

PROJECT WORK

CHEMISTRY OF COFFEE AND POTENTIAL IMPACT ON HUMAN HEALTH

SUBMITTED TO



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Abstract

Today's coffee is the most popular beverage amongst people from younger to older. Everyday millions of people around the world begin their day with a morning cup of coffee. But many scientific researchers showed that coffee seemed to found off liver disease, liver cancer, type 2 diabetes, heart disease and stroke. Coffee even appears to protect against depression, Parkinson's and Alzheimer's diseases. These results taken as a whole might explain the most astonishing findings of all. So it is very interesting to know about chemical composition caffeine, Polyphenols, trigonelline that how to react and effect human bodies.

INTRODUCTION:

Throughout history, coffee has taken on several physical transformations. initially serving as an energy source when nomadic tribes combined coffee berries with animal fat as an early form of an energy bar. Later it was consumed as a tea, then wine and finally to the beverage we've come to identify. But how much of coffee's chemical composition do we actually know? over the past half century scientists have made significant process which as allowed them to unlock the nearly 1,000 components found in roasted coffee.

In this issue of coffee science we'll briefly discuss the family of compounds called 'alkaloids' which serve an important role in coffee's unique chemical composition.

chemical constituents :

The main constituents of coffee are caffeine, tannin, fixed oil, carbohydrates, and proteins. It contains 2-3% caffeine, 3-5% tannins, 13% proteins and 10-15% fixed oils. In the seeds, caffeine is present as a salt of chlorogenic acid (CGA). Also it contains oil and wax.

Coffee is often used as antioxidants, but more importantly coffee is a good source of chromium and magnesium that assist in controlling blood sugar by ensuring proper usage of insulin.

The main chemical ingredients in coffee beans are given below:

- Caffeine
- Tannin
- Thiamin
- Xanthine
- Spermidine
- Guaiacol
- Citric acid

- chlorogenic acid
- Acetaldehyde
- spermine
- Putrescine
- Scopoletin

The carbohydrate content of green and roasted coffee (Santos) was identified and measured. Green coffee contained about 6-7% of sucrose as soluble sugars and low amount of glucose. The experiment was also carried out for the isolation of holocellulose fractions of green and roasted coffee.

The holocellulose of green coffee was hydrolyzed by a novel method consisting of anhydrous sulfuric acid and 10% potassium insoluble hydroxide, which was partially solubilized on roasting.

Green coffee seeds contain up to 14% CGA, (chlorogenic acids), which are present in high concentrations and have a greater influence for determining the quality of coffee and play a vital role in the formation of the coffee flavor. The various constituents along with components of coffee as shown in Table 1.

Table 1:

constituents along with components of coffee

Constituent	components
Soluble Carbohydrates	Monosaccharides Fructose, glucose, galactose, arabinose (traces).
oligosaccharides	Sucrose, raffinose, stachyose
Polysaccharides	Polymers of galactose, mannose, arabinose, glucose, Insoluble Polysaccharides.
Hemicelluloses	Polymers of galactose, arabinose, mannose cellulose Acids and phenols volatile acids
Nonvolatile aliphatic acids	citric acid, malic acid, avinic acid.
chlorogenic acids	Mono-, dicaffeyl- and feruloylavinic acid, Lignin, Lipids, Wax
oil	Main fatty acids : N compounds
Free amino acids	Main amino acids : Glu, Asp , Asp-NH ₂ Proteins.
Caffeine	Traces of theobromine and theophylline Trigonelline Minerals.

Carbohydrates:

Most of the carbohydrates present, such as cellulose and polysaccharides consisting of mannose, galactose and arabinose are insoluble.

Lipids:

The lipid fraction appears to be very stable and its composition is given below.

Linoleic acid is the predominant fatty acid, followed by palmitic acid.

Lipid composition.

Triacylglycerols.

Diterpene esters.

Diterpenes.

Triterpene esters.

Triterpenes (sterols).

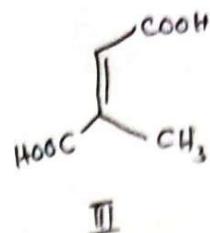
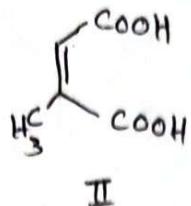
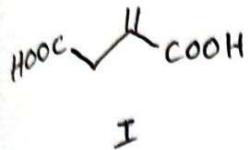
Unidentified compounds.

Acids:

The volatile acids include formic acids and acetic acids, while nonvolatile acids include lactic, tartaric, pyruvic and citric acid. Minor constituents include higher fatty acids and malonic, succinic, glutaric and malic acids.

The degradation products of citric acid are itaconic (I), citraconic (II) and mesaconic acids (III), while fumaric and maleic acids are degraded

products of malic acid.



chlorogenic acids are the mainly rich acids of coffee.

Trigonelline and nicotinic acid

green coffee contains trigonelline (N-methylnicotinic acid) up to 0.6% and 50% decomposed during roasting. The degradants include nicotinic acid, pyridine, 3-methyl pyridine, nicotinic acid, methyl ester and other compounds.

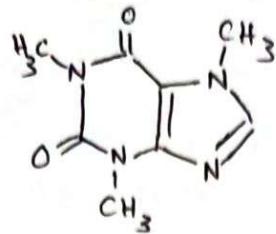
Aromatic principle

The aroma profile of coffee is composed of the following notes: sweet/caramel-like, earthy, sulfurous/roasty, and smoky/phenolic.

Minerals

Potassium is major in coffee ash (1.1%), calcium (0.2%), and magnesium (0.2%). The major anions includes phosphate (0.2%) and sulfate (0.1%), along with traces of other elements.

CAFFEINE

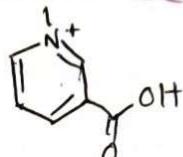


For many, coffee drinking is simply a delivery medium for a potent alkaloid we have come to identify as caffeine or otherwise known as 1,3,7-trimethylxanthine. Although caffeine is typically associated with coffee, its production within the plant kingdom spans across numerous other plant species. Mate, for example, which is traditionally consumed in parts of Uruguay and Argentina, contains less than one percent by weight. Whereas, teas of *Camellia sinensis* which originated in China contain almost three times the concentration of caffeine than Arabica.

But for humans caffeine is very unique. Thus far we are the only living forms on Earth that readily seek caffeine for both its stimulatory and psychological effects. For all other life forms, caffeine is a potent toxin capable of sterilization, phytotoxicity and antifungal properties. As such scientists believe that caffeine, with its intensely bitter taste, has evolved as a primitive defense mechanism in coffee ensuring its survival in the wild for thousands of years.

It's no surprise then, that the caffeine content of the more "robust" Robusta species is almost double that of the more delicate Arabica. The belief is that as insects attack the coffee cherry, they are deterred by the bitter taste of caffeine and simply move on to other crops.

TRIGONELLINE



Trigonelline Molecule coffee

Another less known alkaloid that shadows in the light of caffeine is that of trigonelline. In Arabica coffee, trigonelline concentrations make up roughly 1% by weight with a slightly less concentration (0.7%) found its Robusta counterpart. Although its concentration is slightly less than that of caffeine, it plays a significant role in the development of important flavor compounds during roasting. But unlike that of caffeine, which survives the roasting process, trigonelline readily decomposes as temperatures approach 160°C (320°F).

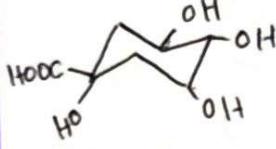
Another important byproduct produced during the decomposition of trigonelline is nicotinic acid or vitamin B₃ - more commonly known as niacin. Depending on roasting conditions, niacin can increase up to ten times its initial concentration, providing anywhere between 1mg of niacin per cup.

EFFECT on HEALTH :

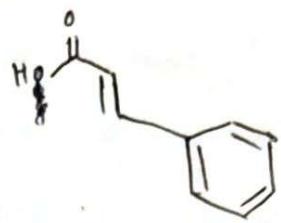
Drinking coffee has been associated with a variety of harmful and beneficial health effects. Coffee contains huge numbers of compounds, including antioxidant chlorogenic acids. Recent evidence suggests coffee could help prevent type 2 diabetes and neurodegenerative diseases like Alzheimer's. The absorption and profile of both helpful and harmful compounds in coffee is complex and depends on many factors. It is hard to avoid stories about the latest must-eat food to join the anticancer brigade. First it was select vegetables and berries, then red wine, dark chocolate and coffee.

Coffee is indeed one of the richest sources of phenolics in the western diet and can potentially pack a strong antioxidant punch, in theory protecting cells if the body's natural mechanisms fail to keep levels of reactive oxygen species under control. Yet the story is far more complex than a simple battle between antioxidants and free radicals. All of the antioxidant-rich products, from red wine to coffee, have far subtler modes of action than previously thought, says Alan Crozier, a plant biochemist.

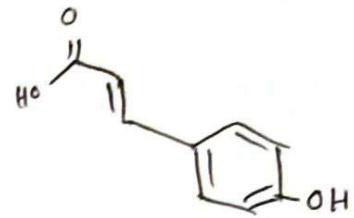
Acid House:



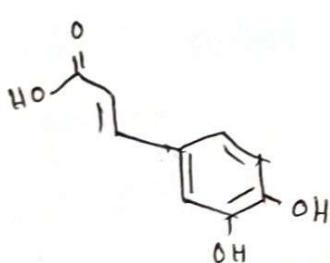
quinic acid



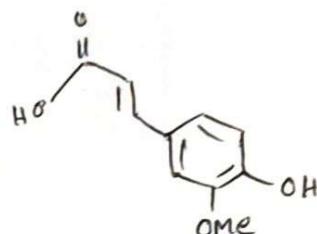
trans-cinnamic acid



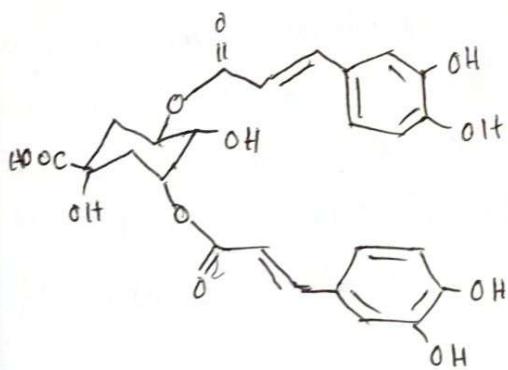
p-coumaric acid



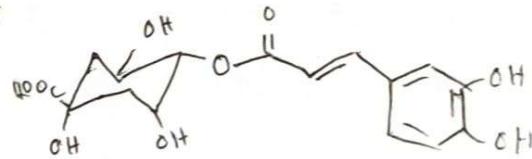
Caffeic acid



ferulic acid



3,5-dicaffeoylquinic acid



4-C-caffeoylelagic acid

Coffee contains a tremendous number of chemicals, with over 1000 aroma compounds. If you are looking for antioxidants, the most abundant phenolic compounds in coffee are chlorogenic acids (CGAs), which account for up to 12 percent of the dry weight of green unroasted coffee beans. Much of coffee's bitter taste comes from CGAs, which also cause the acid reflux that is sometimes experienced by coffee drinkers.

Blood Sugar

Experiments on human fat cells showed coffee doubled the levels of glucose uptake. In the body, such an increase in uptake would lower glucose levels in the blood. But it is not yet clear which coffee compounds induce cells to take up more glucose.

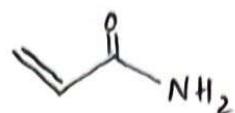
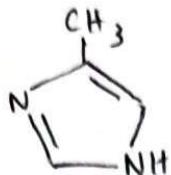
Caffeine in the Bloodstream

Caffeine is known to improve memory and the speed with which our brains process information. It binds to some of the same receptors as adenosine, a compound that promotes sleep, amongst other things. Caffeine is a non-selective antagonist at A1 and A2A adenosine receptors in the heart and the brain, having an opposite effect to adenosine and producing a stimulant effect.

Moderate coffee intake could have significant health benefits, but excess is best avoided.

Carcinogens in coffee

of course, there are negatives. For example, coffee contains 4-methylimidazole, which the US National Toxicology Program (NTP) has identified as a carcinogen. The compound is used to manufacture many products, from dyes to agricultural chemicals and rubber. But it can also form through the Maillard reaction in foods and drinks, particularly those with a caramel flavor such as Cola.



Carcinogens including 4-methylimidazole and acrylamide are found in small amounts in coffee.

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CONCLUSION :

Coffee drinking and caffeine intake stimulate the cascade of hormones and the body's stress hormones. Being beneficial and harmful for body, scientists have yet to fully ascertain just how coffee works. So it is necessary to work on the process on substituting or replacing a non-caffeinated, alkaline herbal coffee that brews and tastes just like coffee.

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