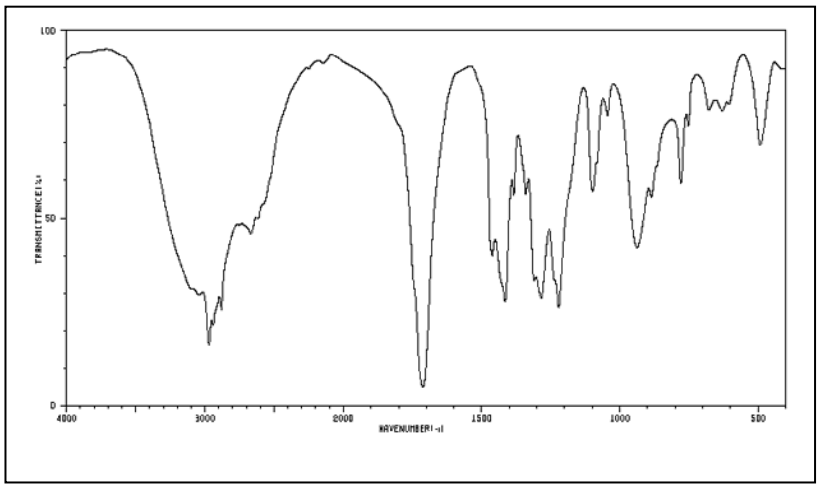
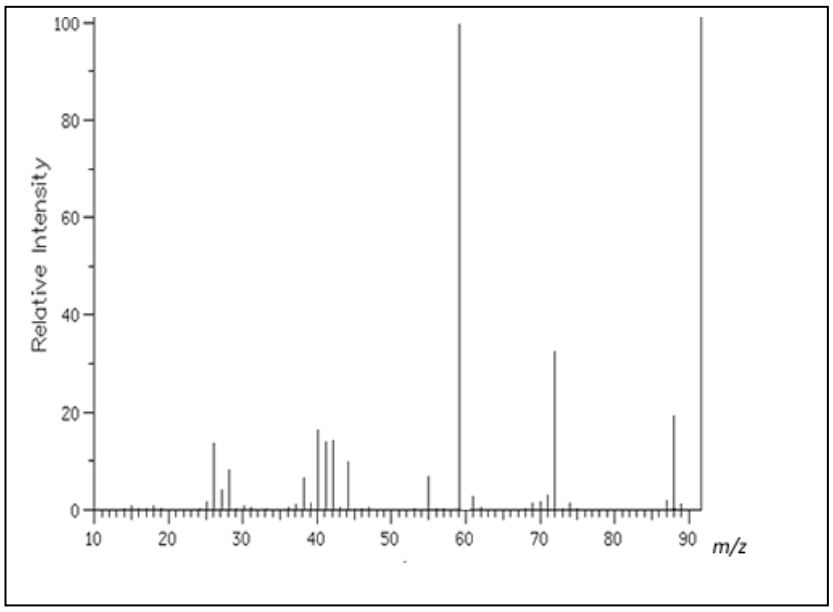
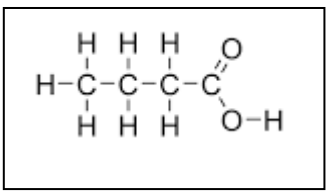
Friday Worksheet 4
Infared Radiation (IR) **Name: …….**

1) An organic molecule has the empirical formula of C_2H_4O. The IR spectrum and mass spectrum of this compound are shown below.







a) What is the molecular formula for this compound. *$C_4H_8O_2$. The molecular mass is shown clearly in the MS as 88 hence the empirical formula is multiplied by 2 to derive the molecular formula.*

b) With reference to the IR spectrum, what strong signals, outside of the fingerprint region, exist. Give the wavelength and the possible functional group that is present in the molecule. *A strong trough at wavenumber 1720 indicates a C=O. It is not always clear if it is an ester an acid ketone or aldehyde. Hence the next signal is a broad trough stretching between 2500 and 3500. Clearly indicates an acidic O-H.*

c) Name the compound. *Butanoic acid.*

d) Draw the structural formula for this molecule.

e) What fragment may have produced the peak at m/z 59? *CH_2COOH^+*

f) What caused the small peak at m/z 89? *$C^{12}H_3C^{13}H_2\ C^{12}H_2\ C^{12}OOH^+$ A parent ion with just one C^{13} isotope.*