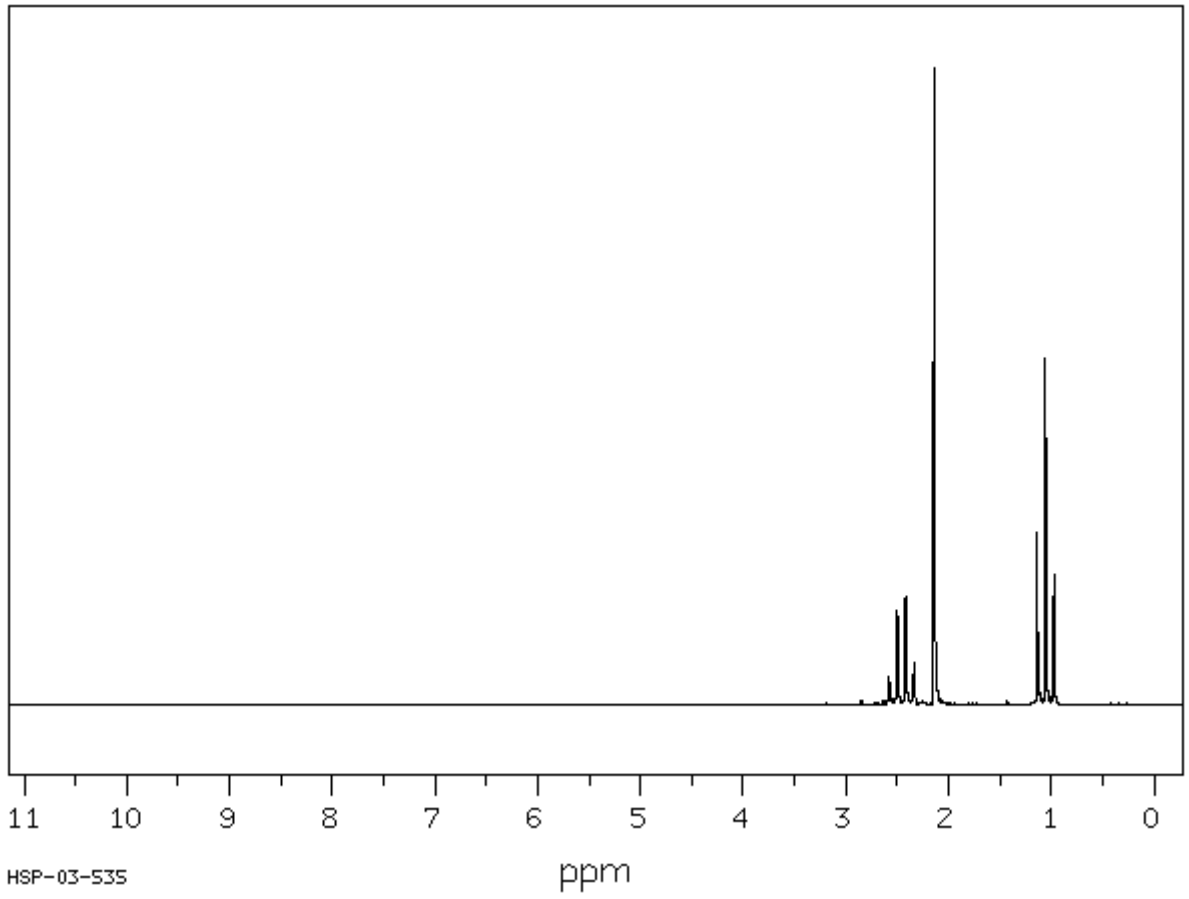
H-1 NMR: HIGH RESOLUTION

The spectral data in this file are taken from the SDBS (SDBSWeb : http://sdbs.db.aist.go.jp (National Institute of Advanced Industrial Science and Technology, 28/8/2014).

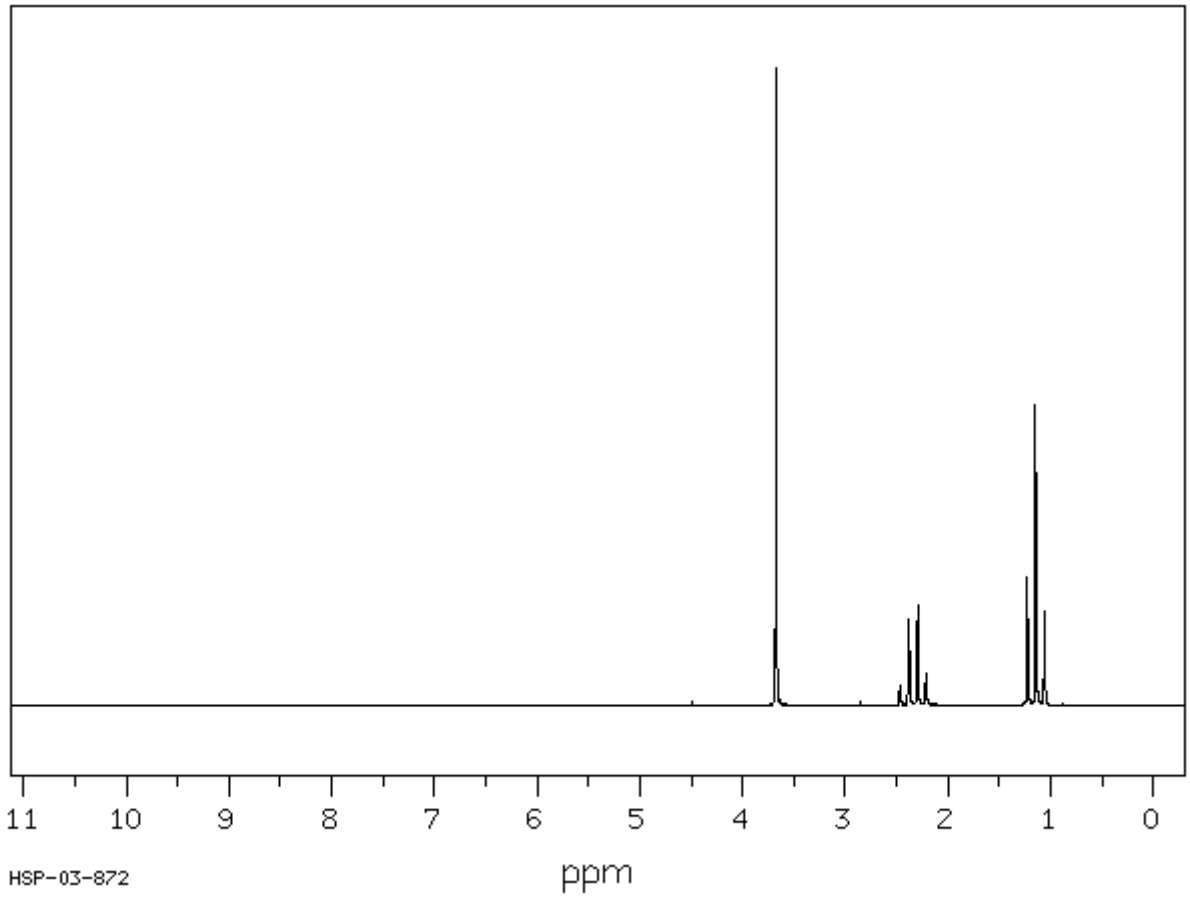
1. For the high resolution ^1H NMR data below, work out the structure of the molecules concerned. You will find a short table of useful chemical shifts at the end of the questions.

   a) A molecule with the molecular formula C_4H_8O :



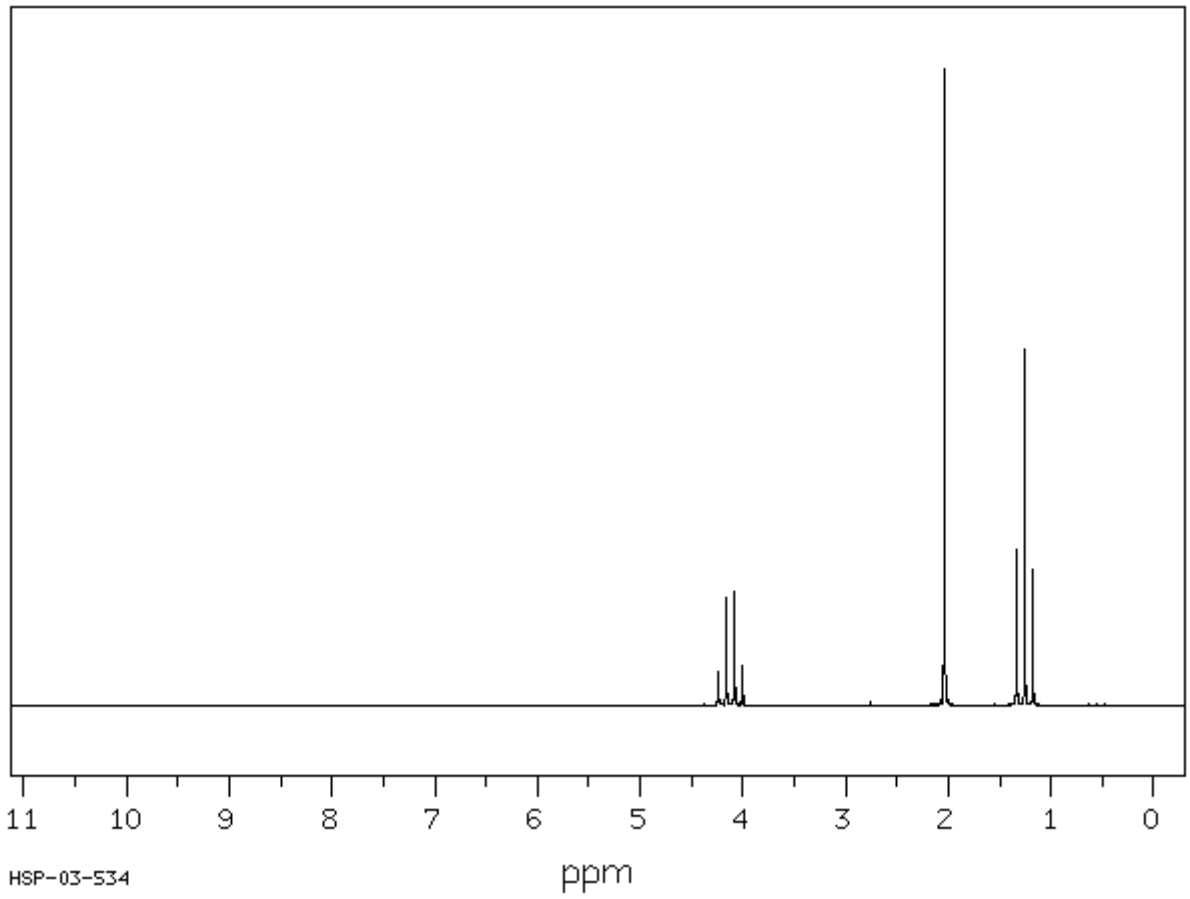
chemical shift (ppm)	2.449	2.139	1.058
ratio of areas under the peaks	2	3	3
splitting	quartet	singlet	triplet

b) A molecule with the molecular formula $C_4H_8O_2$:



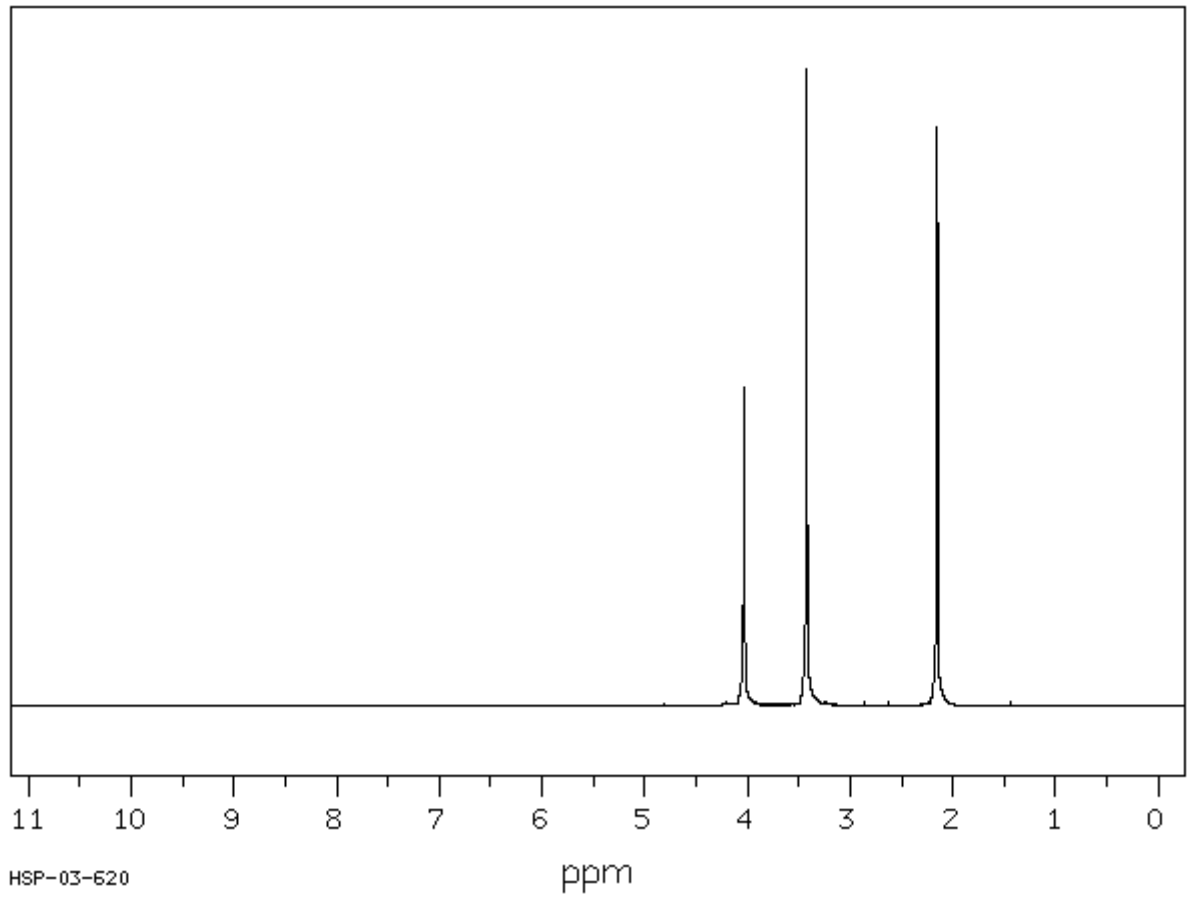
chemical shift (ppm)	3.674	2.324	1.148
ratio of areas under the peaks	3	2	3
splitting	singlet	quartet	triplet

c) Another molecule with the molecular formula $C_4H_8O_2$:



chemical shift (ppm)	4.119	2.038	1.260
ratio of areas under the peaks	2	3	3
splitting	quartet	singlet	triplet

d) Yet another molecule with the molecular formula $C_4H_8O_2$:



chemical shift (ppm)	4.029	3.421	2.148
ratio of areas under the peaks	2	3	3
splitting	singlet	singlet	singlet

2. a) The ^1H NMR peak for the hydrogen in an O-H bond in an alcohol is very variable in position in the spectrum. If someone suspected that they had a peak due to an O-H hydrogen, how could they easily confirm that?

b) How many peaks would you get for the hydrogens in the molecule CH_2ClCH_2Cl, and how would they be split?

c) How many peaks would you get for the hydrogens in the molecule CH_2ClCH_2Br and how would they be split?

Chemguide – questions

Chemical shifts

	chemical shift, δ
R-C**H**$_3$	0.7 - 1.6
R-C**H**$_2$-C(=O)-	2.0 - 2.9
-O-C**H**$_3$ or -O-C**H**$_2$-R	3.3 - 4.3
H-C(=O)-	9.0 - 10.0
-COO**H**	11.0 - 12.0