Chemguide – answers

H-1 NMR: HIGH RESOLUTION

1. a)

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

In an exam, you wouldn't be given the data above - just the spectrum. However, spectra in exams at 16 - 18 year old level are often simplified a bit so that the splitting is a bit clearer. Since this is just an introduction, I want to make it as clear as possible for you.

First of all, the sum of the ratio of the areas corresponds exactly to the number of hydrogen atoms in the formula (as it usually does, but check it anyway).

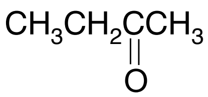
Both of the first two peaks correspond to hydrogens on a carbon atom attached to a C=O double bond. The singleton at 2.139 with 3 hydrogens attached is obviously a CH_3 group, and there can't be anything else attached to it other than the C=O because it only has one bond left apart from those attached to hydrogens.

So you have a $-COCH_3$ group.

The quartet (with two hydrogens) at 2.449 is obviously a CH_2 group attached to C=O. The fact that it is a quartet means that it is next door to a carbon with 3 hydrogens attached - a CH_3 group.

That CH_3 group is a triplet, and so must be attached to a carbon with 2 hydrogens on it. The combination of these two peaks is typical of an ethyl group, CH_3CH_2-.

Remember that the CH_2 group is attached to a C=O, and so putting this all together you get the structure



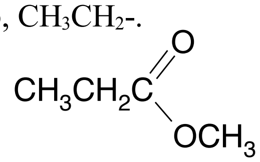
b)

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

Start with the singlet at 3.674. The 3 hydrogens are in a CH_3 group attached to an oxygen atom.

The quartet at 2.324 with 2 hydrogens is due to a CH_2 group next to a C=O bond. The fact that it is a quartet means that there are 3 hydrogens on the adjacent carbon. The two peaks at 2.234 and 1.148 are again from an ethyl group, CH_3CH_2-.

Putting this together gives you



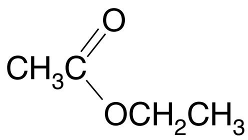
c)

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

The quartet at 4.119 shows a CH_2 group attached to an oxygen. It is also likely to be attached to a CH_3 group because of the splitting.

Looking at the other two peaks, they are both going to be CH_3 groups because of the number of hydrogens attached.

The 2.038 peak will be a CH_3 group attached to a C=O bond. The other one, the triplet, is going to be at the end of a chain and attached to the CH_2 group.

The molecule is therefore 

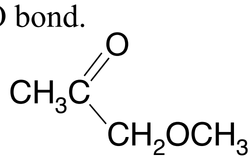
d)

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

The odd thing about this one is that all the peaks are singlets. There are two CH_3 groups and a CH_2 group, none of which are next door to each other.

The 4.029 peak and the 3.421 peak are both due to hydrogens on carbons attached to an oxygen. That suggests a group like $-CH_2-O-CH_3$.

The other peak is due to a CH_3 group attached to a C=O bond.

There is only one way that you can fit this together: 

2. a) Add some heavy water, D_2O, and redo the spectrum. The peak due to an OH group in an alcohol will disappear.

   b) You would get a single peak with no splitting. All the hydrogens are in exactly the same environment, and are said to be equivalent. Equivalent hydrogens have no effect on each other.

   c) You would get two peaks, each split into triplets. The hydrogens on the two CH_2 groups are no longer in exactly the same environment.