Identification of Unknown Compounds Report.

Name: _____   ## Bench Number   _____

Complete the sheets below for all three of your unknown compounds. Attach the proton and carbon NMR spectra you obtain via Mestre-C. Ensure that you show justification for the structure you propose – remember most of the marks are for the deduction process rather than just the structure of the unknown.

Write the unknown number here: _____

1.   Molecular formula – fill in the table below for the elements present. Look at the mass spec. data to find the molecular weight of the compound. This will usually be the largest ion, and use this to work out the molecular formula. Be aware that sometimes the molecular ion may not be present in a mass spectrum, but in the case of this exercise they all show a molecular ion.

Element	C	H				
percentage divided by 100						
multiply by mol weight						
Divide by atomic weight	12	1				
To give no. of atoms						

Round up or down to give whole numbers. So the molecular formula is: _____

Next calculate the number of double bond equivalents (*dbe*) using the method in the lab manual. Remember that halogens count as hydrogens for this calculation.

Number of *dbe* is :   _____

2. IR Spectrum   Record characteristic group absorptions only.

Peak position /wavenumber	Functional Group Assignment

3. ¹H NMR spectrum

Record each set of signals separately in the table below. Spectra are recorded at **250 MHz**.

Chemical Shift (δ, ppm)	Splitting Pattern *d, t etc*	Coupling (*J*, Hz)	Integral (no. of H's)	Inference

Note: Record a doublet as 'd', a triplet as 't' *etc*. If there are overlapping resonances, record them as 'm' for multiplet.

4. ¹³C NMR spectrum

Chemical Shift	DEPT 135 signal?	DEPT 90 signal?	Inference

5. Mass spectrometry

Peak	Suggested Structure of Fragment

6. Suggested structure of unknown (with explanation)