

Structure determination

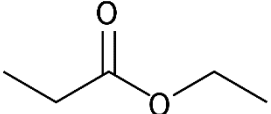
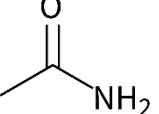
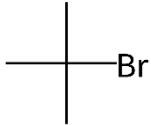
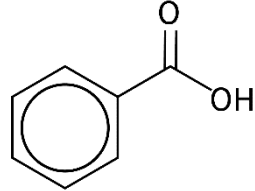
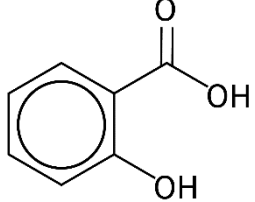
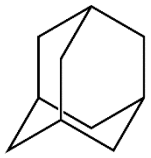
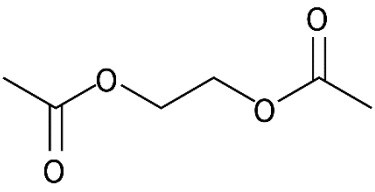
Learning objective

- 1 Analyse and interpret infrared, ^{13}C NMR and ^1H NMR spectra
- 2 Suggest chemical structures based on spectral evidence

Activity

Below are the skeletal structures for 7 compounds.

Decide which set of spectra sets **A-G** from the following pages belong to each compound.

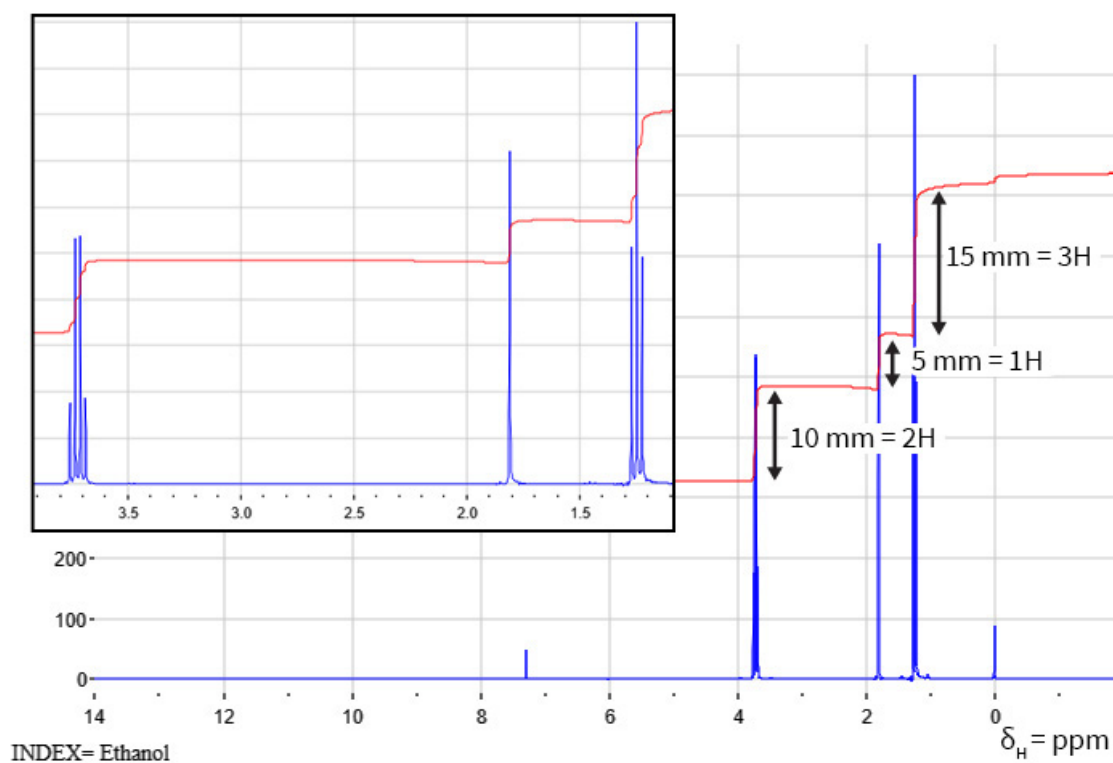
ethyl propanoate  Spectra set ____	ethanamide  Spectra set ____	2-bromo-2-methyl propane  Spectra set ____
benzoic acid  Spectra set ____	2-hydroxybenzoic acid  Spectra set ____	adamantane  Spectra set ____
	1,2-diacetoxyethane  Spectra set ____	

Before you begin read the **Helpful information** on the next page.

Make sure you have a data book or sheet available to help you identify key bonds and groups present.

Helpful information

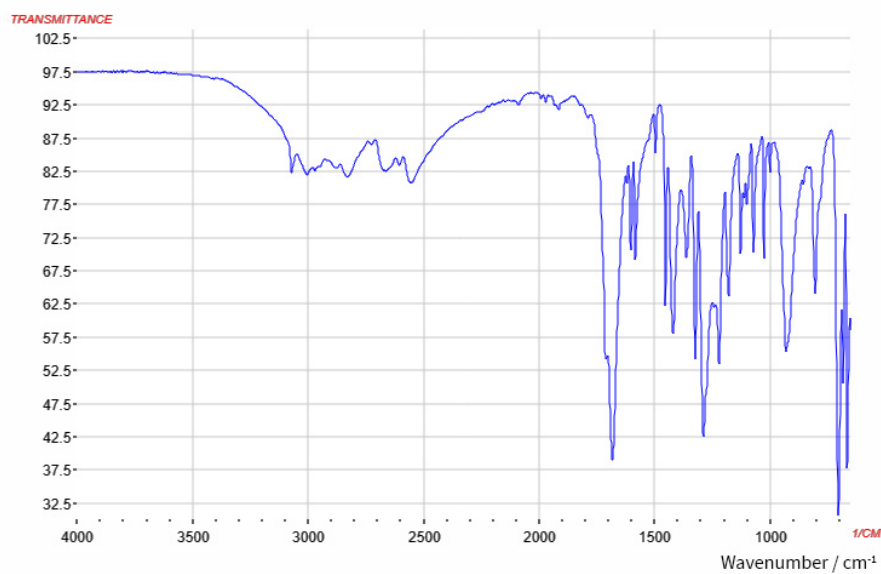
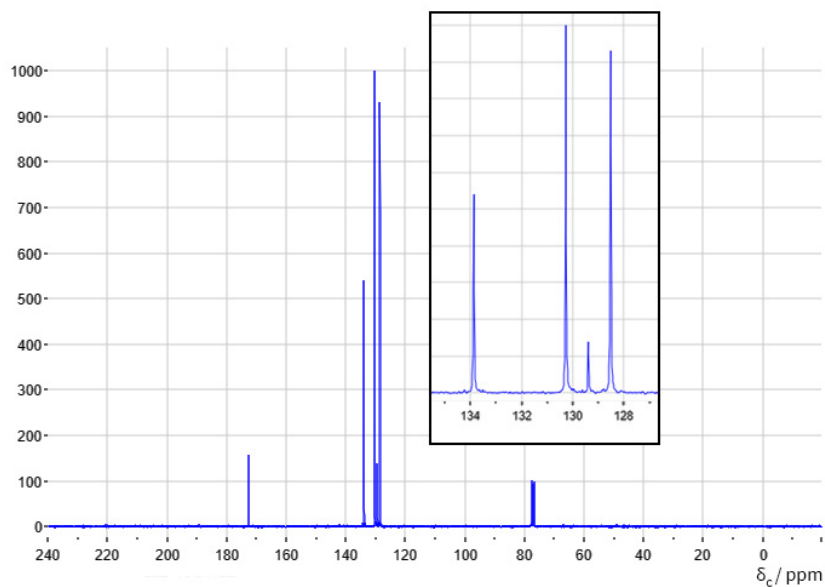
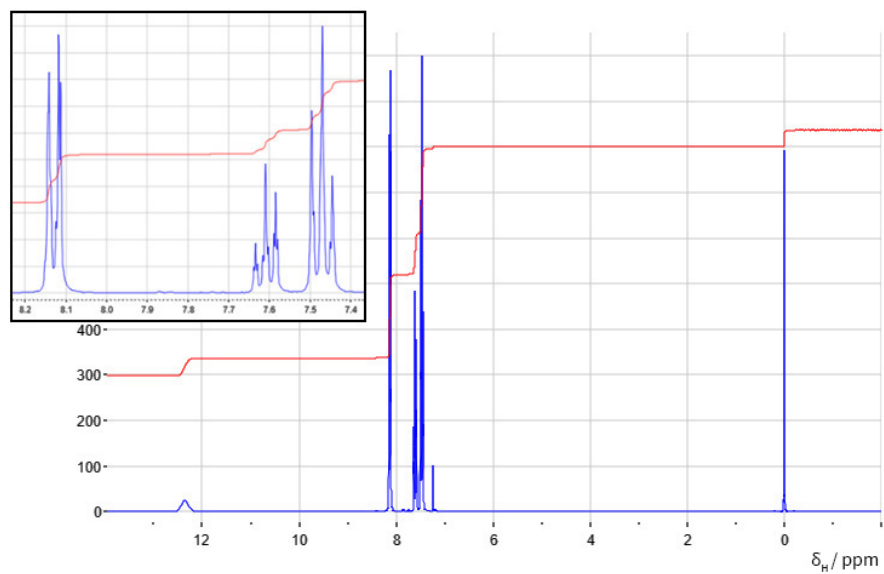
1. In the ^1H NMR the relative height of the red line shows the integration of each of the peaks. Where peaks are split a zoomed in section of the spectrum is given to show the splitting pattern.



2. These are real spectra so in some instances small peaks of impurities are seen.
3. You may also see peaks owing to the solvent used to dissolve the sample.
 CDCl_3 δ_{C} 77 ppm (three lines 1:1:1) and δ_{H} 7.25 ppm
DMSO δ_{C} 39.5 ppm (septet) and δ_{H} 2.50 ppm (quintet)

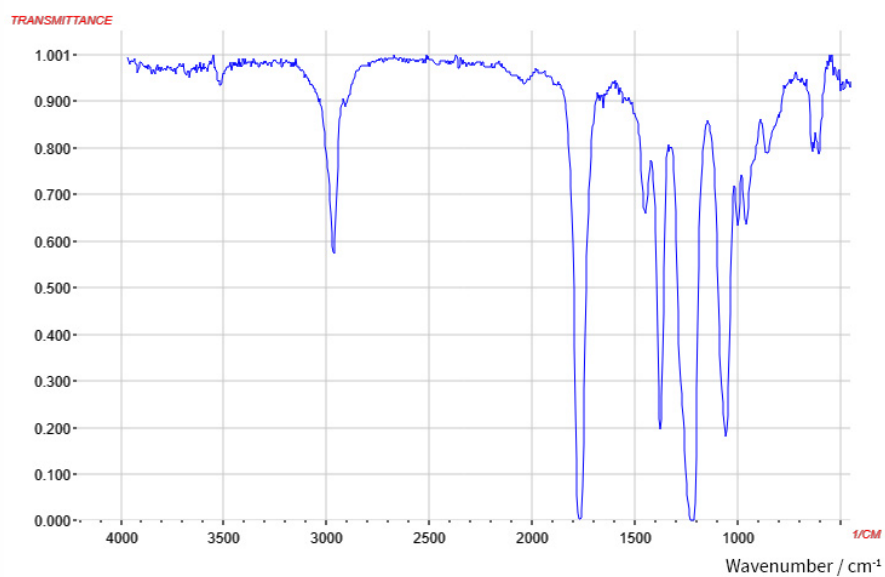
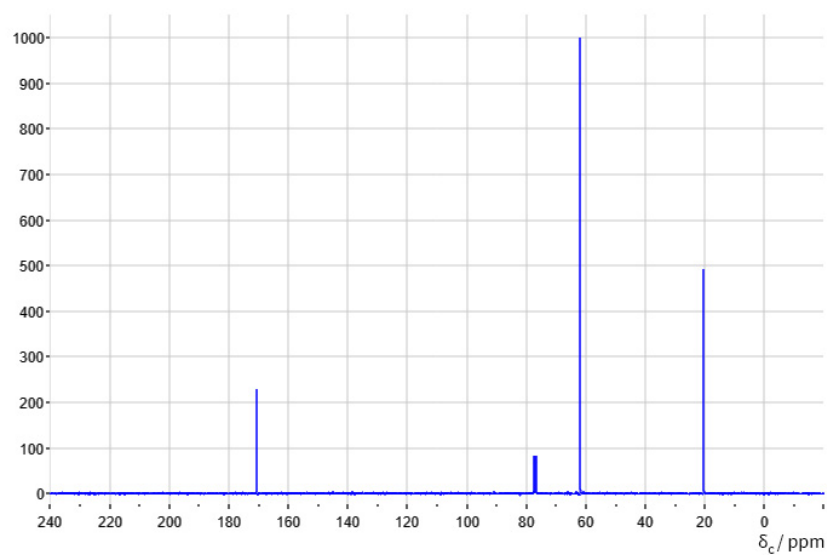
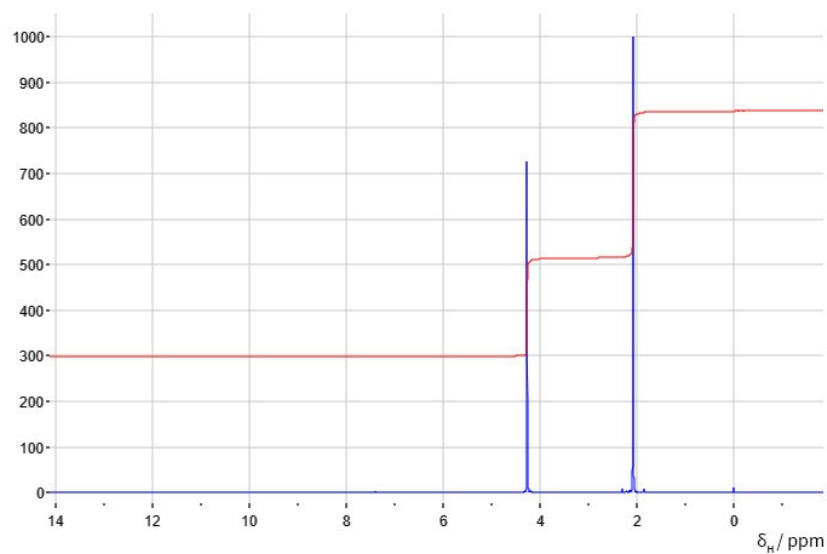
Spectra set A

Infrared

 ^{13}C NMR ^1H NMR

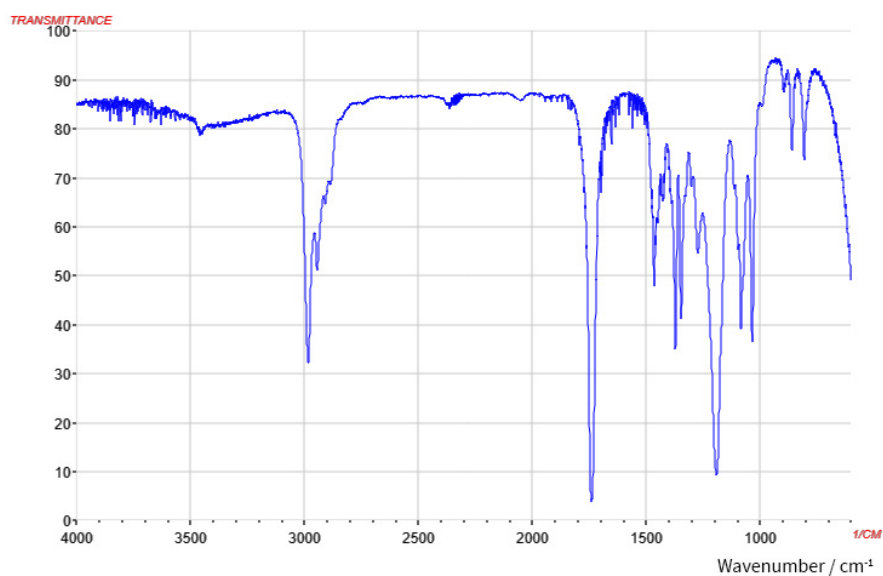
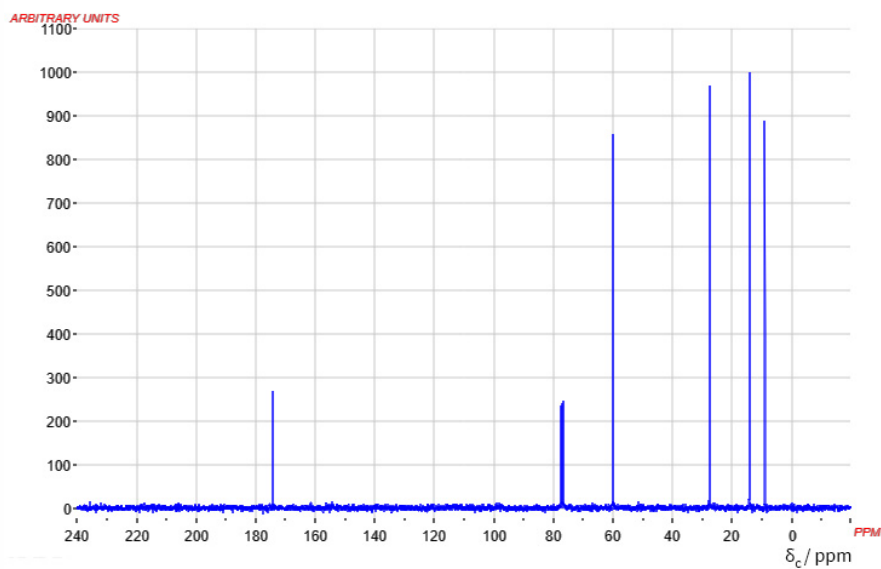
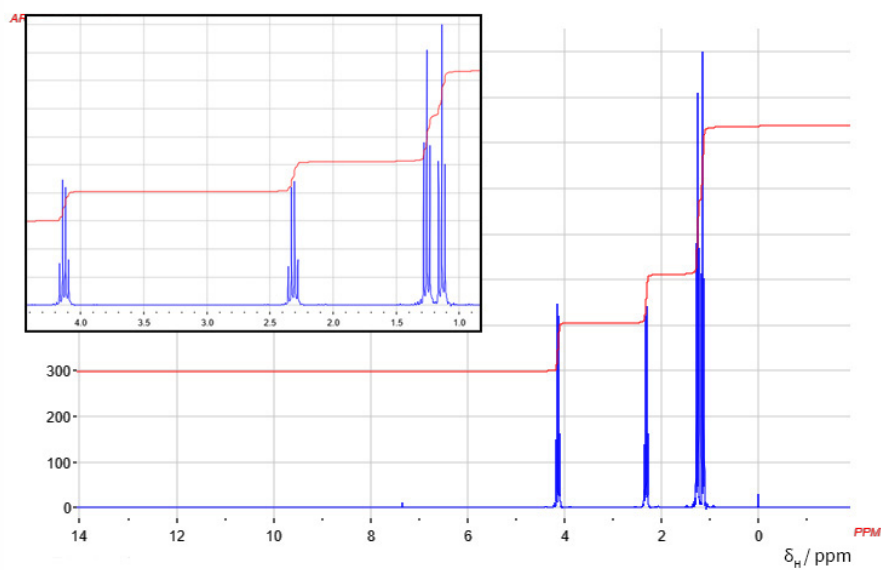
Spectra set B

Infrared

 ^{13}C NMR ^1H NMR

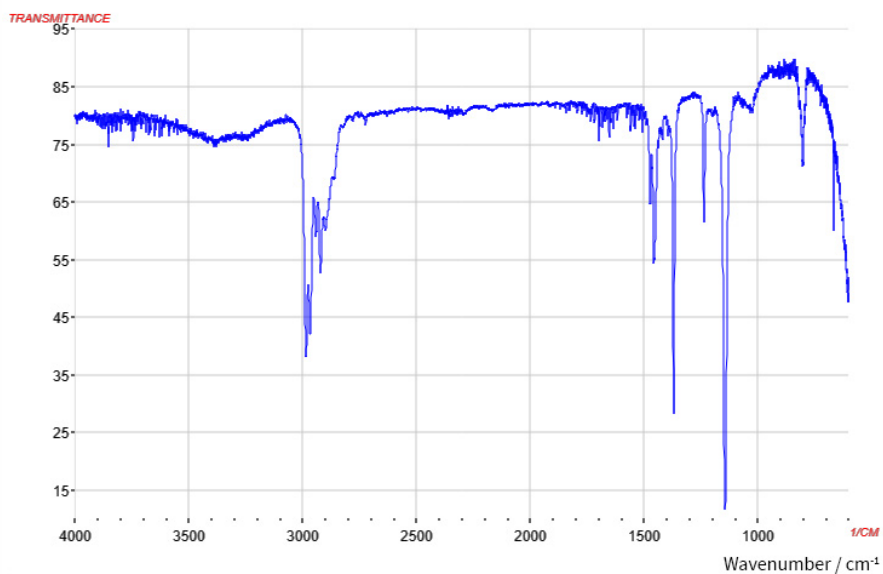
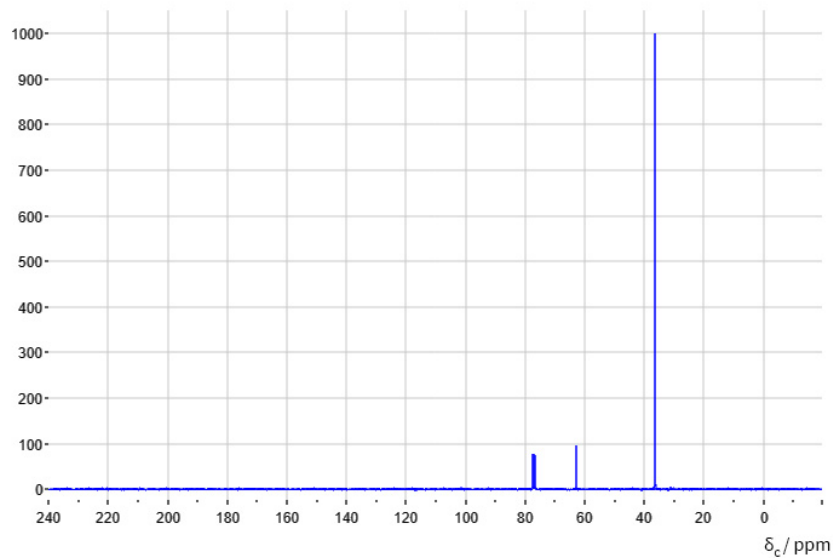
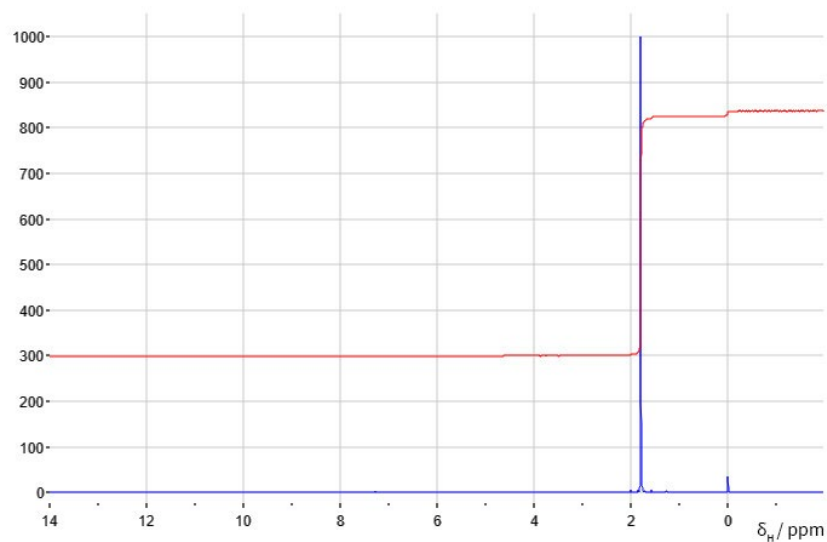
Spectra set C

Infrared

 ^{13}C NMR ^1H NMR

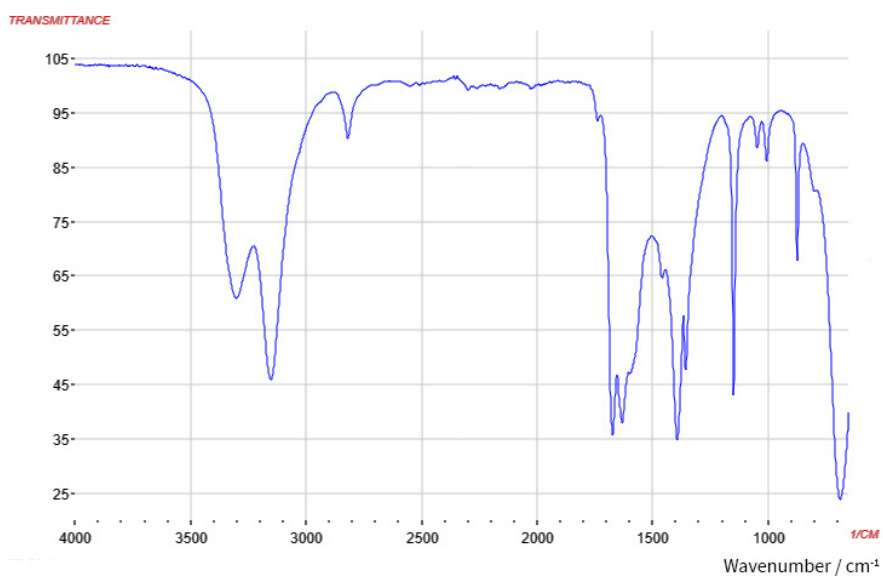
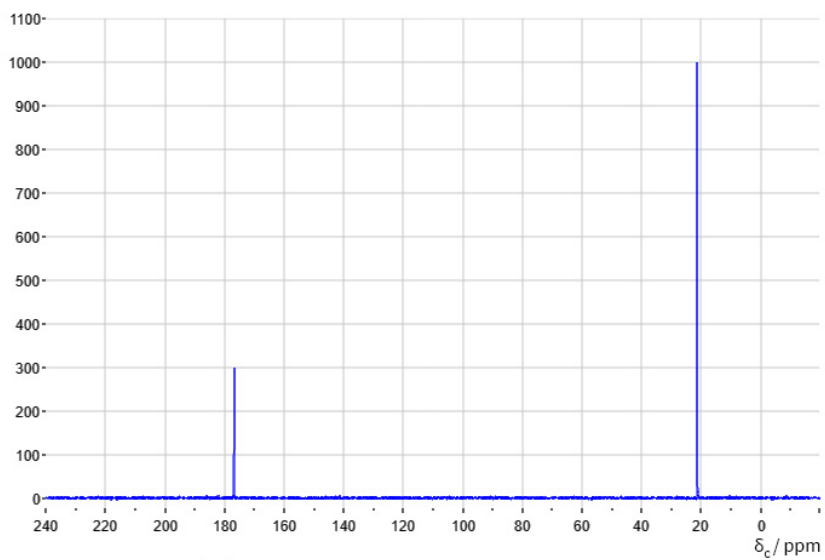
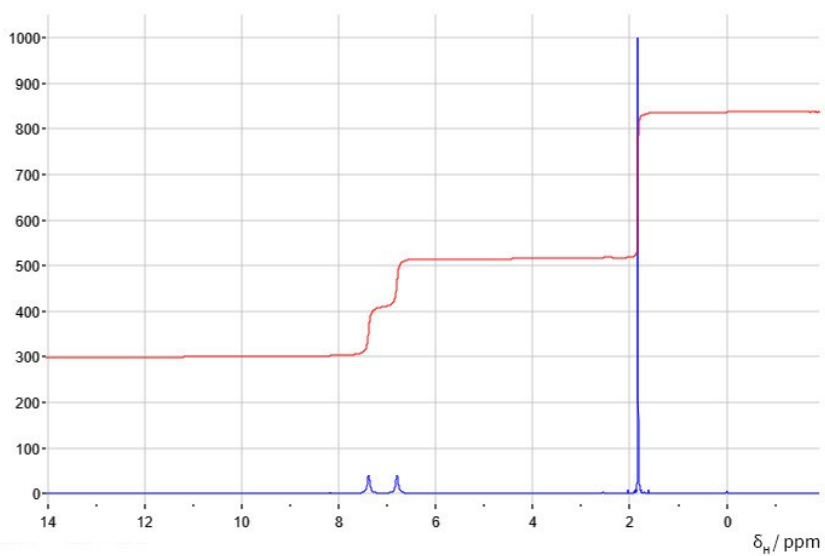
Spectra set D

Infrared

¹³C NMR¹H NMR

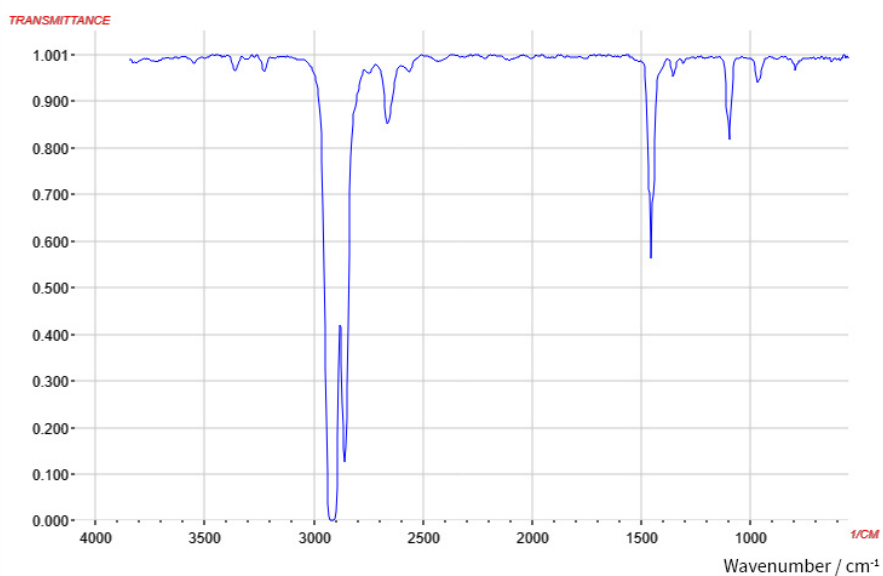
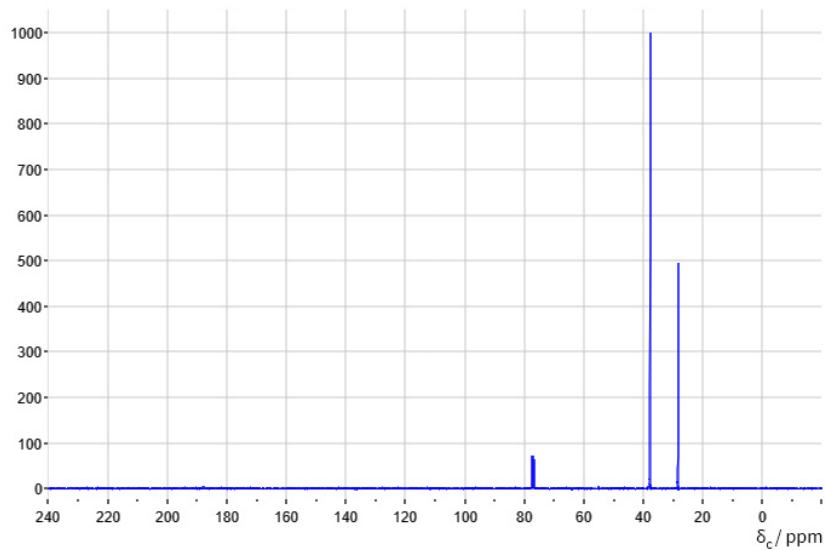
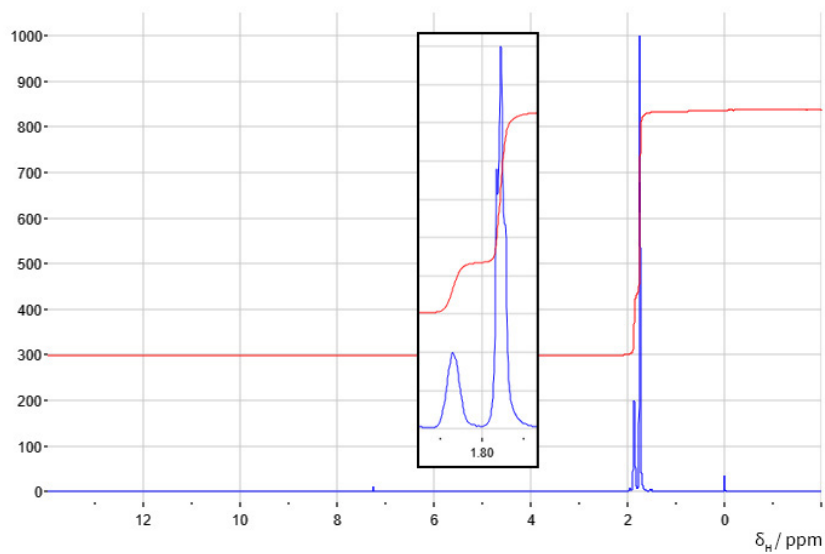
Spectra set E

Infrared

 ^{13}C NMR ^1H NMR

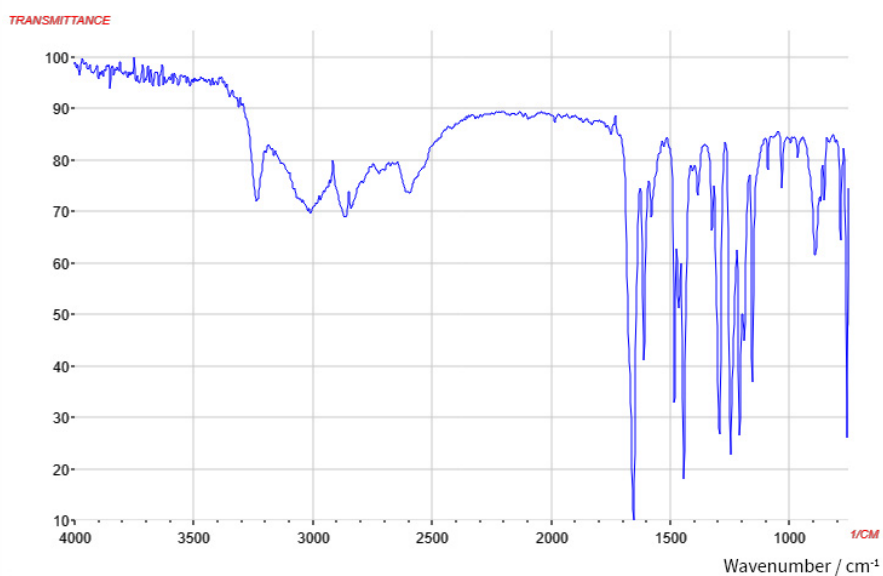
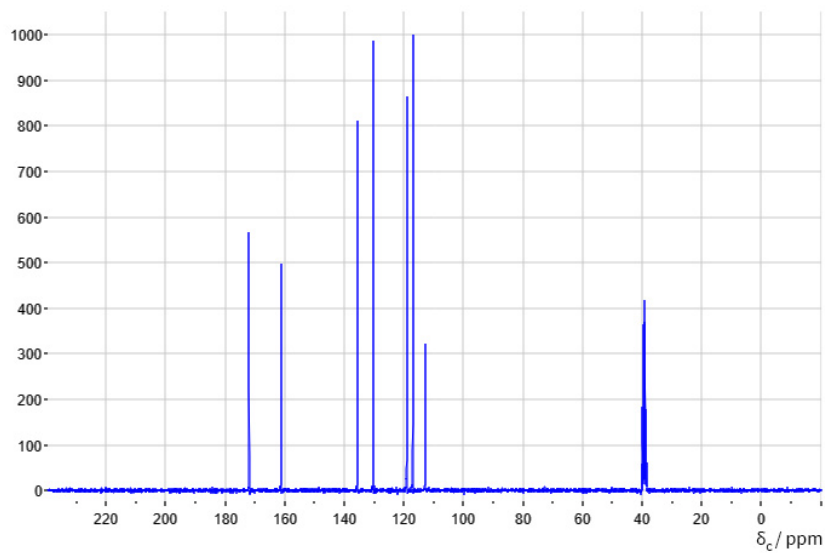
Spectra set F

Infrared

¹³C NMR¹H NMR

Spectra set G

Infrared

 ^{13}C NMR ^1H NMR