

Determining the structure of compounds

Here are real results obtained by analysing compounds using mass spectrometry, IR spectroscopy and NMR spectroscopy.

Do your best to work out the structure of the compounds in as much detail as you can.

You are given the empirical formula and the relative molecular mass of each compound.

Some clues

Compound 1

The molecule fragments so easily that we do not see the molecular ion peak – the highest is at 59, which is M-1.

Compounds 2 and 3

These are complete unknowns.

Compound 4

This substance was obtained from heating plastic to a high temperature.

Compound 5

This compound was produced during the oxidation of methyl benzene in ethanoic acid.

Compound 6

This compound was produced as a product during the reduction of phenol.

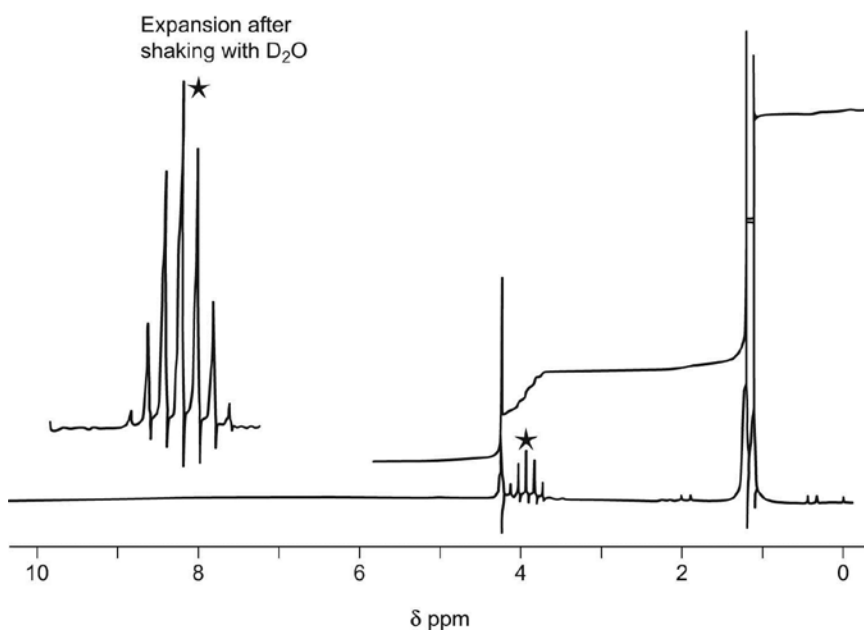
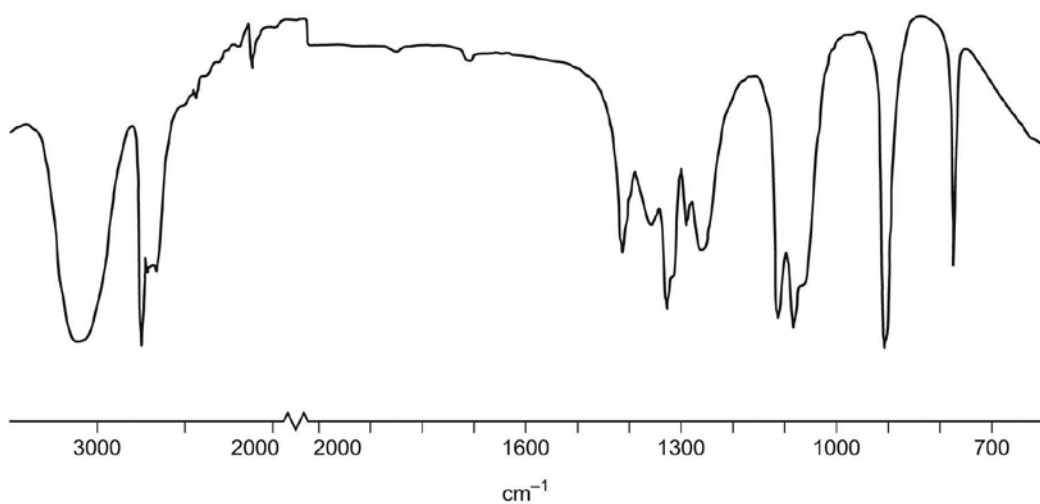
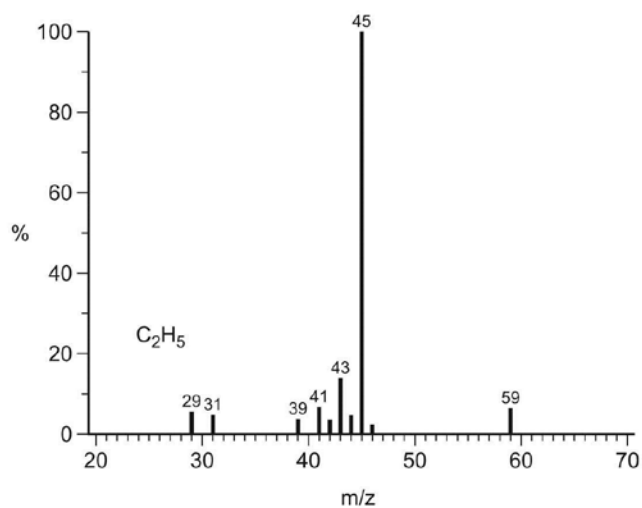
Compound 7

This compound was extracted from a reaction mixture containing hydrochloric acid. The molecular ion is absent again and the relative molecular mass is thought to be 73.

Compound 1

C_3H_8O

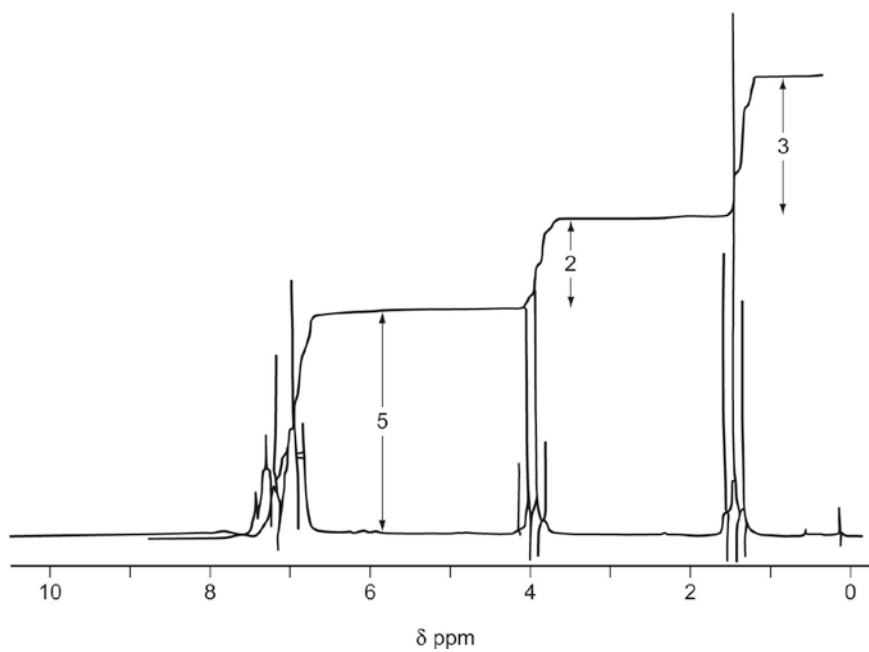
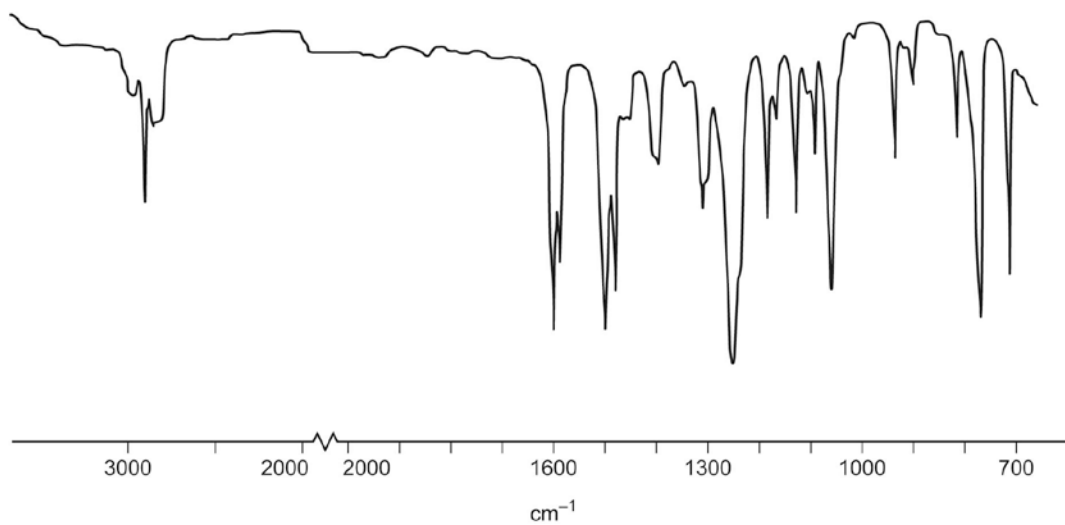
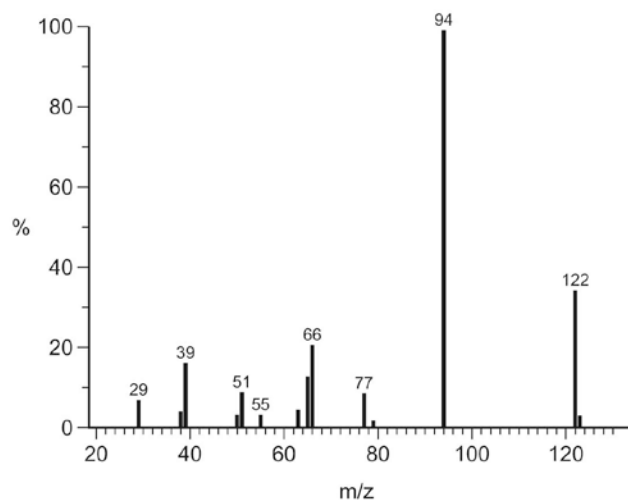
RMM 60



Compound 2

C₈H₁₀O

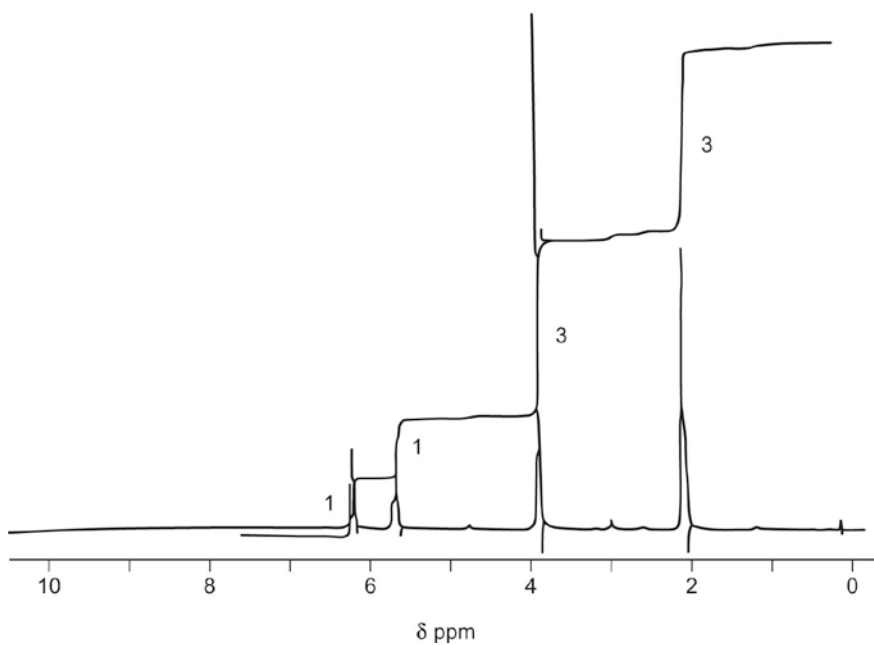
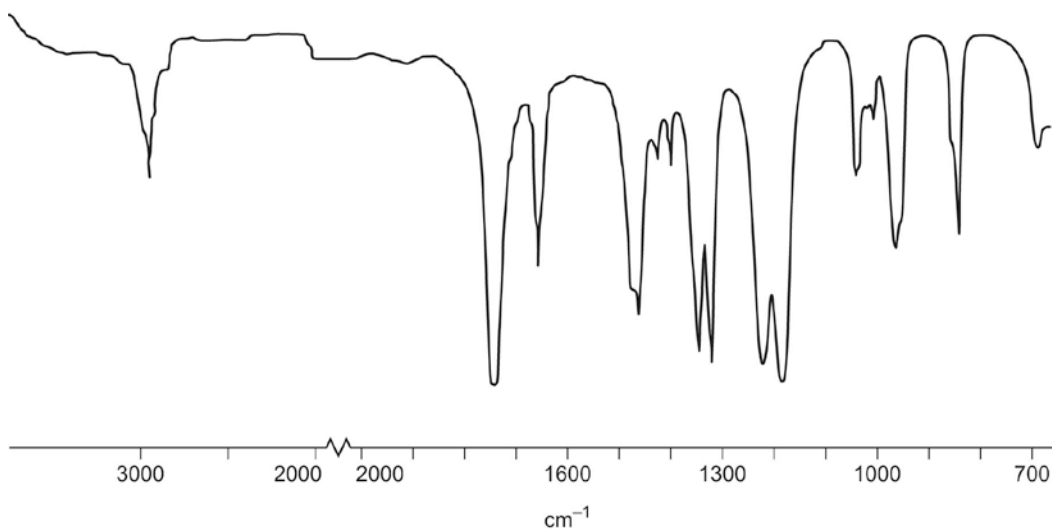
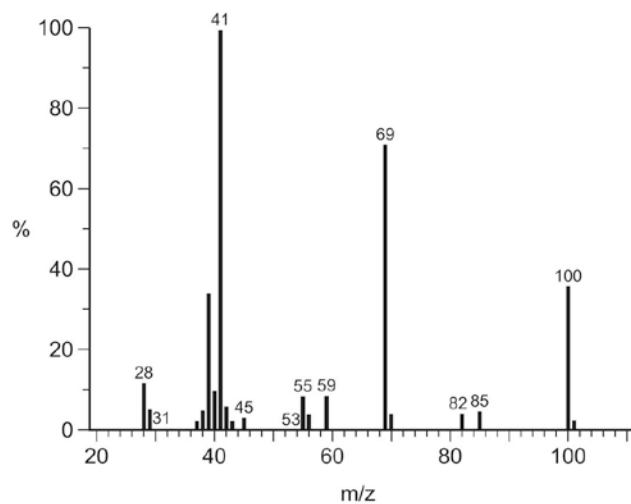
RMM 122



Compound 3

$C_5H_8O_2$

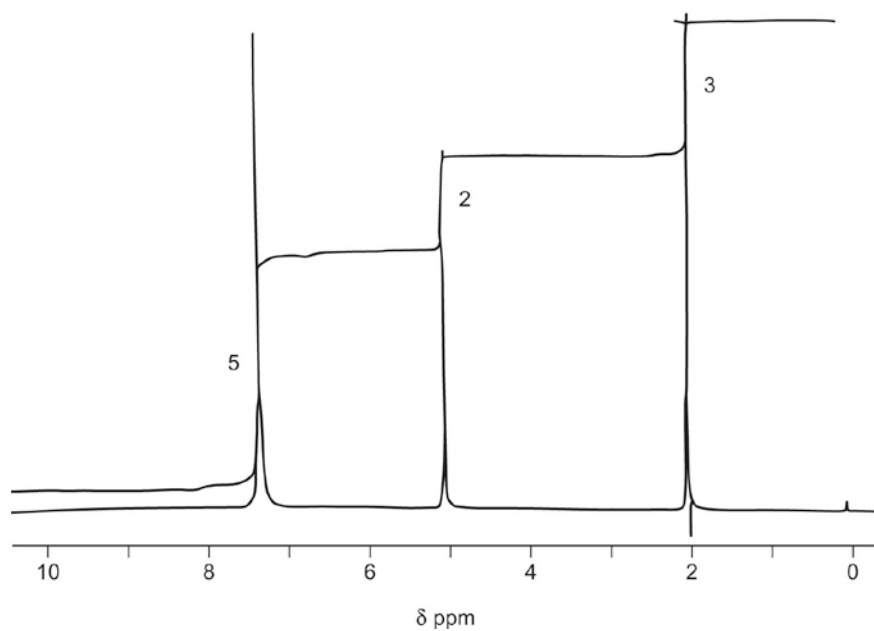
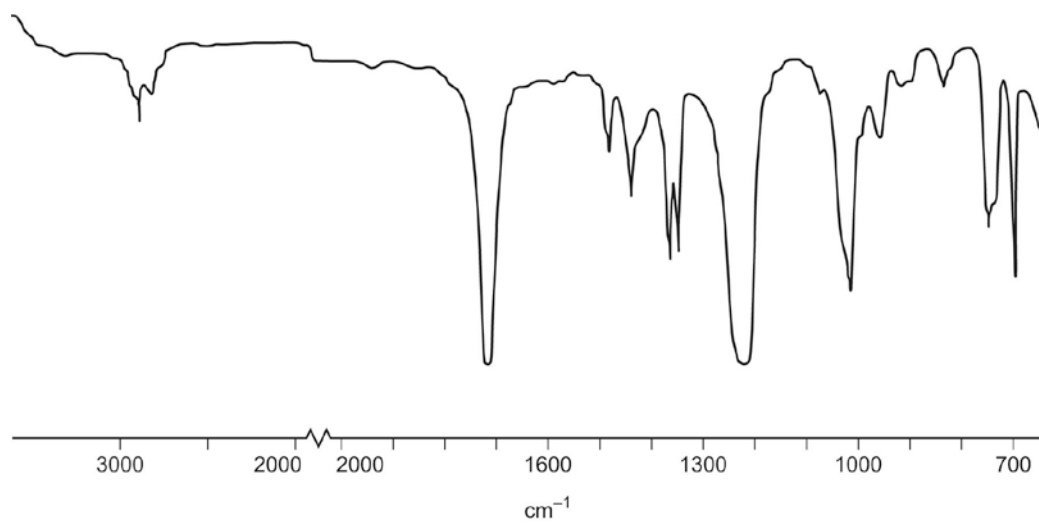
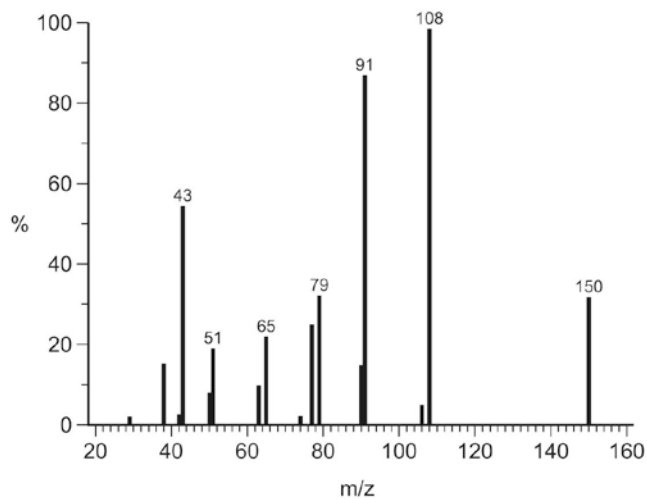
RMM 100



Compound 4

$C_9H_{10}O_2$

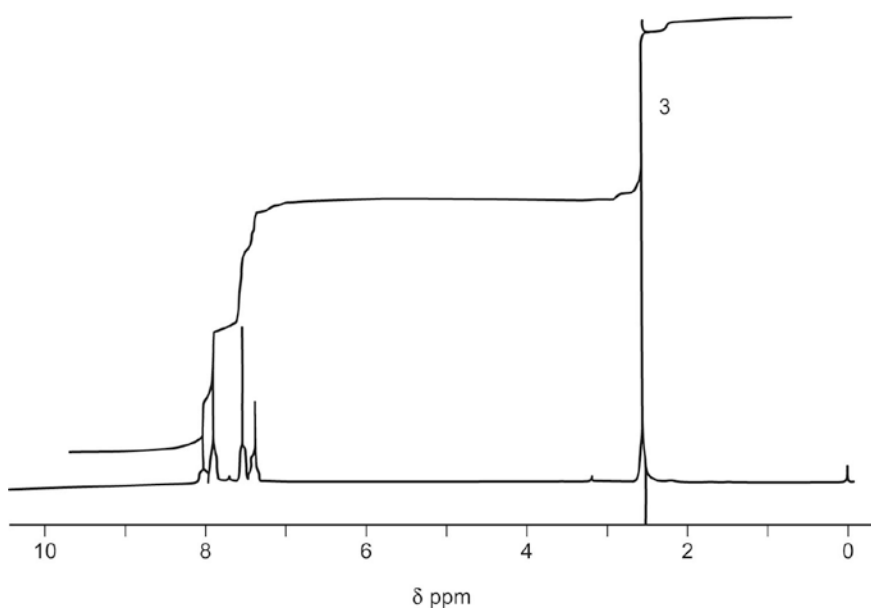
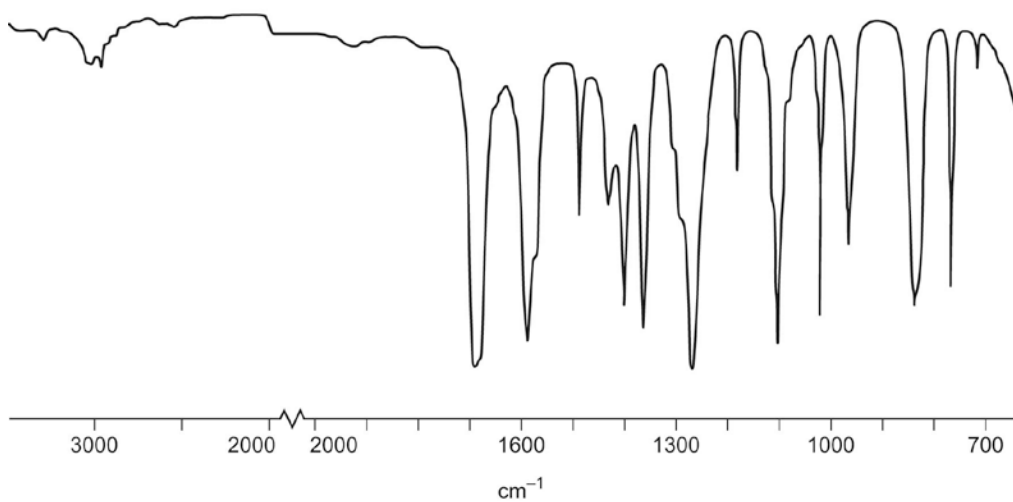
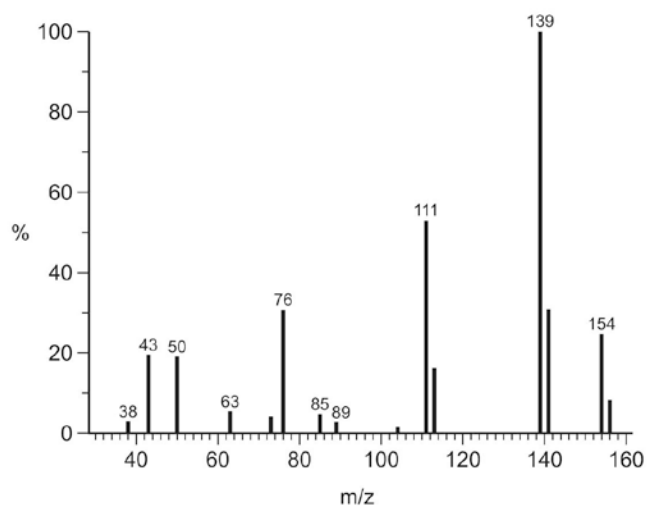
RMM 150



Compound 5

C₈H₇Cl

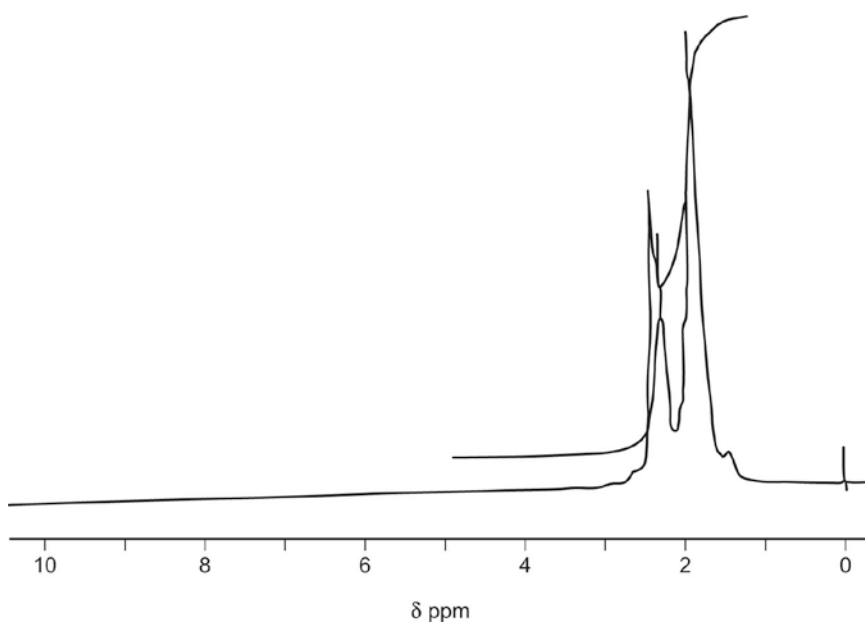
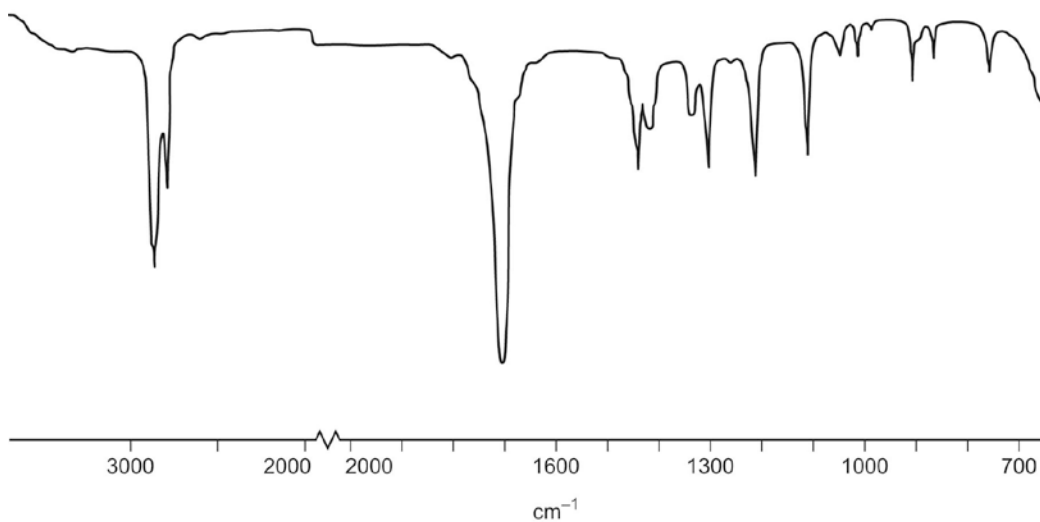
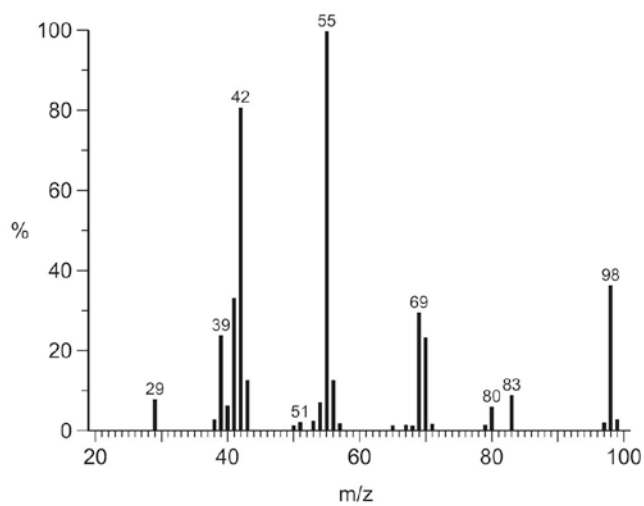
RMM 154



Compound 6

$C_6H_{10}O$

RMM 98



Compound 7

$C_4H_{11}N$

RMM 73

