Solving NMR Structures Step by Step.

1. If you are given the chemical formula calculate the degrees of unsaturation:

$$°unsaturation = \quad pi-bonds + rings = C+1- \frac{H+X-N}{2}$$

   hint: four or more °unsaturation often implies the presence of an aromatic ring

2. If this IR spectrum is given look for "give away" peaks such as C=O, OH, NH,C C, C N.

3 If you have the ^{13}C spectrum, determine the number of non-equivalent carbons in your spectrum.

4 From your ^{1}H nmr spectrum, look for "give away" chemical shifts.
     7.0- 8.0 ppm => aromatic
     10.0 – 11.0 ppm => aldehyde
     12 – 15 ppm => carboxylic acid
     2 – 5 ppm broad => alcohol or amine (also exchanges with D_2O)

5. Look at the integration and determine the number of hydogens associated with each set of peaks. Remember the number of hydrogens in your spectrum must equal the number of hydrogens in your molecule. You can use these two steps to solve for the number of hydrogens associated with each peak

$$integral\ height\ per\ hydrogen = \frac{total\ integral\ height\ for\ all\ peaks}{total\ number\ of\ hydrogens\ in\ molecule}$$

$$number\ of\ hydrogens\ under\ specific\ peak(s) = \frac{integral\ height\ of\ specific\ peak(s)}{integral\ height\ per\ hydrogen}$$

6. Look at the splittings. Use the N+1 rule and write down the fragments.
   Remember, when there are more than four peaks, it is better to say it is a multiplet. The splitting must come from hydrogens on more than one adjacent carbon.

7. Put the fragments together as many ways as possible leaving no unfilled valences. Also your structures should not break any Lewis rules. Make sure that you have accounted for all atoms in your original formula and that there are the correct ° unsaturation.

8. Use the chemical shift data to determine which functional groups are next to which hydrogen atoms. Remember the effects are additive. This will allow you to choose between the molecules drawn in the previous step. When you have some experience, you will skip step 7 and do this directly.