Caffeine term paper sample

Environment, Plants

Caffeine is the name that is used to commonly refer to the trimethylxanthine and has a molecular formula of C8H10N4O2 (Helmenstine, 2013). The compound has two major systematic name, which are 1, 3, 7-trimethylxanthine and 3, 7-dihydro-1, 3, 7-trimethyl-1H-purine-2, 6-Dione. Other common names that are used to refer to caffeine include guaranine, coffeine, mateine, theine, and methyltheobromine. The molecular structure for caffeine is as illustrated in Figure 1 below. Caffeine is usually produced by a number of plants that include guarana, coffee beans, cacao beans, and tea. It usually acts as a natural pesticide in plants where it kills or paralyzes insects that intend to feed on the plants (Lovett, 2005).

Figure 1: The molecular structure of caffeine

Caffeine molecule is achiral in nature and has no stereoisomers (Klosterman, 2006). The two groups of amide in caffeine exist mainly as zwitterionic resonance structures in which the atoms of carbon and nitrogen are joined by a double bond to each other making the nitrogen atoms to be planar atoms that are in sp2 orbital hybridization. This results in a fused ring system that has a total of ten pi electrons. This makes the structure to be aromatic according to the rule of Hückel. The synthesis of caffeine in plants starts from the purine nucleotides such as the Adenosine monophosphate, guanosine monophosphate and inosine monophosphate. The nucleotides are then transformed making xanthosine and finally theobromine. Theobromine acts as the immediate precursor of caffeine (Ashihara, Monteiro, Gillies, & Crozier, 1996). This process is illustrated in Figure 2 below, where EC 2. 1. 1. 158 7 is the methylxanthosine synthase, EC2. 1. 1. 160 caffeine synthase, EC 2. 1. 1. 159 theobromine synthase, EC 3. 2. 2. 25 N-methyl nucleosidase and

EC 3. 1. 3. 5 5'-nucleotidase.

Figure 2: Caffeine biosynthesis process in plants (Enzyme Database, 2007)

Caffeine is readily available as a decaffeination byproduct and is thus not usually synthesized through chemical processes. In the laboratory, caffeine is synthesized using malonic acid and dimethylurea as the starting materials as in Figure 3.

Figure 3: Caffeine laboratory synthesis

A pure compound of anhydrous caffeine is a powder that is colorless and has a melting point of between 227 and 228°C. The solubility of caffeine in water is moderate at room temperature with about 2 g of caffeine dissolving in 100 mL of water. However, the compound has a very high solubility in boiling water with about 66 g of caffeine dissolving in 100 mL of boiling water. It has a moderate solubility (1. 5 g/100 mL) in ethanol.

The first isolation of the molecule was done in 1819 by a German chemist known as Friedrich Ferdinand Runge. The isolation was then independently done by French chemists known as Pierre Pelletier, Pierre Robiquet, and Joseph Caventou in the year 1821. Pelletier is the one who coined the word caffeine using a French word, café, which means coffee.

Humans have been taking caffeine ever since the Stone Age. Those people who lived in those days realized that chewing the bark, seeds or even the leaves of some plants resulted to effects that eased the fatigue, elevated moods and stimulated awareness. The effect of caffeine was later realized to be increased when the plants were put in hot water. There is no clear history of coffee, although there are popular myths that trace the discovery of coffee to Ethiopia. It is in Ethiopia that Coffea arabica originated. The myth credits a

goat farmer named Kaldi who observed goats that had sleepless nights and were elated after grazing on coffee shrubs. The farmer then tried the berries that were eaten by the goat and experienced the same vitality.

Once the caffeine is taken in to the body, it is absorbed within the first 45 minutes after ingestion by the small intestine and distributed throughout the tissues in the body (Liguori, Hughes, & Grass, 1997). Peak of caffeine concentration in the blood is reached within an hour with the elimination taking place by first-order kinetics. The biological half-life, which is the time needed for one-half of the total amount of caffeine to be eliminated varies among individuals. The half-life is dependent on factors such as liver function, age, pregnancy, the enzyme levels in the liver that are needed for the metabolism of caffeine, as well as some concurrent medications. The measured half-life of caffeine is between 4. 9 and 6 hours (Liguori, Hughes, & Grass, 1997).

Caffeine molecules have the capability to pass through the blood–brain barrier separating the interior of the brain from the bloodstream. Once the caffeine has entered to the brain, the main mode of action is by acting as an antagonist of the receptors of adenosine non-selectively. The structure of caffeine molecule is similar to that of adenosine and is thus capable of binding to the receptors of the adenosine although they do not activate the receptor. This means that the caffeine molecule does work as a competitive inhibitor (Smith, 2001). The molecules of adenosine are located in all the body parts since they are involved in the energy metabolism processes that are ATP-related. Adenosine is also important in the synthesis of RNA molecules. Some secondary effects have been recorded resulting from

caffeine and are not related to caffeine. It competitively inhibits the phosphodiesterase reading to an increase in the intracellular cAMP. It activates the PKA, inhibits leukotriene and TNF-alpha synthesis, and causes a reduction in both the inflammation, as well as, innate immunity (Smith, 2001).

The metabolism of caffeine takes place in the liver and is done by a system of cytochrome P450 oxidase enzyme producing three dimethylxanthines with different effects on the body. The first product is the paraxanthine, which is the most abundant and accounts for 84% of the products. Paraxanthine works by increases the process of lipolysis causing an increase in the level of glycerol as well as that of free fatty acid in the blood plasma. The other product of metabolism is theobromine which accounts for 12% and is involved in the dilation of the blood vessels and urine volume increase. The third product is theophylline accounting for the 4% and is involved in the relaxation of smooth muscles that are in the bronchi and is used in the treatment of asthma. The metabolism process of caffeine is as shown in Figure 4 below.

Figure 4: The metabolism process of caffeine

Reference List

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