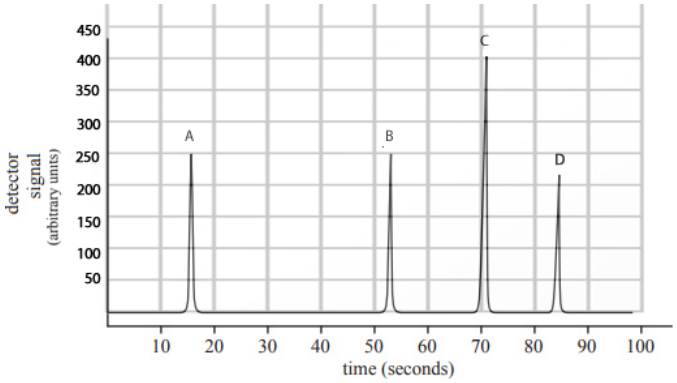
Ongoing revision 13 – organic, pathways, naming, chirality, HPLC, HNMR, proteins, fats and lipids.

1. A mixture of the amino acids, threonine, serine, isoleucine and aspartic acid was separated using reverse phase chromatography and the chromatogram on the right was obtained.

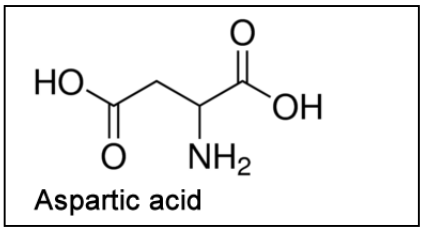


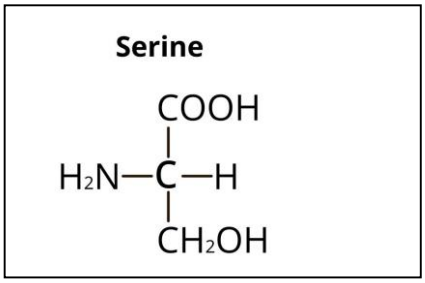
   a. Name the amino acid forming peak:
      - A *aspartic acid*
      - B *serine*
      - C *threonine*
      - D *isoleucine*

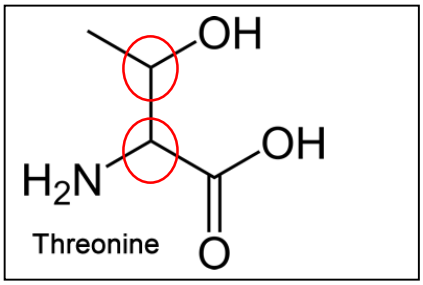
   b. Explain your answer in question a. above.
      The order of polarity of the molecules is critical to their retention time. The less polar a molecule the greater its affinity for the stationary phase in reverse-phase HPLC.
      Aspartic acid is the most polar so it will have a greater affinity for the mobile phase and hence it will pass through the column and come out in the eluent the quickest. Next will serine and then threonine while isoleucine, being the most hydrophobic molecule, will be last to leave the column.

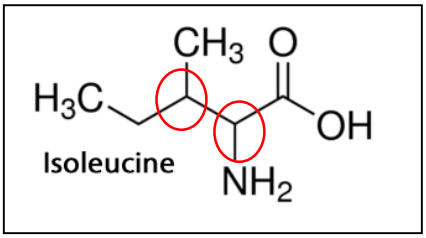
   c. Give the systematic names of:
      i. Threonine -*2-amino-3-hydroxybutanoic acid*
      ii. Aspartic acid - *2-aminobutandioic acid*
      iii. Serine – *2-amino-3hydroxyproapnoic acid*
      iv. Isoleucine-*2-amino-3-methylpentanoic acid*

   d. Which amino acids have 4 isomers able to rotate polarised light? *Threonine and isoleucine – they have two chiral centres, circled in the skeletal formula on the right, hence has 4 optical isomers.*

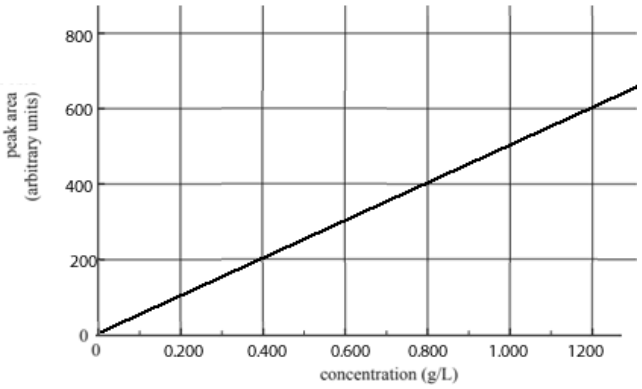








e. The mass of threonine in a particular vitamin drink was determined by high-performance liquid chromatography (HPLC). The calibration curve produced from running standard solutions of threonine through an HPLC column, in the exact same conditions as the those used to derive the chromatogram above, is shown on the right.
A 10.0 mL aliquot of the 350 mL can vitamin drink was diluted to 100.0 mL with de-ionised water. A sample of the diluted drink was run through the HPLC column under identical conditions to those used to obtain the calibration curve, shown here.



Calibration curve

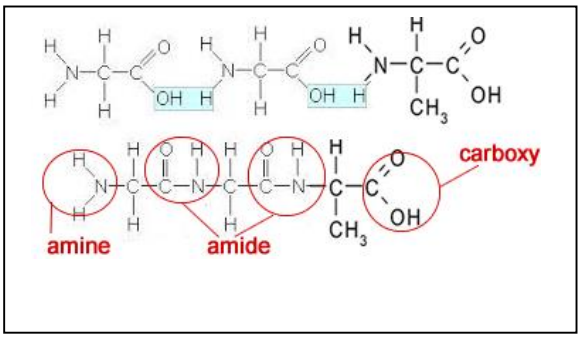
i. Calculate, to the right number of significant figures, the concentration of threonine (119.12 g/mol), in mol/L, in the 350 mL drink can.

Step 1 Calculate the concentration of the diluted sample.
=> threonine shows an absorbance of 400 unit. From the calibration curve this equates to a concentration of 0.800g/L
Step 2 Calculate the concentration in g/L in the original sample
=> (100/10) X 0.800g/L = 8.00g/L
Step 3 Calculate the concentration of threonine in mol/L
=> (8.00 / 119.12) /L = 6.72 X 10^{-2} M

ii. Which one of the following would make a good solvent to use as the mobile phase in the column? Explain your reasoning.
CCl_4, ethanol, hexan-1-ol or octane.
Since it is reverse-phase HPLC the stationary phase is non polar hence the mobile phase must be polar and so the most polar molecule is ethanol. This will give good separation of the amino acids.

f. Consider the peptide Gly-Gly-Ala

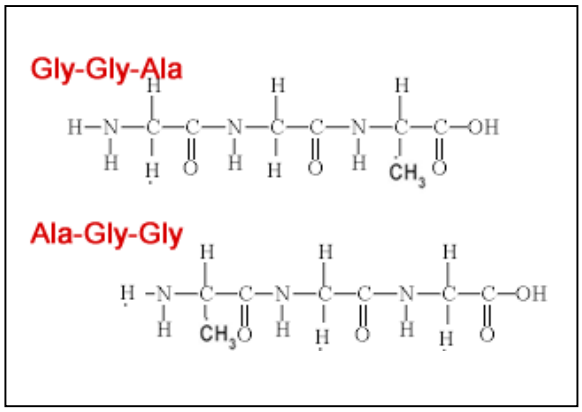
i. Draw the structural formula of the peptide in the space provided, circle and name all the functional groups.



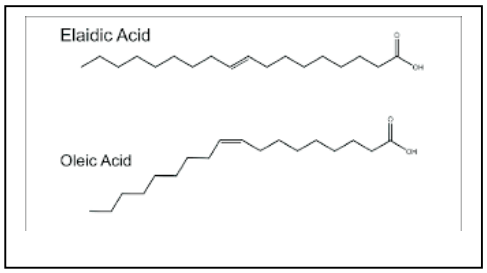
ii. Calculate its formula mass.
(75 + 75 + 89) – 2 X 18 = 203 g/mol

iii. Are the two peptides Gly-Gly-Ala and Ala-Gly-Gly the same? *No.*

iv. Draw the structural formulae of both and justify your answer to iii. Above.

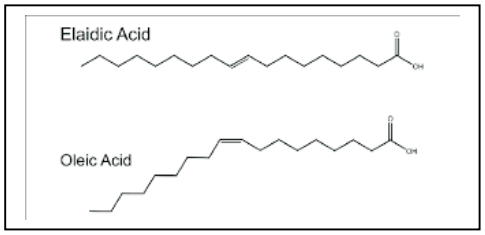


2. Consider the two fatty acids, oleic ($C_{17}H_{33}COOH$) and elaidic ($C_{17}H_{33}COOH$).
   a. Although both have the same chemical formula elaidic acid melts at 45°C while oleic acid melts at 13.4°C. Account for the difference in melting temperatures.



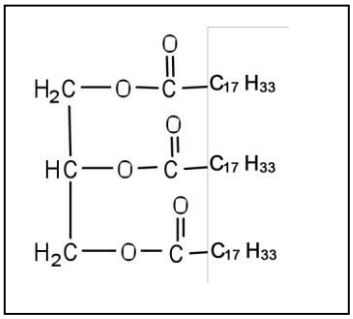
The difference in melting temperature is due to the nature of the C=C bond. A cis configuration, oleic acid, causes a kink in the molecule which prevents oleic acid from packing tightly in the solid lattice where dispersion force can take hold. Elaidic on the other hand has trans configuration which does not cause a kink to form and hence elaidic molecules can pack tightly together and dispersion forces can exert a greater force of attraction.

   b. Oleic acid has a boiling temperature of 360°C while elaidic acid boils at 288 °C. Account for the difference in boiling temperatures.

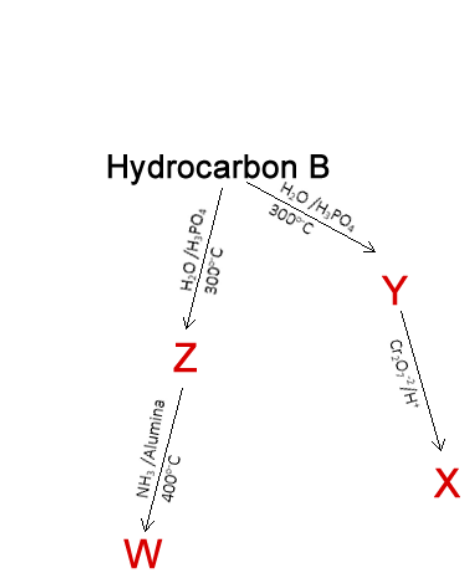


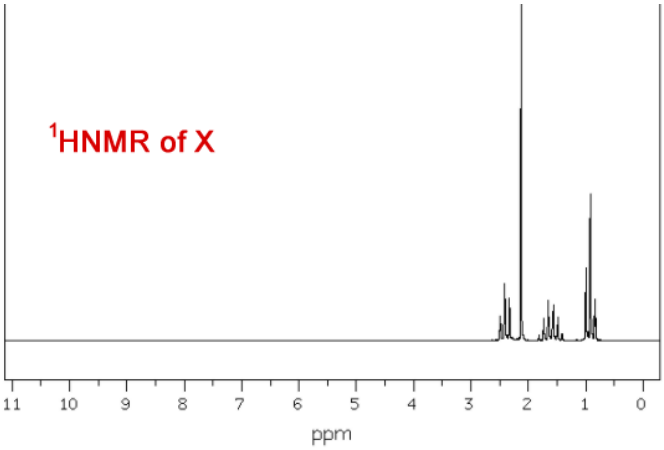
This is due to the fact that the cis C=C bond is polar. Unlike a trans C=C, dipoles form at the site of the cis C=C and hence provides a greater intermolecular force of attraction consisting of dispersion forces and dipole-dipole bonding. Unlike the trans configuration which only relies on dispersion forces as its intermolecular force of attraction. Since the molecules are in the liquid state movement of molecules results in dipoles coming close to each other and exerting a force of attraction.

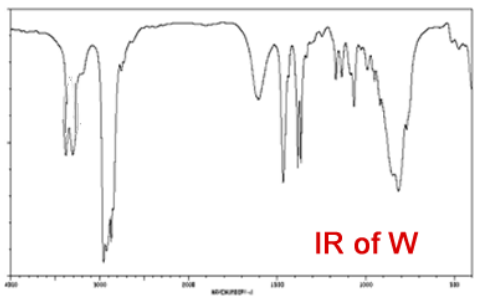
   c. Draw the structural formula of the triglyceride that contains only oleic acid fatty acids. You may abbreviate oleic acid to $C_{17}H_{33}COOH$.

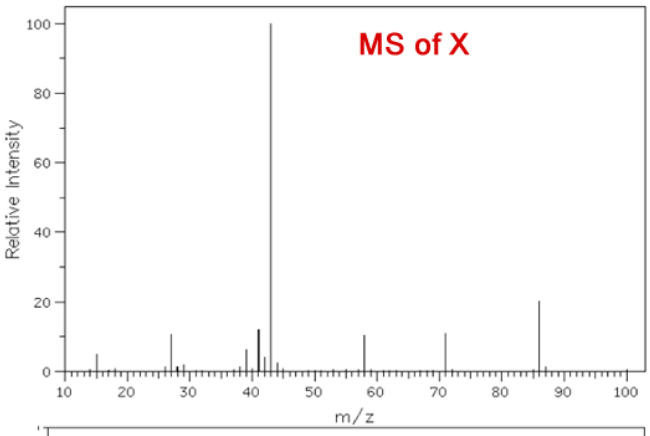


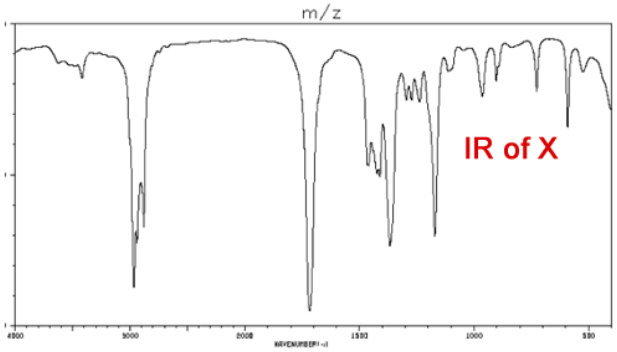
3. Consider the reaction pathway shown below and the different spectra of some compounds.











a. Identify compounds :
   - Y – *pentan-2-ol*
   - Z – *pentan-1-ol*
   - W - *pentan-1-amine*
   - B - *pent-1-ene*

b. Identify the class of compounds that X belongs to. *ketones*