1. By noting the integer mass of the molecular ion, what can you state about the presence or absence of nitrogen in this compound?

2. How many different environments of carbons and hydrogens are present in the compound? (see note below).

3. How many hydrogens of each environment are present?

4. Give two items of data that suggest the presence of a di-substituted benzene ring.

5. Define the substitution pattern of the benzene ring as being either 1,2 or 1,3 or 1,4. What data did you use to draw this conclusion?

6. What spectroscopic evidence is there that supports the presence of two different oxygen containing functional groups? What are the two-oxygen containing functional groups?

7. The exact mass as determined by high resolution mass spectroscopy (E1) is 164.0473: propose a molecular formula for the compound that is consistent with the observed NMR data.

8. Draw possible molecular structures for the compound. Make sure that the proposed structures make chemical sense.

9. Assign as many of the $^{13}$C NMR signals as you can to carbons in your proposed structure.

10. Assign as many of the $^1$H NMR signals as you can to protons in your proposed structure.

11. Draw a fragmentation scheme to show how your structure accounts for the ions observed at m/z 163, 133 and 105.

Mass spectrum:

Electron impact ionization: m/z 164 (10%), 163 (20%), 135 (25%), 133 (15%), 105 (100%).

High resolution exact mass of molecular ion: 164.0473

Note: NMR solvent (CDCl3) signals are visible as three equal height signals in the $^{13}$C NMR spectrum at 77.0 ppm.
1. How many different environments of carbons and hydrogens are present in the compound? (see note below).
2. What are relative number of hydrogens of each environment that are present?
3. The exact mass as determined by high resolution mass spectrometry (EI) is 168.0786. Given that the compound only contains the elements C, H and O, propose a molecular formula for the compound.
4. Draw possible molecular structures for the compound. Make sure that the proposed structures make chemical sense. Hint: consider the presence of an aromatic ring in the compound!
5. Assign the $^{13}$C NMR resonances observed to specific carbons in your proposed structure.
6. Assign the $^1$H NMR resonances observed to specific protons in your proposed structure.

Mass spectrum:

Electron impact ionization: m/z 168 (100%).

High resolution exact mass of molecular ion: 168.0786

Note: NMR solvent (CDCl3) signals are visible as three equal height at 77.0 ppm in the $^{13}$C NMR spectrum.