Answer Sheet

1. a) $2\ NaHCO_3 \xrightarrow{\text{heat}} Na_2CO_3 + CO_2 + H_2O$

   b) Mass of $NaHCO_3$ = 5.00 g

   Molecular weight of $NaHCO_3$ = 84.01 g/mol

   Number of moles = mass / molecular weight = 5.00 g / 84.01 g/mol = 0.0595 mol

   To account for stoichiometry, number of moles of Na_2CO_3 = 0.0595 / 2 = 0.0298 mol

   Molecular weight of Na_2CO_3 = 105.99 g/mol

   Mass of Na_2CO_3 = 0.0298 mol x 105.99 g/mol = <u>3.15 g</u>

   c) In order to separate tannins from caffeine and to increase the purity of the caffeine product, tannins are converted into their sodium salt derivatives by the action of an inorganic base. When they become ionic, they remain dissolved in water while caffeine gets extracted by the organic solvent during the water-ethyl acetate liquid-liquid extraction. Since tannins are polyphenols, the base needs to be sufficiently strong to deprotonate phenolic hydroxyl groups. While sodium carbonate is strong enough to achieve that, sodium bicarbonate is not.

2. Note: All the drawings and examples shown below are merely illustrative – other plausible, clearly labelled and chemically correct diagrams are acceptable.

   a) Example of a separating funnel (Figure 1).

   b) The organic solvent used in this experiment was ethyl acetate. It forms as the upper layer because its density is lower than that of water (Figure 1).

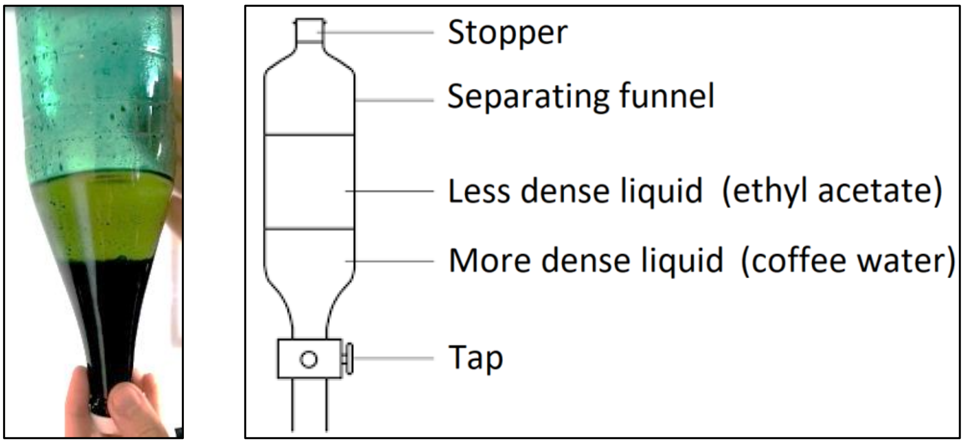

Figure 1. Example of a separating funnel.

c) Examples of a gravity filtration setup (Figure 2).

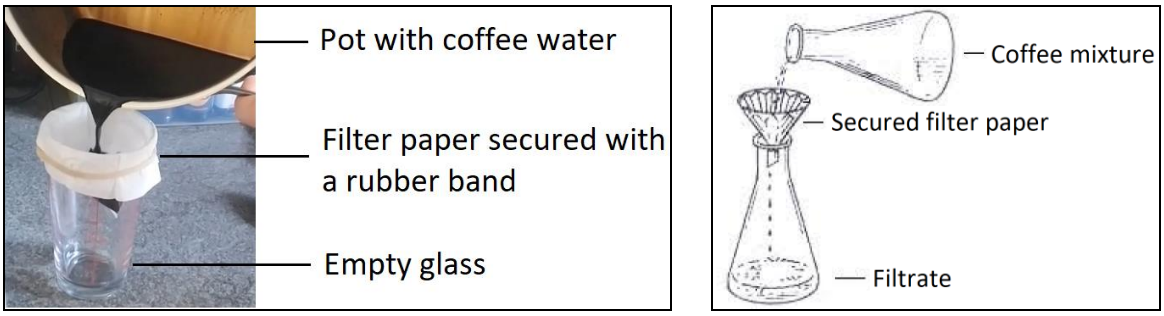

Figure 2. Examples of a gravity filtration setup.

Example of a crystallisation process (Figure 3). As the solvent evaporates over time, the concentration of the sample in solution increases, and eventually, the solution becomes saturated. At that point, should any more solvent evaporate, the solid will start to crystallise out of the solution.

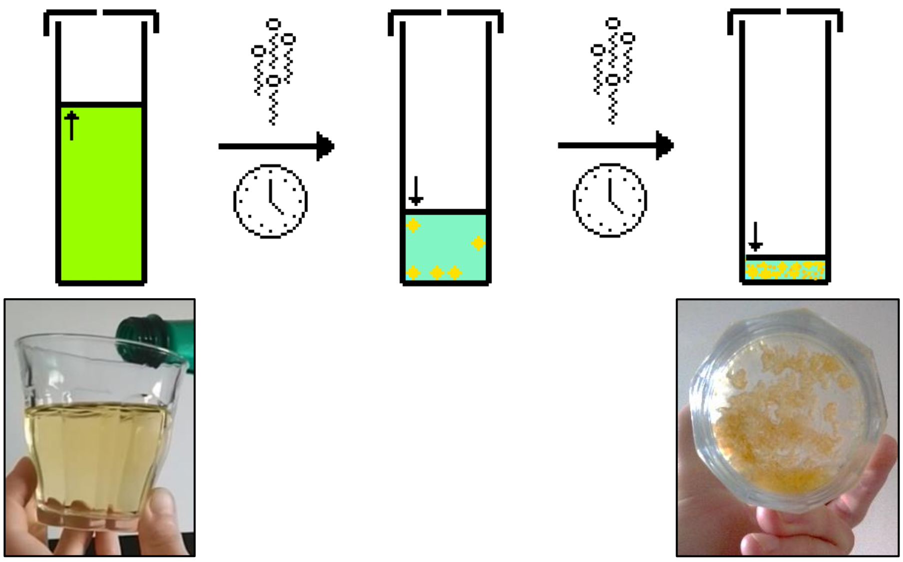

Figure 3. Example of a crystallisation process.

d) Chemical structure of caffeine (Figure 4). Caffeine is a heterocycle because it is a cyclic compound that has atoms of at least two different elements as members of its rings – nitrogen and carbon.

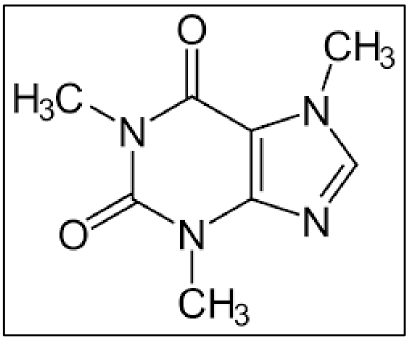

Figure 4. Chemical structure of caffeine.

3. a) The solubility of salt in water at room temperature is 357 mg/mL. To make a saturated solution with 50 mL of water, we need 0.357 g/mL x 50 mL = 17.85 g of salt.

   b) The solubility of water in ethyl acetate is 3%. In 150 mL of ethyl acetate, there is therefore:

   150 mL x 3 / 100 = 4.5 mL of water.

   c) Since the solubility of ethyl acetate in water is 83 mg/mL, there is approximately 83 mg/mL x 100 mL = 8.3 g of ethyl acetate in the aqueous layer (depending on how much water was in the filtrate). To minimise the solubility of the organic solvent and caffeine in water, we could add salt to the aqueous layer. This effect is called salting out – the aqueous layer becomes very highly ionic and the solubility of ethyl acetate and caffeine in it is reduced.

4. a) By measuring its melting point. Alternatively, nuclear magnetic resonance spectroscopy, gas chromatography or high-performance liquid chromatography may be used as well.

   Note: Infrared spectroscopy or mass spectrometry would not be as suitable because impurities are typically less distinguishable using these techniques.

   b) For adolescents, the maximum recommended daily intake of caffeine is 2.5 mg/kg of body weight, however, no more than 100 mg. Since the athlete weighs 60 kg, 60 kg x 2.5 mg/kg = 150 mg. This is above the 100 mg limit and hence 100 mg would be recommended as the maximum daily dose.