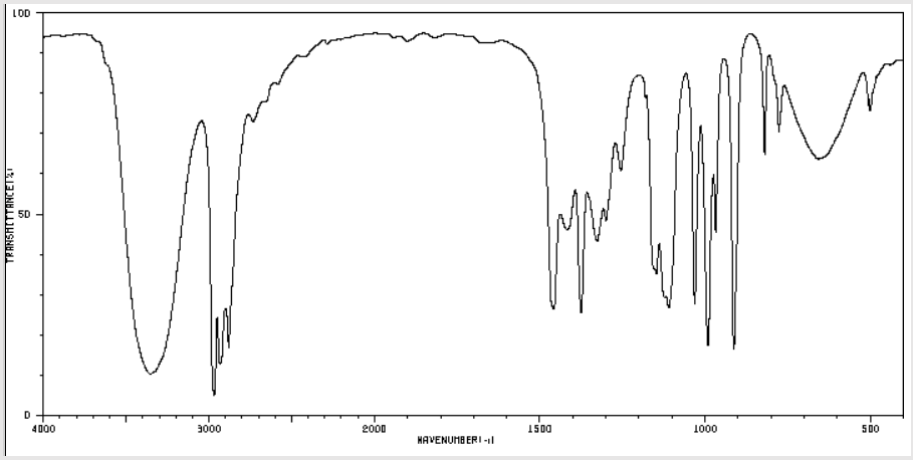
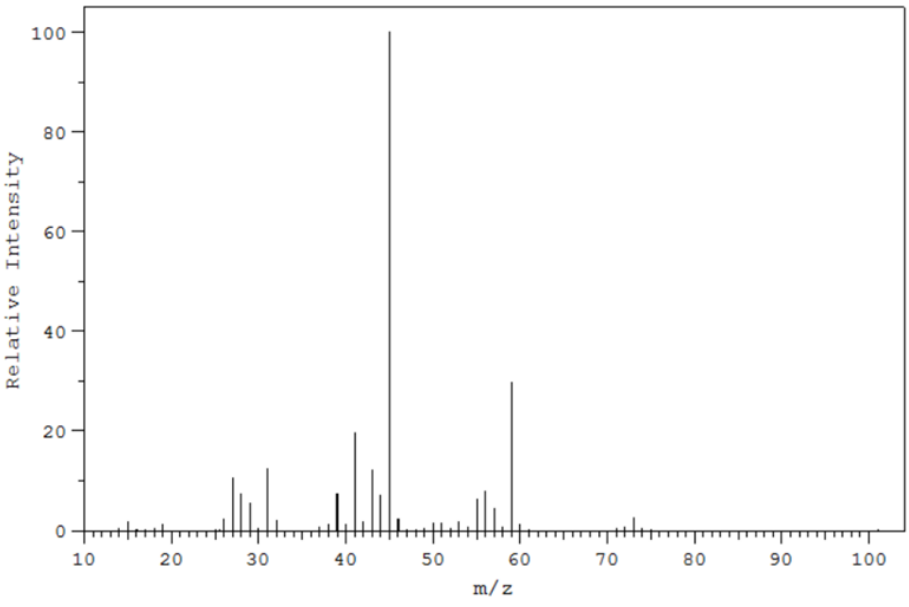
Proton NMR peak data

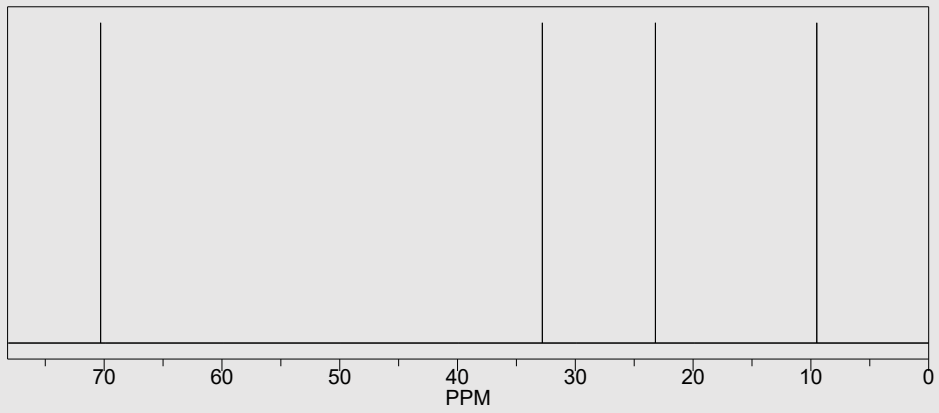
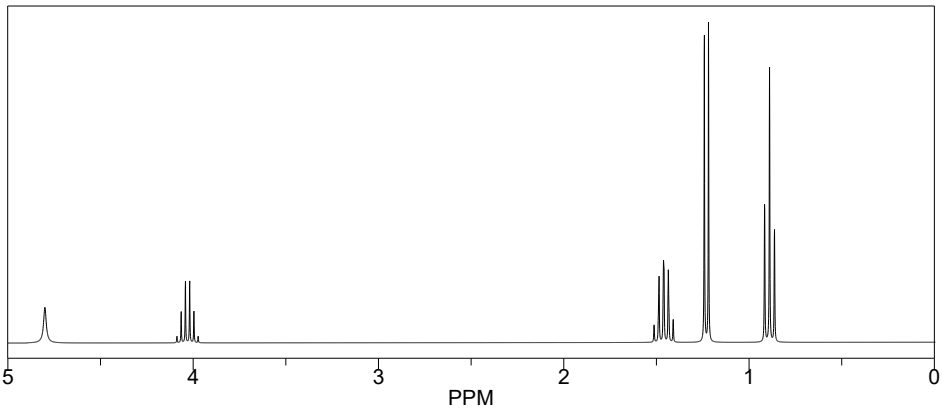
Shift (ppm)	Number of peaks	Peak area ratio
4.70	1	1
3.63	3	2
1.53	5	2

Shift (ppm)	Number of peaks	Peak area ratio
1.39	6	2
0.94	3	3

Check the solution to Sample L and see a work-through of the problem in this video on YouTube.

Sample M

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Solution turns green
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 74**	

Test	Result
Carbon-13 NMR	
Proton NMR	

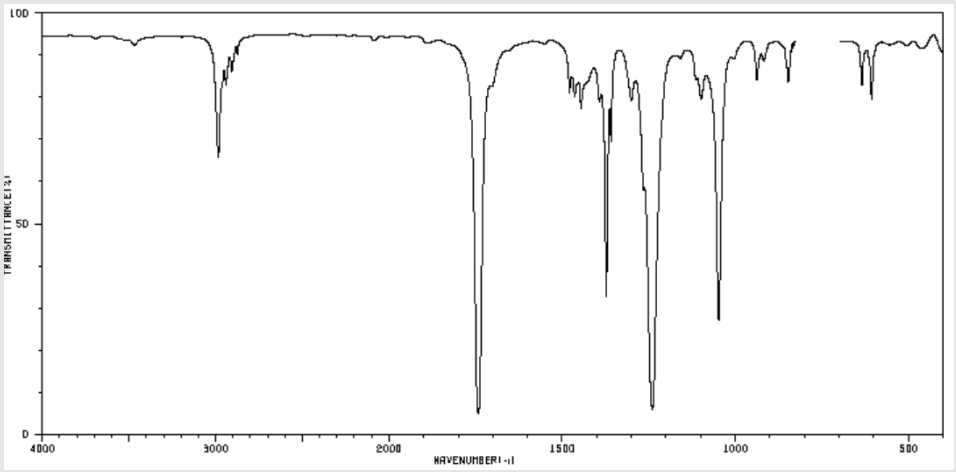
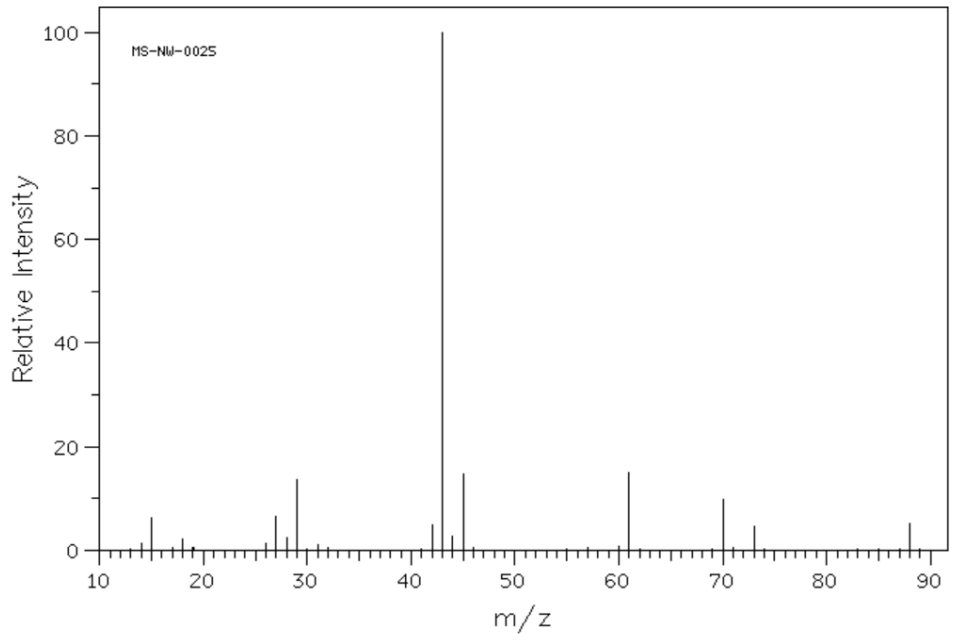
Proton NMR peak data

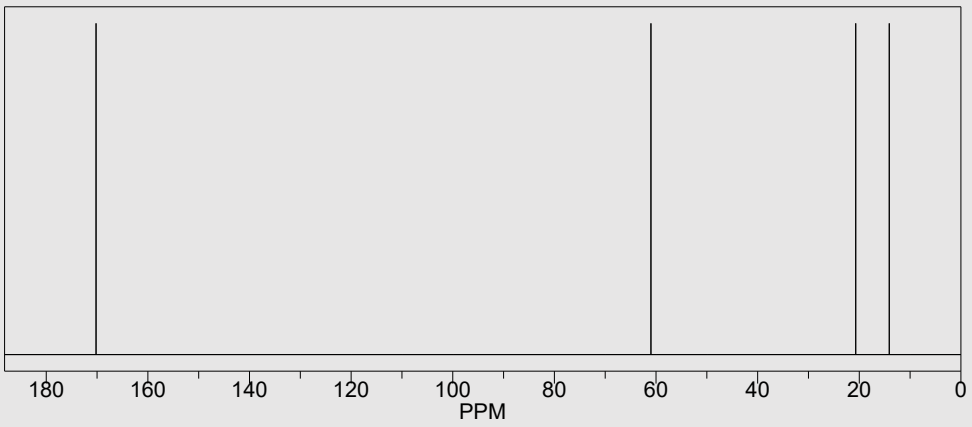
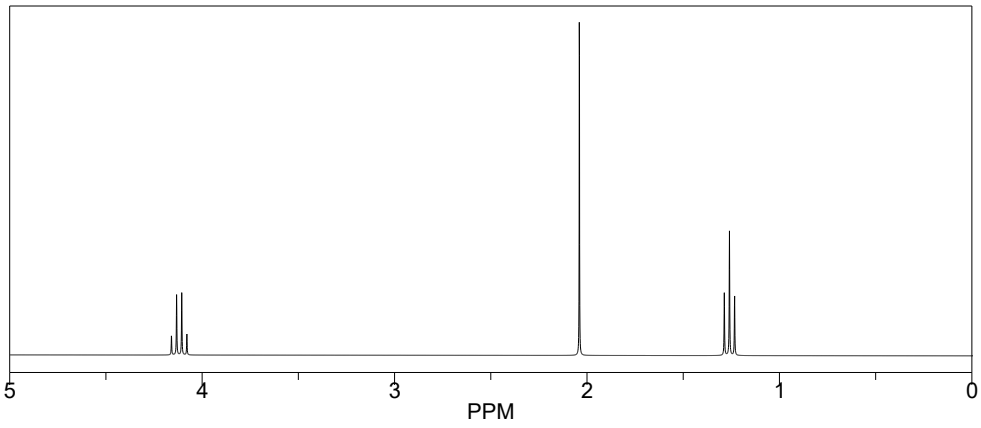
Shift (ppm)	Number of peaks	Peak area ratio
4.80	1	1
4.03	6	1
1.46	5	2

Shift (ppm)	Number of peaks	Peak area ratio
1.23	2	3
0.89	3	3

Check the solution to Sample M and see a work-through of the problem in this video on YouTube.

Sample N

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 74**	

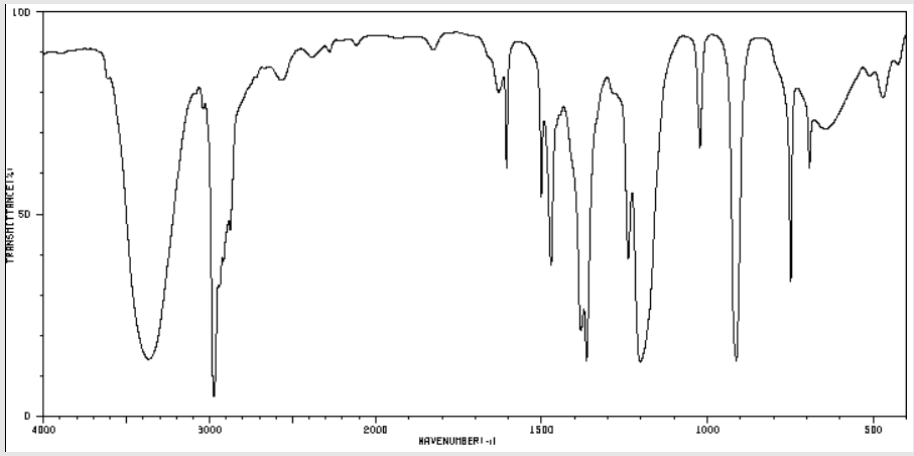
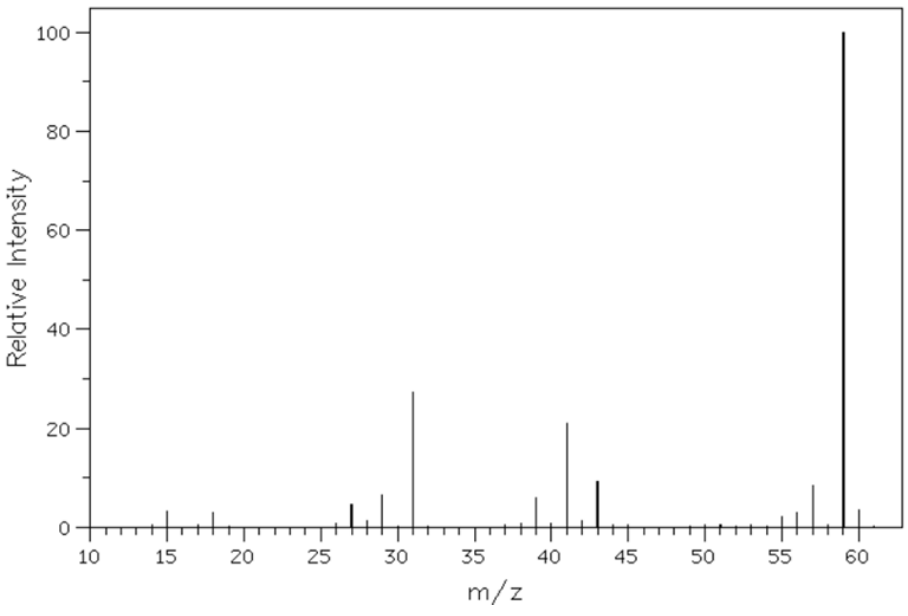
Test	Result
Carbon-13 NMR	
Proton NMR	

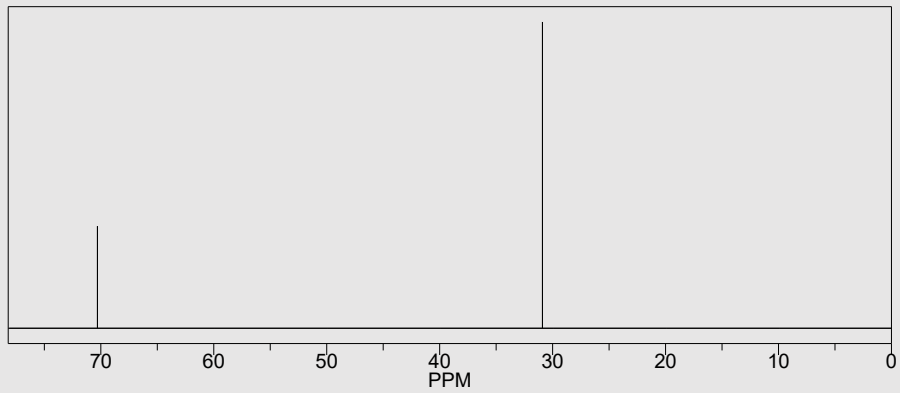
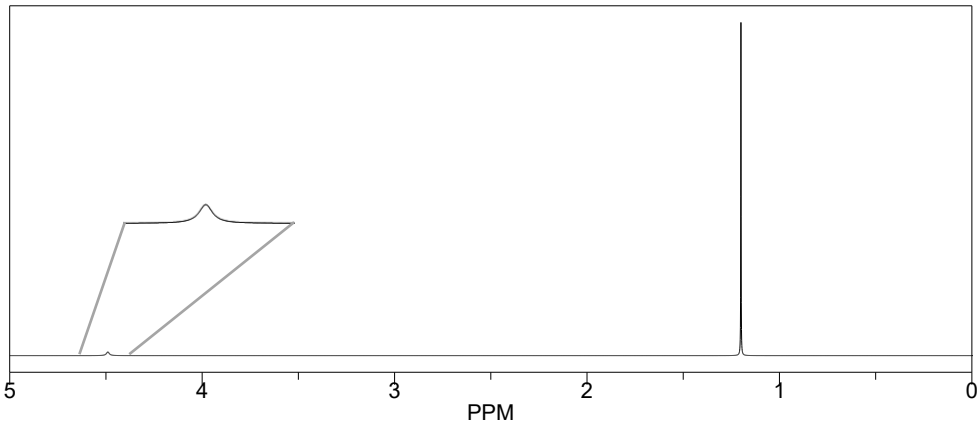
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
4.12	4	2
2.04	1	3
1.26	3	3

Check the solution to Sample N and see a work-through of the problem in this video on YouTube.

Sample O

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 74**	

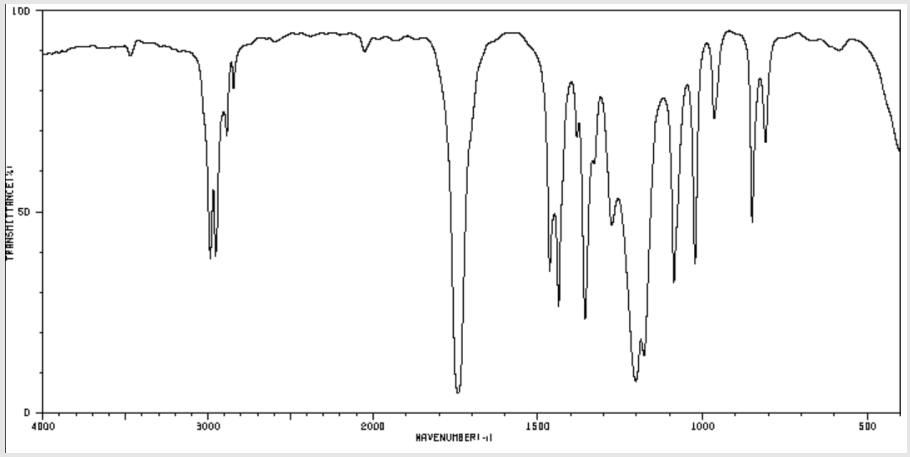
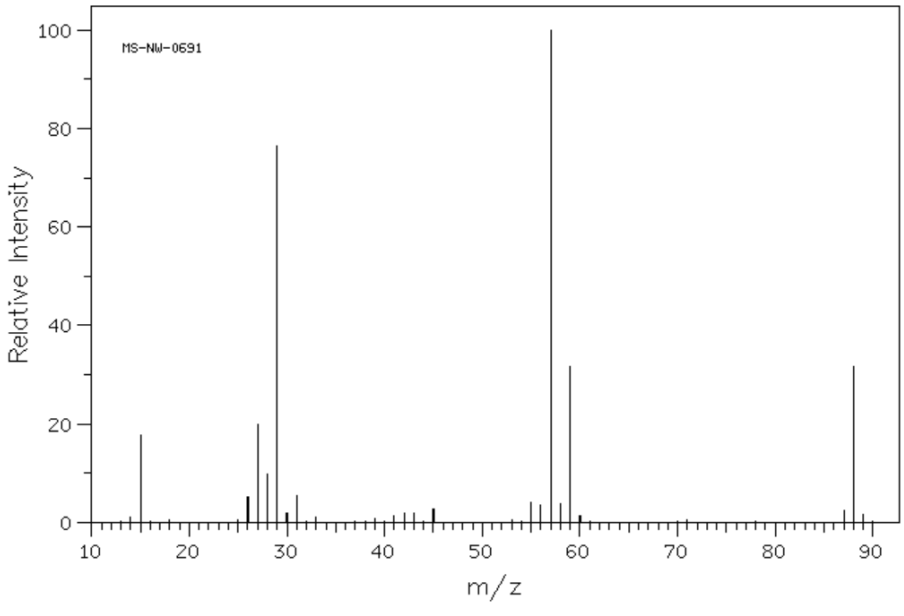
Test	Result
Carbon-13 NMR	
Proton NMR	

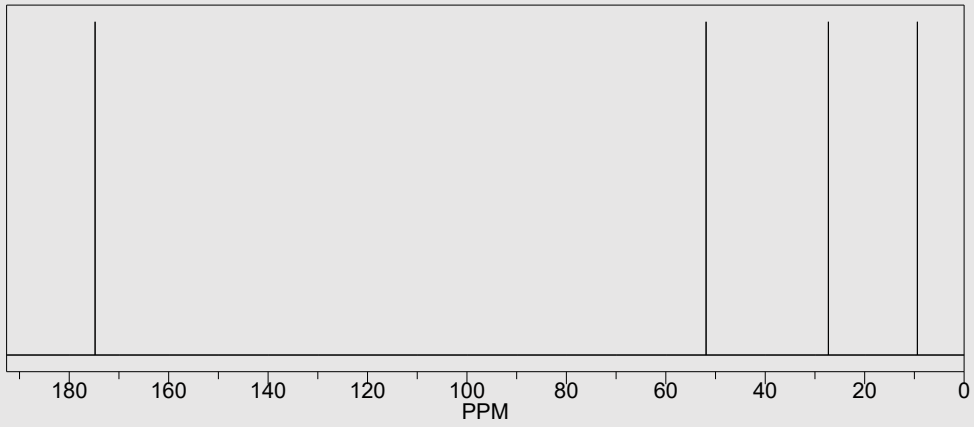
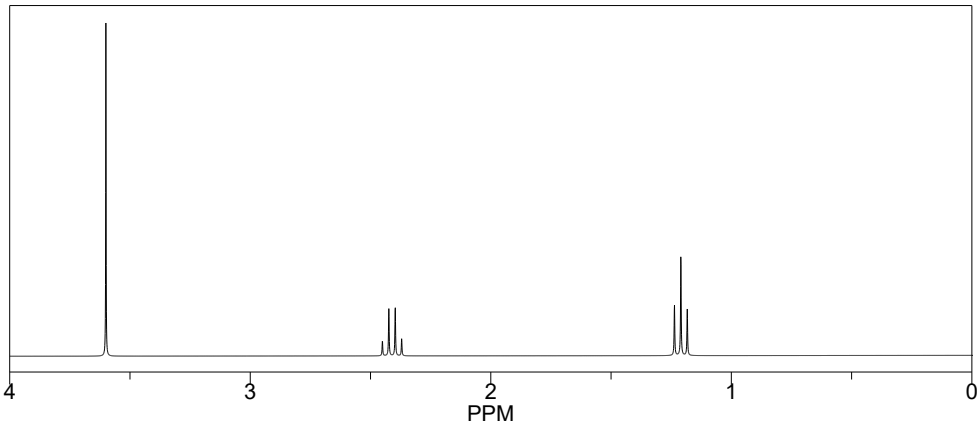
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
4.49	1	1
1.26	1	9

Check the solution to Sample O and see a work-through of the problem in this video on YouTube.

Sample P

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 88**	

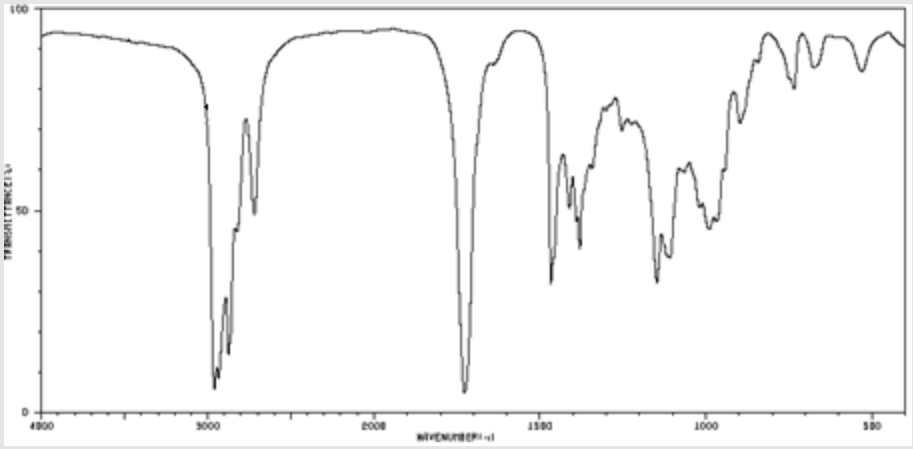
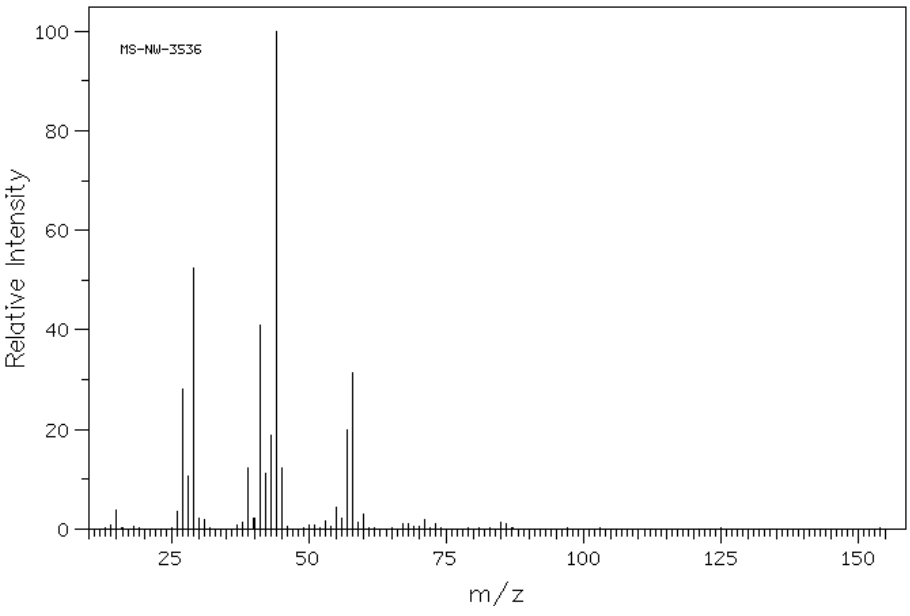
Test	Result
Carbon-13 NMR	
Proton NMR	

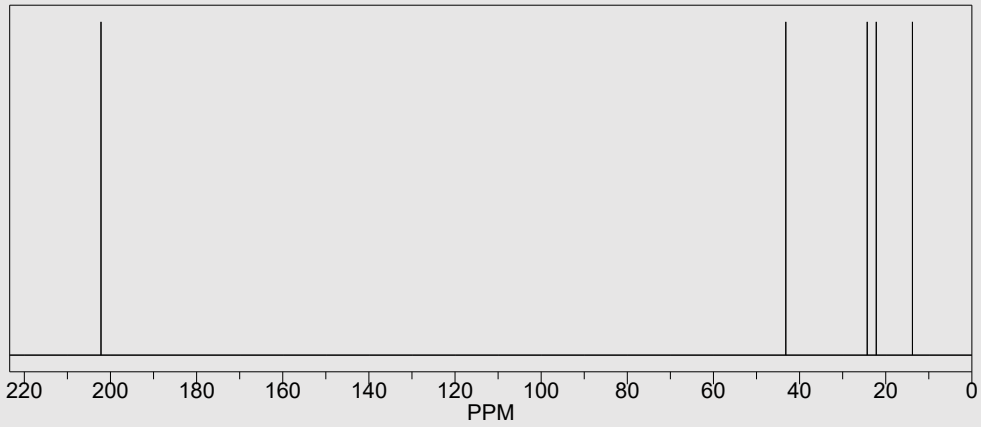
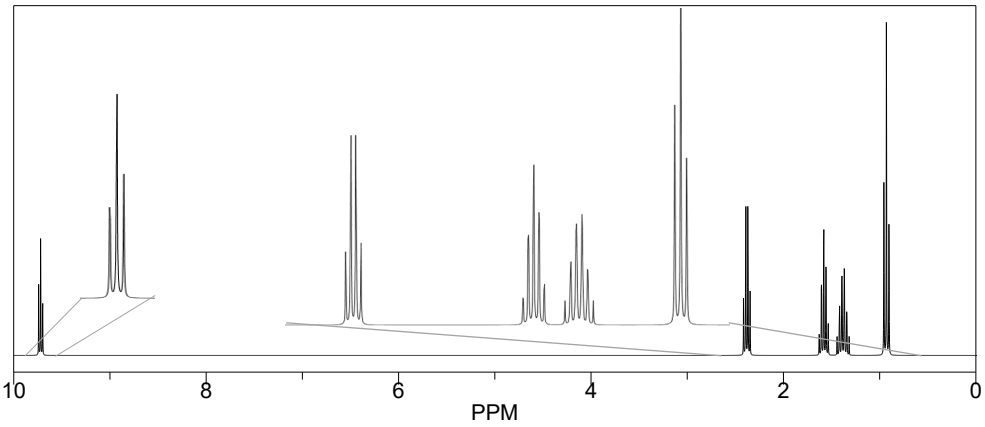
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
3.60	1	3
2.41	4	2
1.21	3	3

Check the solution to Sample P and see a work-through of the problem in this video on YouTube.

Sample Q

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Solution turns green
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 86**	

Test	Result
Carbon-13 NMR	
Proton NMR	

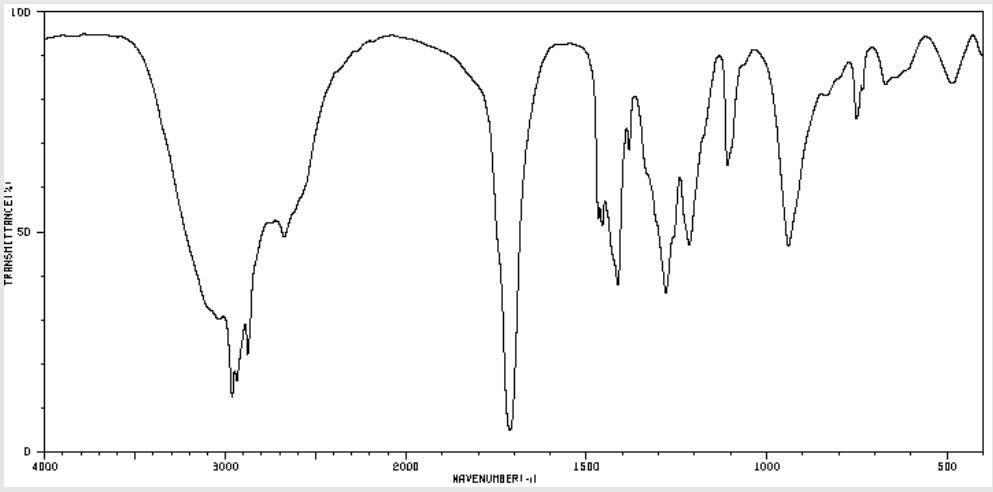
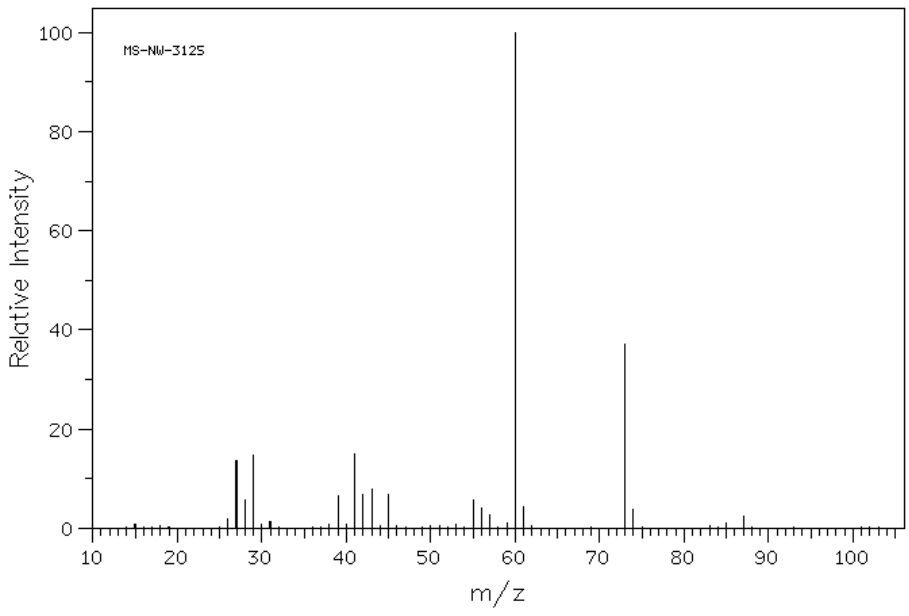
Proton NMR peak data

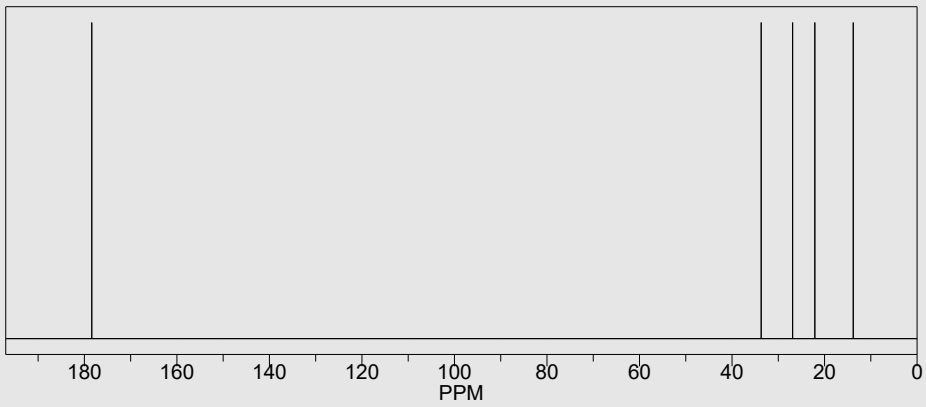
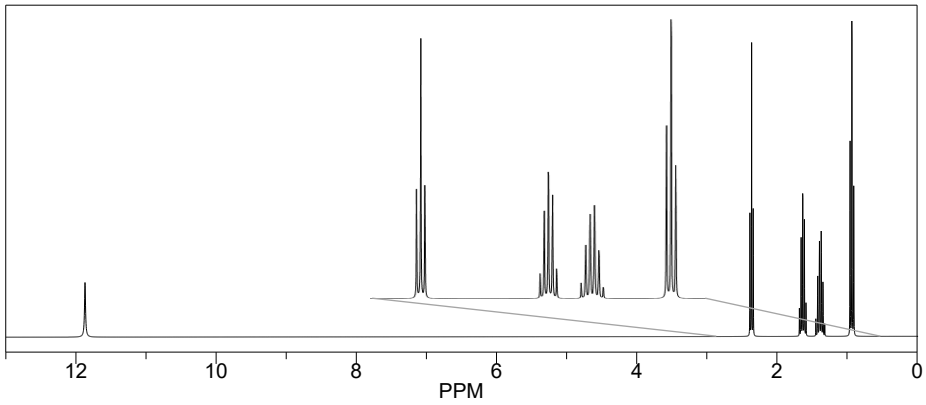
Shift (ppm)	Number of peaks	Peak area ratio
9.76	3	1
2.42	4	2
1.59	5	2

Shift (ppm)	Number of peaks	Peak area ratio
1.35	6	2
0.93	3	3

Check the solution to Sample Q and see a work-through of the problem in this video on YouTube.

Sample R

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	Bubbles of carbon dioxide
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 102**	

Test	Result
Carbon-13 NMR	
Proton NMR	

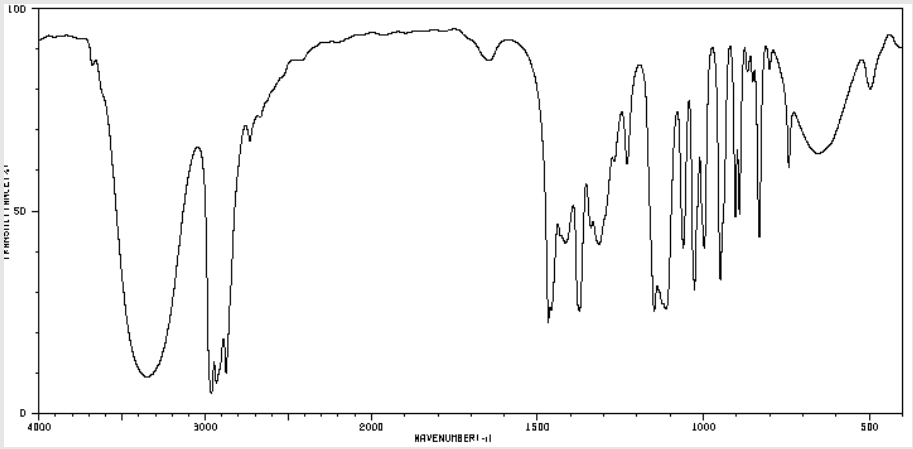
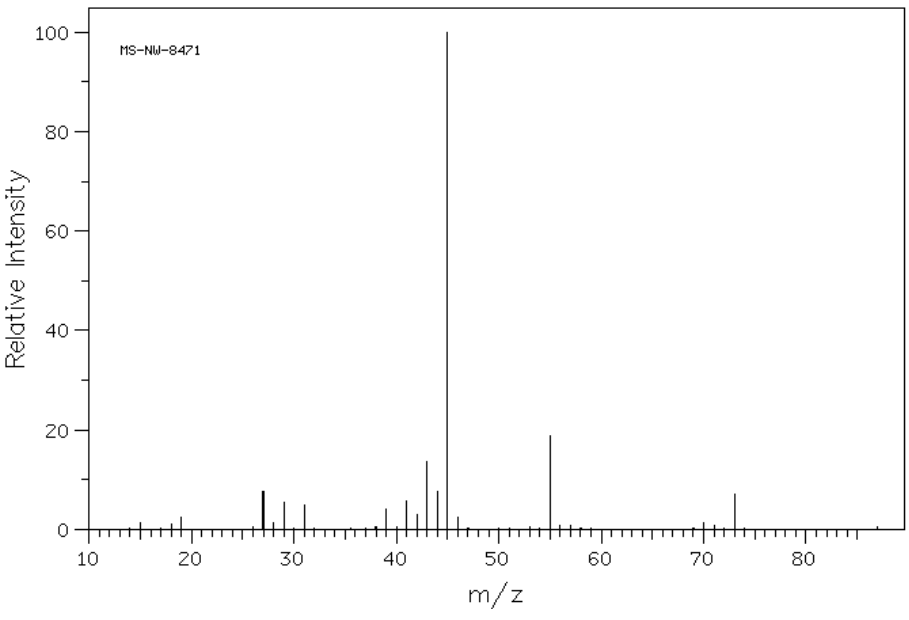
Proton NMR peak data

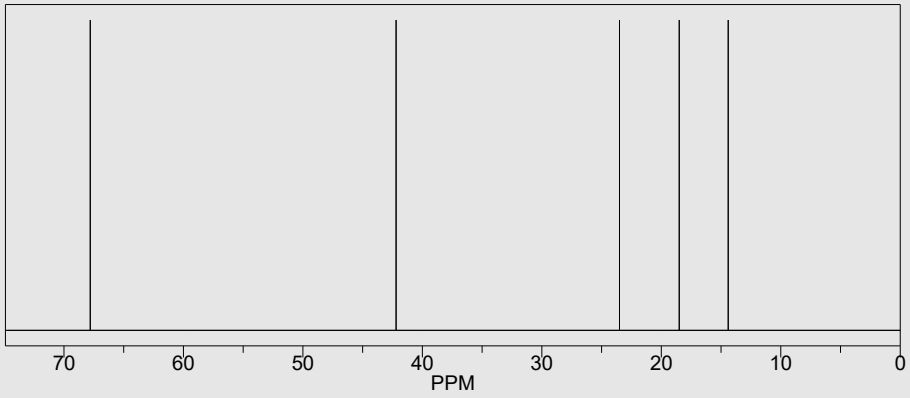
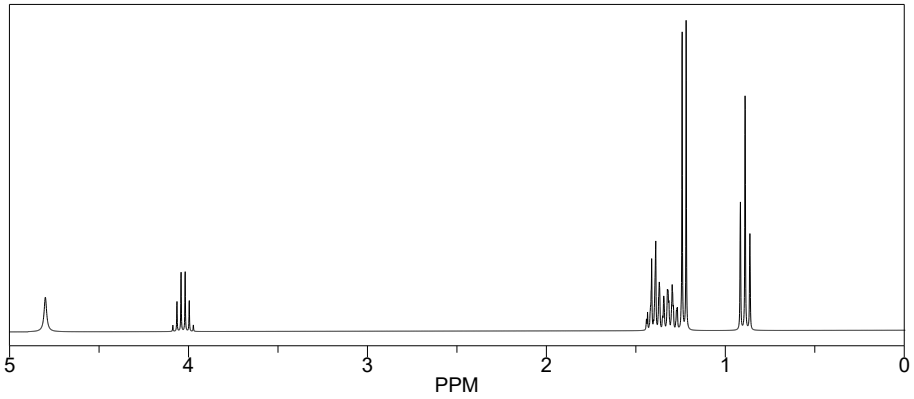
Shift (ppm)	Number of peaks	Peak area ratio
11.96	1	1
2.35	3	2
1.62	5	2

Shift (ppm)	Number of peaks	Peak area ratio
1.39	6	2
0.93	3	3

Check the solution to Sample R and see a work-through of the problem in this video on YouTube.

Sample S

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Solution turns green
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 88**	

Test	Result
Carbon-13 NMR	
Proton NMR	

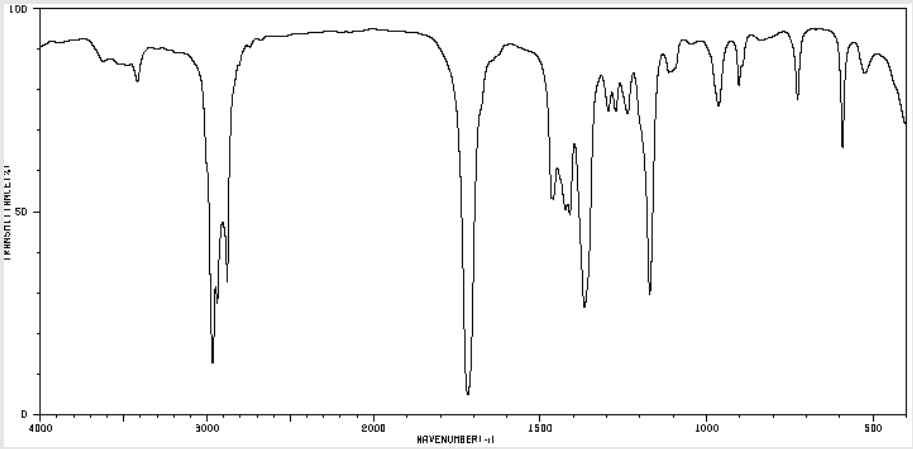
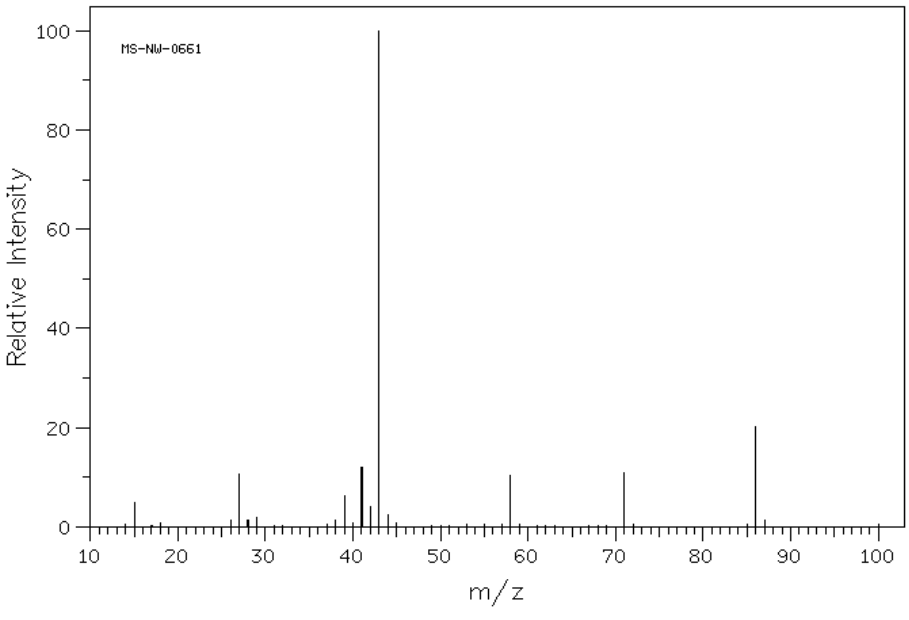
Proton NMR peak data

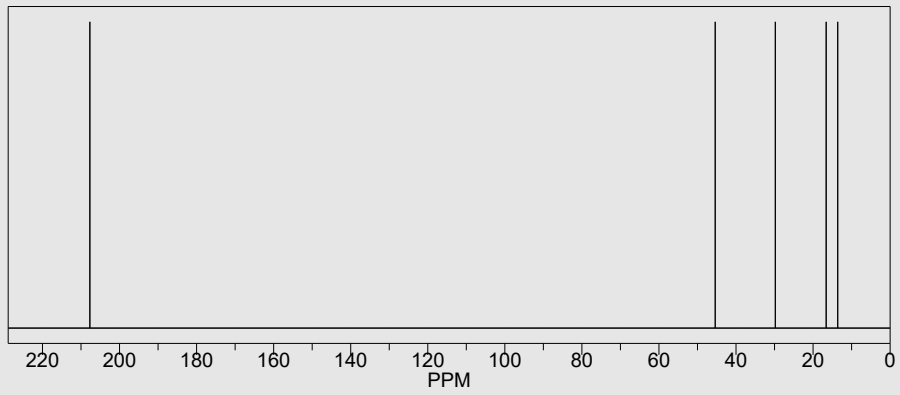
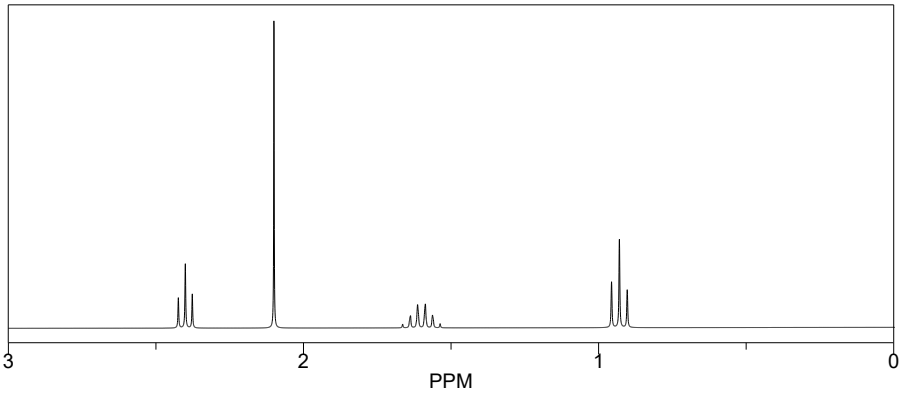
Shift (ppm)	Number of peaks	Peak area ratio
2.66	1	1
3.79	6	1
1.44	4	2

Shift (ppm)	Number of peaks	Peak area ratio
1.36	6	2
1.17	2	3
0.92	3	3

Check the solution to Sample S and see a work-through of the problem in this video on YouTube.

Sample T

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 86**	

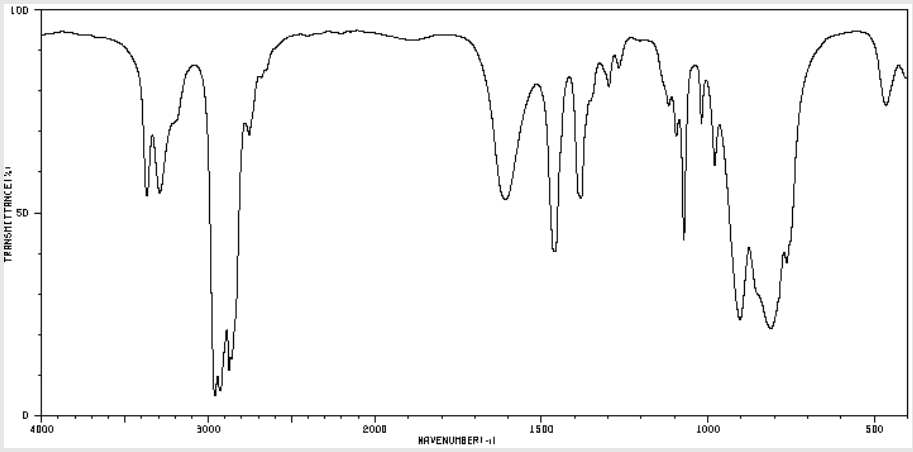
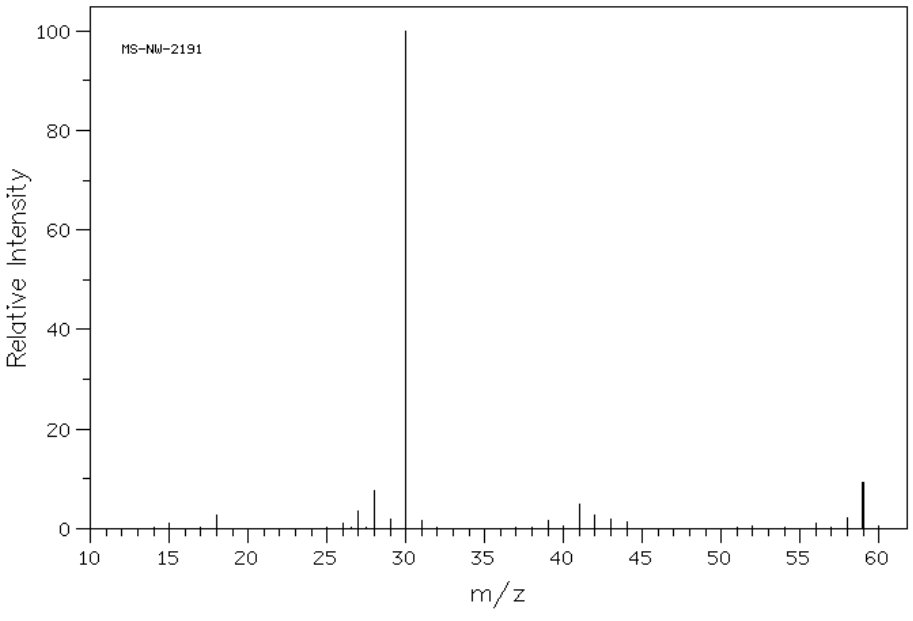
Test	Result
Carbon-13 NMR	
Proton NMR	

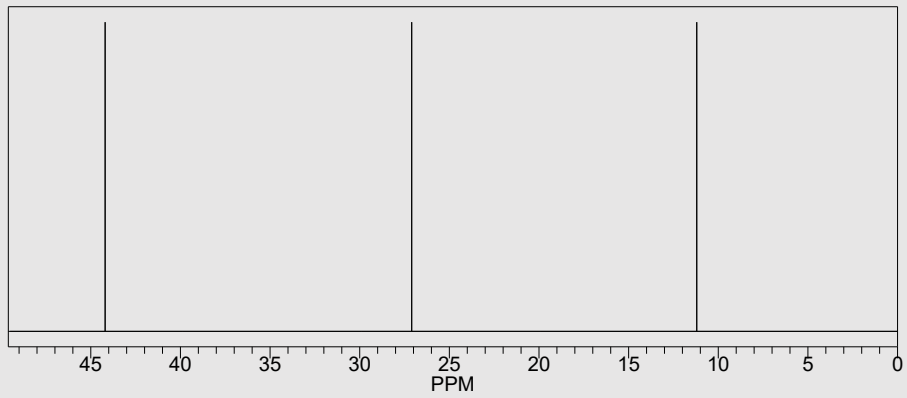
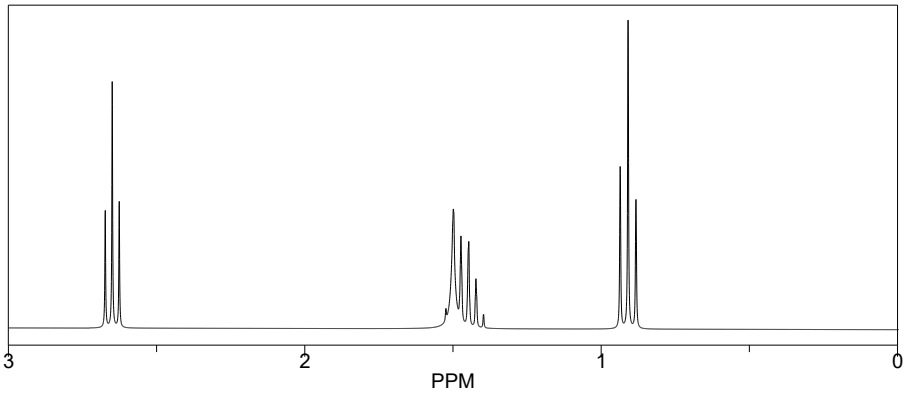
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
2.40	3	2
2.13	1	3
1.60	6	2
0.93	3	3

Check the solution to Sample T and see a work-through of the problem in this video on YouTube.

Sample U

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 59**	

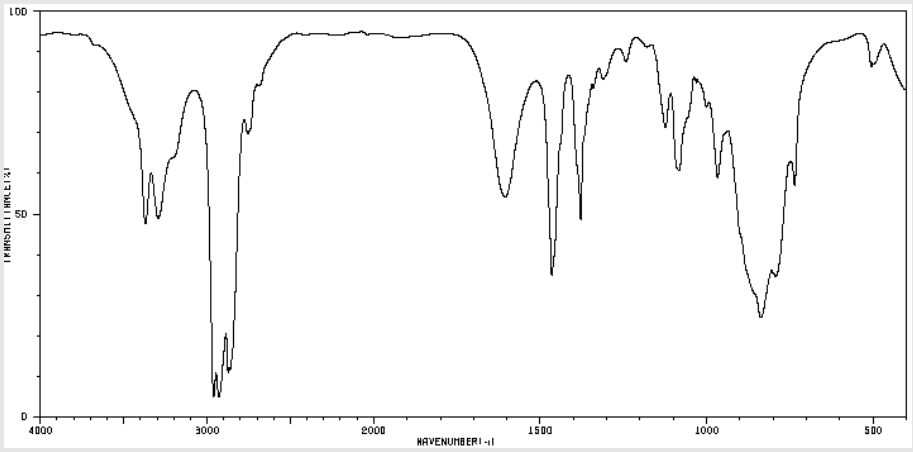
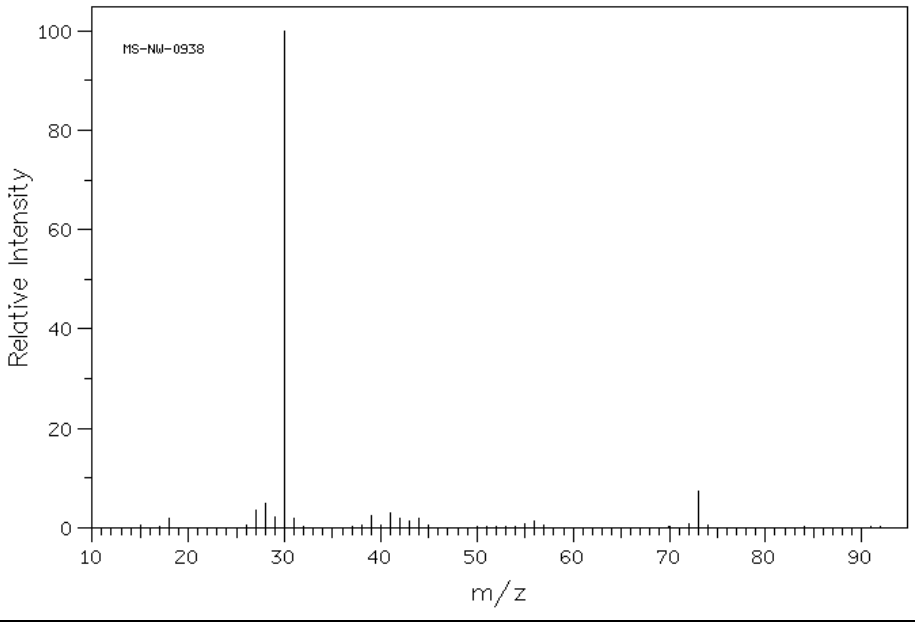
Test	Result
Carbon-13 NMR	
Proton NMR	

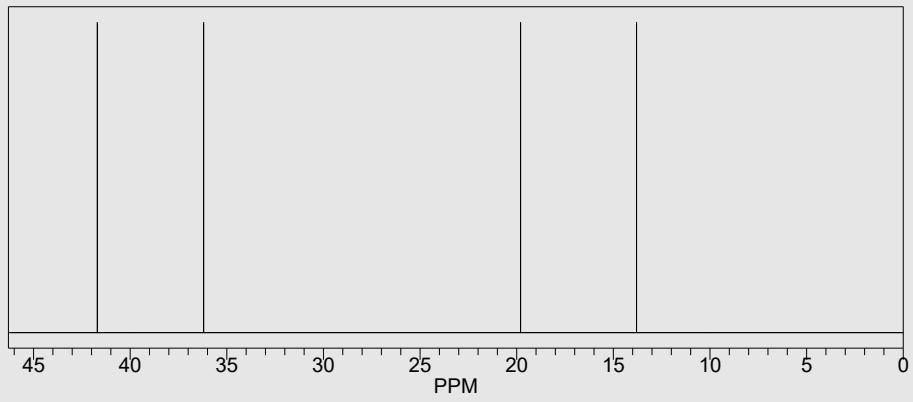
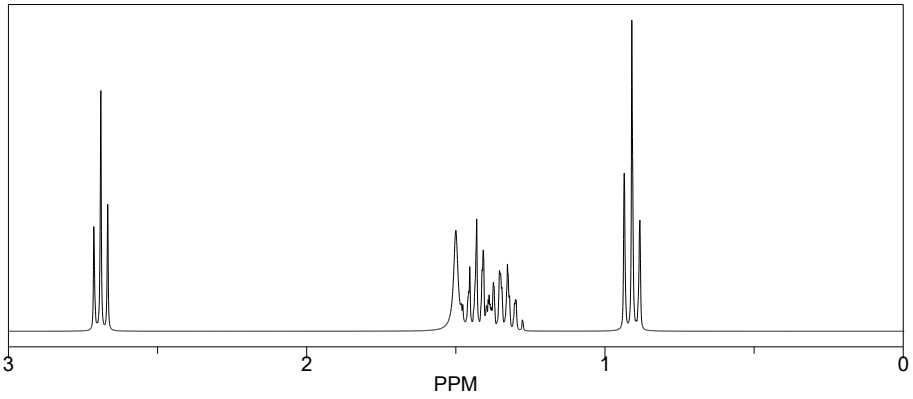
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
2.65	3	2
1.50	1	2
1.46	6	2
0.92	3	3

Check the solution to Sample U and see a work-through of the problem in this video on YouTube.

Sample V

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 73**	

Test	Result
Carbon-13 NMR	
Proton NMR	

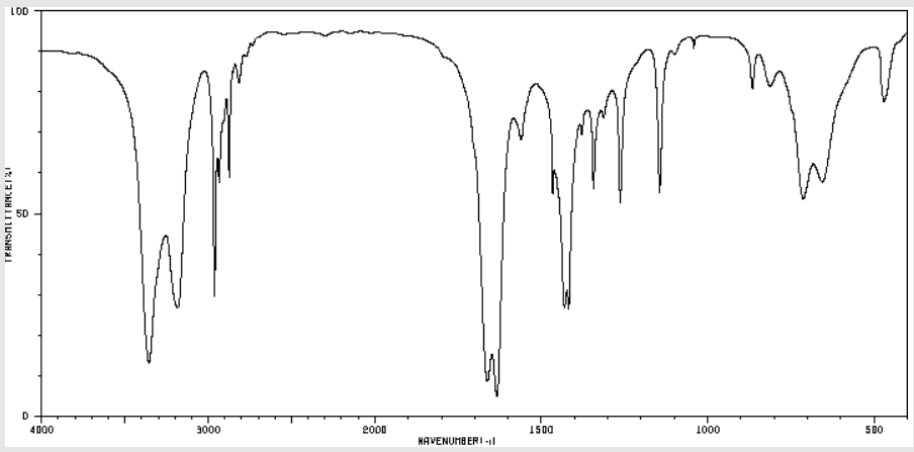
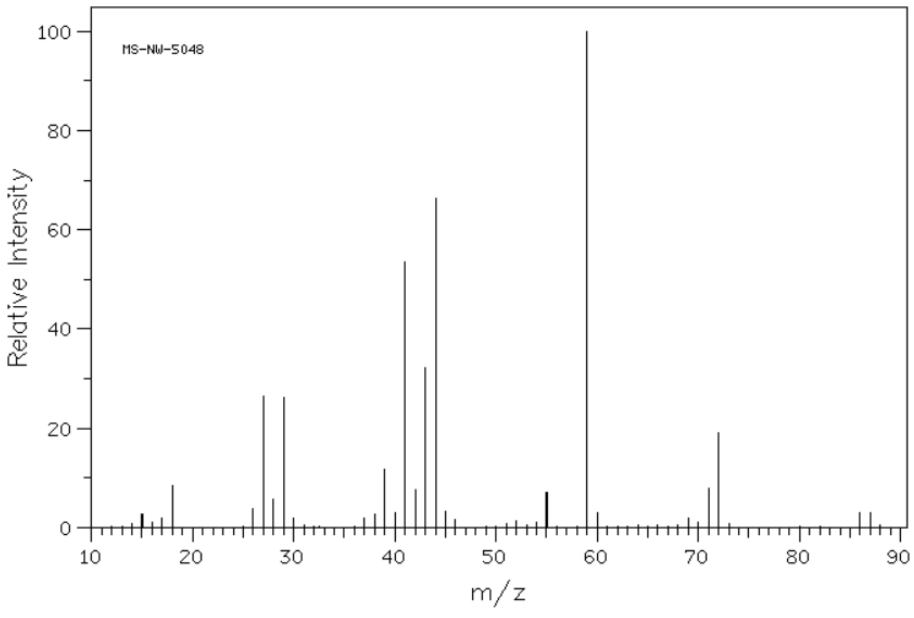
Proton NMR peak data

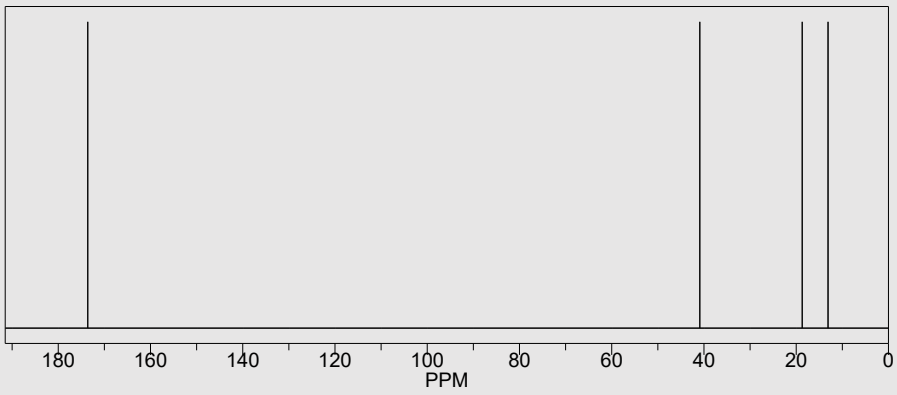
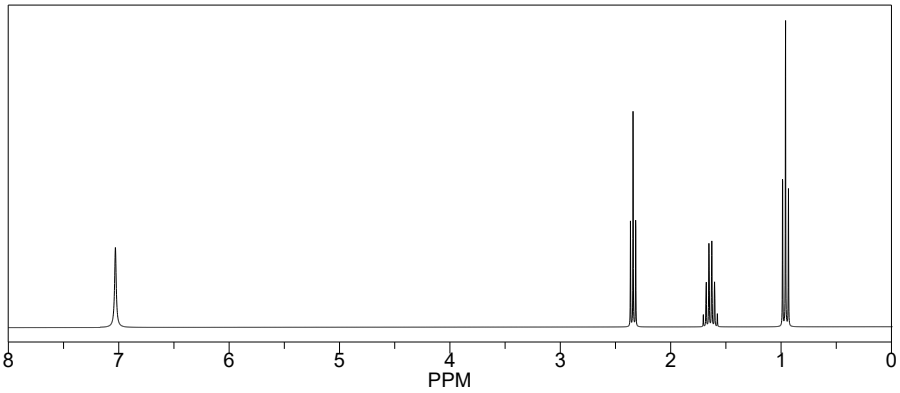
Shift (ppm)	Number of peaks	Peak area ratio
2.68	3	2
1.50	1	2
1.43	5	2

Shift (ppm)	Number of peaks	Peak area ratio
1.33	6	2
0.92	3	3

Check the solution to Sample V and see a work-through of the problem in this video on YouTube.

Sample W

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 87**	

Test	Result
Carbon-13 NMR	
Proton NMR	

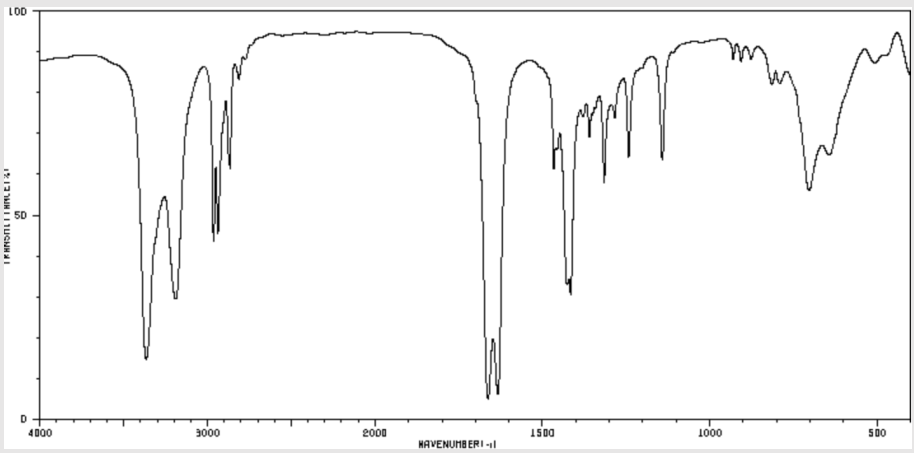
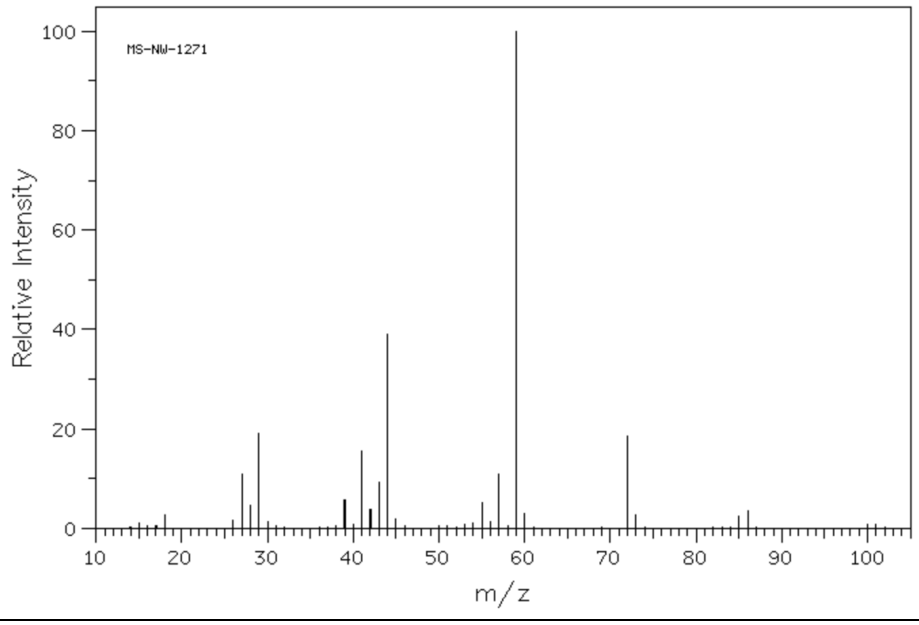
Proton NMR peak data

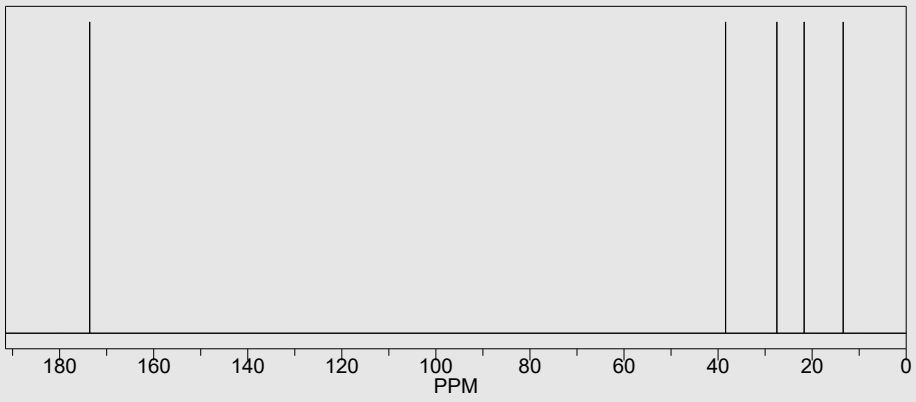
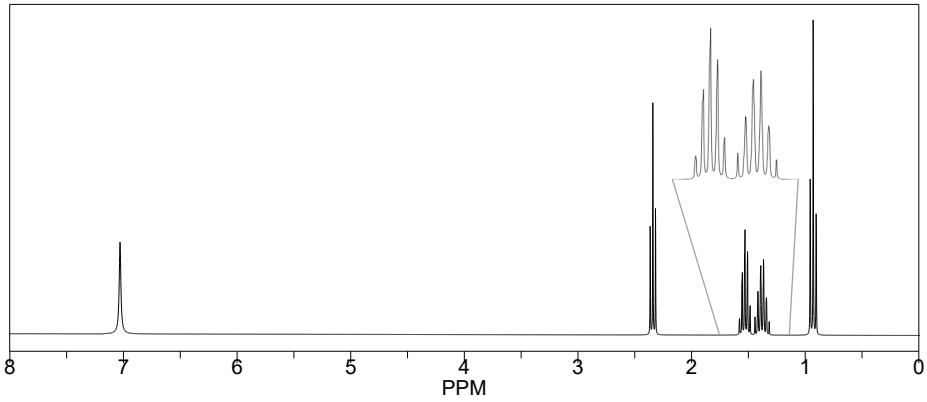
Shift (ppm)	Number of peaks	Peak area ratio
7.03	1	2
2.02	3	2

Shift (ppm)	Number of peaks	Peak area ratio
1.64	6	2
0.96	3	3

Check the solution to Sample W and see a work-through of the problem in this video on YouTube.

Sample X

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 101**	

Test	Result
Carbon-13 NMR	
Proton NMR	

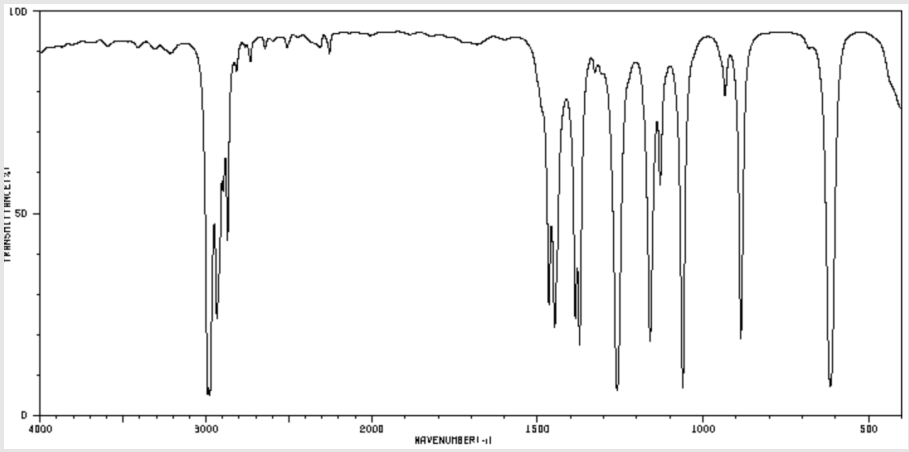
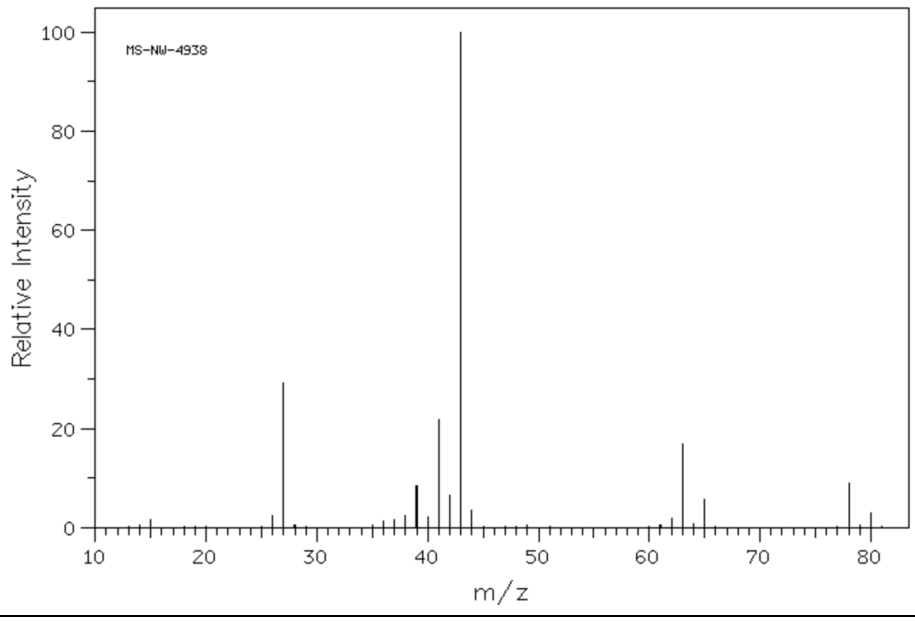
Proton NMR peak data

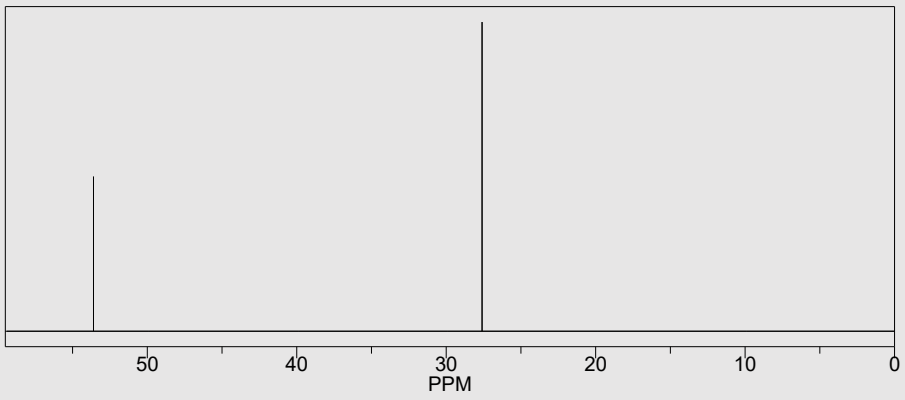
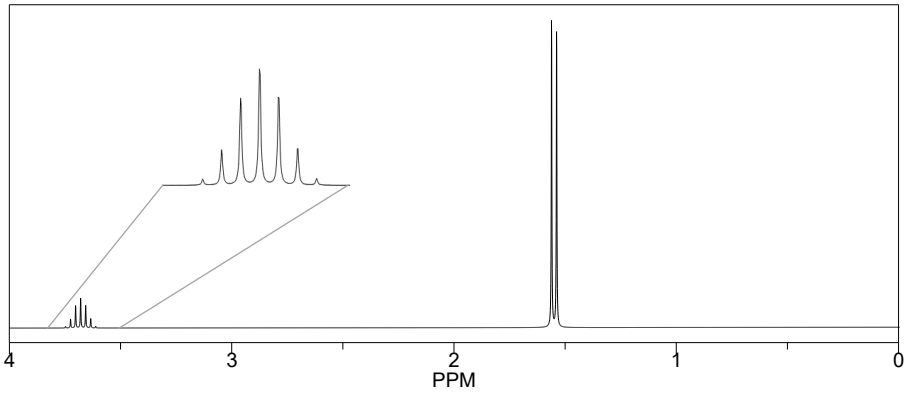
Shift (ppm)	Number of peaks	Peak area ratio
7.03	1	1
2.34	3	2

Shift (ppm)	Number of peaks	Peak area ratio
1.53	5	2
1.37	6	2
0.93	3	3

Check the solution to Sample X and see a work-through of the problem in this video on YouTube.

Sample Y

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 78**	

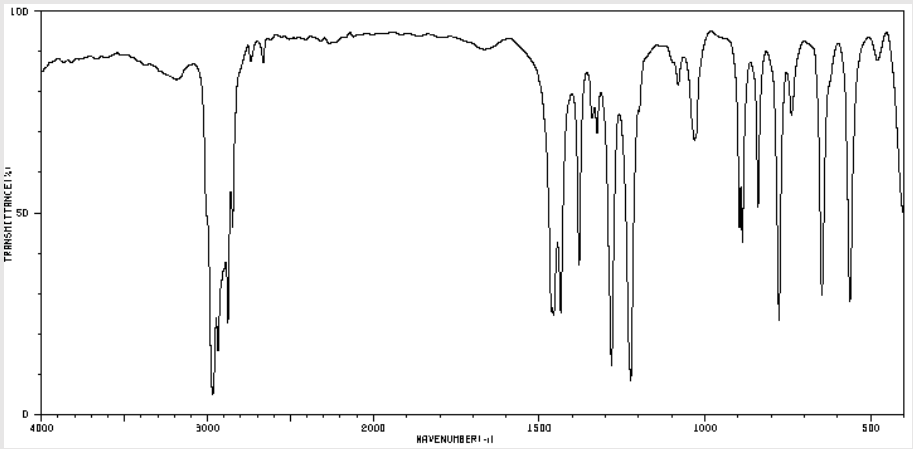
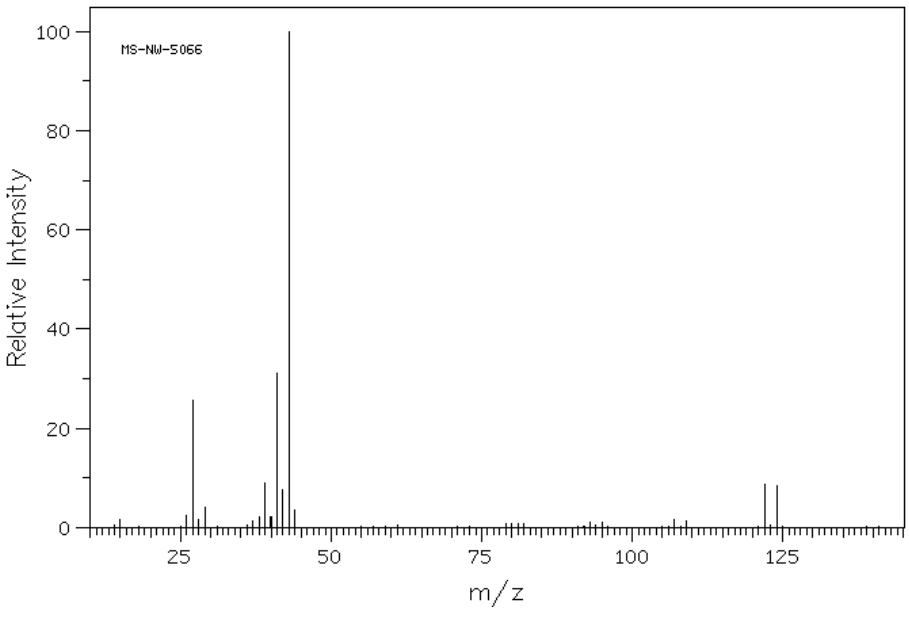
Test	Result
Carbon-13 NMR	
Proton NMR	

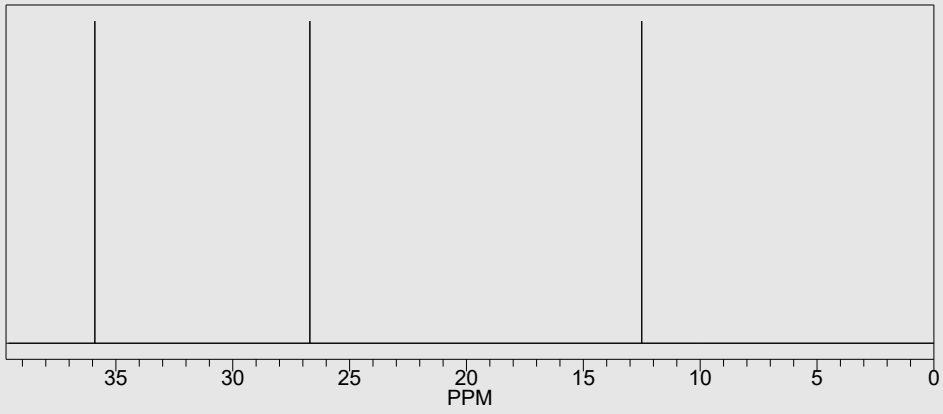
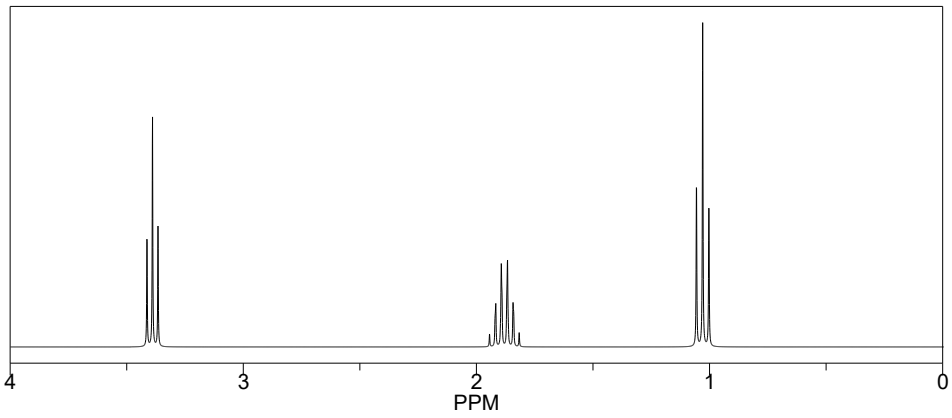
Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
3.68	7	1
1.55	2	6

Check the solution to Sample Y and see a work-through of the problem in this video on YouTube.

Sample Z

Test	Result
Unsaturation test using bromine water	Orange colour remains
Oxidation test using acidified potassium dichromate	Orange colour remains
Carboxylic acid test using sodium carbonate	No bubbles
Infrared spectroscopy	
Mass spectrometry **Mass of molecular ion:** **m/z = 122**	

Test	Result
Carbon-13 NMR	
Proton NMR	

Proton NMR peak data

Shift (ppm)	Number of peaks	Peak area ratio
3.39	3	2
1.87	6	2
1.03	3	3

Check the solution to Sample Z and see a work-through of the problem in this video on YouTube.

References

Bergwerf, H., 2015. *Molview.* [Online]
Available at: http://molview.org/
[Accessed 29 06 2020].

National Institute of Advanced Industrial Science and Technology, Japan, 2018. *Spectral Database for Organic Compounds.* [Online]
Available at: https://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi
[Accessed 06 29 2020].

NSW Education Standards Authority, 2017. *Chemistry HSC Data Sheet.* [Online]
Available at: https://educationstandards.nsw.edu.au/wps/wcm/connect/98664936-221f-4c49-88e1-d002ec69285c/chemistry-data-sheet-2017-02.pdf?MOD=AJPERES&CVID=
[Accessed 30 6 2020].

NSW Education Standards Authority, 2017. *Chemistry Stage 6 Syllabus.* [Online]
Available at: https://educationstandards.nsw.edu.au/wps/portal/nesa/11-12/stage-6-learning-areas/stage-6-science/chemistry-2017
[Accessed 6 29 2020].

NSW Education Standards Authority, 2019. *Chemistry 2019 HSC Exam Pack.* [Online]
Available at: https://educationstandards.nsw.edu.au/wps/portal/nesa/resource-finder/hsc-exam-papers/2019/chemistry-2019-hsc-exam-pack
[Accessed 6 29 2020].