

**April/May 2017 Teacher's Guide**

**Background Information**

**for**

***Espresso, Café Latte, Cappuccino… A Complex Brew***

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# About the Guide

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Articles from past issues of *ChemMatters* and related Teacher’s Guides can be accessed from a DVD that is available from the American Chemical Society for $42. The DVD contains the entire 30-year publication of *ChemMatters* issues, from February 1983 to April 2013, along with all the related Teacher’s Guides since they were first created with the February 1990 issue of *ChemMatters*.

The DVD also includes Article, Title, and Keyword Indexes that cover all issues from February 1983 to April 2013. A search function (similar to a Google search of keywords) is also available on the DVD.

The *ChemMatters* DVD can be purchased by calling 1-800-227-5558. Purchase information can also be found online at <http://tinyurl.com/o37s9x2>.

# Background Information

**(teacher information)**

**History of coffee**

The coffee tree is native to the Horn of Africa on the shores of the Red Sea. The earliest history of the use of the cherries (also known as berries) from the tree being used for food date back to 600 AD. At this time, the cherries were ground up and mixed with animal fat. The mixture was said to give warriors the needed energy for battle (the original power bar). One popular legend of the discovery of coffee tells of a goat herder named Kaldi who noticed his herd became friskier than usual after eating the berries from a wild shrub. Out of curiosity he tasted the berries and was delighted by the effects. He shared his discovery with some nearby monks who decided to investigate the properties of the coffee berries. (The first food chemists?) They boiled the coffee beans to make a tea-like beverage that helped them stay awake during prayers and vigils.

Around 1000 AD, Ethiopians used the coffee cherries to make a sort of wine. Through the earliest reports, the beverage was used for medicinal purposes and to enhance concentration during prayers. It wasn’t until the 1300s that people started roasting the coffee beans (the cherry’s seeds) to make a beverage. In the 1500s Turkish coffee was developed. The coffee beans were deeply roasted, finely ground to a powder, and mixed with hot water. The undissolved solids sank to the bottom of the cup and the supernatant liquid was consumed, leaving a pattern of grounds behind in the cup. (Today in Turkey you can have your coffee ground patterns interpreted by a fortune teller.) At first a drink for palace royalty, it soon became a beverage of the public as well, sold in coffee houses that became popular meeting places. Merchants visiting Constantinople returned to their respective countries with tales of this new drink. The establishment of the first coffee house in Venice in 1645 had a rippling effect, and by the end of the 17th century, there were coffee houses throughout Europe.

Cultivation of coffee spread throughout the Arabian Peninsula. Yemen’s climate and fertile soil offered the ideal conditions for growing coffee. It is felt that coffee as a beverage was further developed there. The exportation of coffee beans was highly controlled. Only after the beans were rendered infertile by either parching or boiling were they exported, thus preventing the spread of coffee plantations in other parts of the world and maintaining their tight grip on the industry. In the early 1600s, an Indian pilgrim, Baba Budan, strapped some fertile seeds to his abdomen as he left Mecca. On returning to India, he planted the seeds and started the expansion of the coffee industry. The Dutch were the first to start a plantation in their colonies in Indonesia. Dutch royalty gave coffee saplings to the royalty of other countries as a gift, and the race was on for each country to establish its own source of coffee beans. The Dutch established plantations in Sri Lanka, Ceylon, and Java. The French began growing coffee in the Caribbean. The Spanish planted coffee in South America, and the Portuguese started their plantations in Brazil.

While coffee houses were gaining popularity in Europe they were not always welcomed, particularly in those countries where women were not allowed in. German women were allowed in the coffee houses in that country, but English women were not allowed into English coffee houses. The anonymous 1674 “Women’s Petition Against Coffee” declared: “the Excessive Use of that Newfangled, Abominable, Heathenish Liquor called *COFFEE* ...has ... *Eunucht* our Husbands, and Crippled our more kind *Gallants*, that they are become as *Impotent*, as Age.” (<https://en.wikipedia.org/wiki/History_of_coffee>)

Sometimes there was entertainment in the coffee houses. Johann Sebastian Bach wrote a Coffee Cantata around 1735 that has a humorous dialog between a father and his coffee drinking daughter that was probably performed in a coffee house. The father is upset that his daughter drinks coffee and desperately wants her to stop. He scolds her and bribes her, to no avail. Finally, she tells him if he will find her a husband she will stop drinking coffee. As she meets with her suitors, she tells them in secret that they must let her drink coffee.

Even though there were coffee houses in what would become the United States (e.g., The King’s Arms, established in 1696), coffee was not a popular drink here. Tea was the beverage of choice, as coffee was more expensive and seen as medicinal. However, after the Boston Tea Party in 1773, switching from tea to coffee became something of a patriotic duty. By 1920, around half of all coffee produced worldwide was consumed in the U.S.

As the coffee drink migrated from Turkey to various countries, different methods of preparation evolved. In the early 1700s, the French put solid beans in cloth bags and boiled them. In 1750, they used a drip pot method where hot water was poured over grounds and collected in a separate pot. In the early 1800s, an American-born British physicist invented the coffee percolator. But it is the Italians who gave us espresso. In 1884 in Turin, Italy, Angelo Moriondo invented the espresso machine. In Moriando’s machine, near boiling water was forced through densely packed, finely ground coffee under very high pressure. In this way, the flavor is quickly extracted from the coffee, and not directly brewed out of it. It was called espresso because the process was fast. Improvements were made to the machine by Luigi Bezzera, a mechanic in Milan whose patents were later purchased by Desiderio Pavoni. Pavoni founded the La Pavoni Company to build commercial espresso machines at a rate of one per day. Espresso is now enjoyed throughout the world.

(<http://www.thecoffeebrewers.com/about-demitasse-spoons.html>)

**Coffee trees and their fruit**

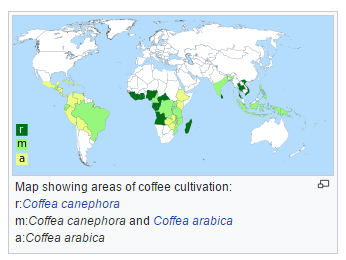
The coffee plant is a member of the family Rubiaceae and is actually an evergreen tree that is a tropical relative to the gardenia. Commercially grown coffee trees are generally trimmed to a shrub in order to increase fruit productivity and to make harvesting easier. There are four species of the tree that are used to produce commercial coffee. These are *Coffea arabica*, *Coffea canephora* or *robusta*, *Coffea liberica*, and *Coffea excelsa*. The Philippines is one of the few countries that has grown all four varieties. The two varieties that are used to produce practically all of the commercially traded coffee are *C. arabica* and *C. canephora*. Two thirds of the coffee in commercial trade is from the arabica variety. Coffee made from arabica beans is smoother, more flavorful, and less bitter. Robusta is more bitter due to its higher percentage of caffeine and phenolic compounds, and the fact that it contains less sugar. It is often used for darker roasts like those for espresso or in blends.

|  |  |  |
| --- | --- | --- |
| Substance | *Coffea arabica* | *Coffea canephora (robusta)* |
| Caffeine | <1.5% | 2.5% |
| Phenolic compounds | 6.5% | 10% |
| Oil | 16% | 10% |
| Sugar | 7% | 3.5% |
| Protein | 10–13% | 10–13% |

*Content of the two major types of coffee*

*(Data taken from McGee, H.* On Food and Cooking: The Science and Lore of the Kitchen*; Scribner: New York, NY, 2004; p 442,* [*http://www.wtf.tw/ref/mcgee.pdf*](http://www.wtf.tw/ref/mcgee.pdf)*)*

Coffee plants grow within a defined area between the Tropic of Cancer and the Tropic of Capricorn. They are not tolerant of cold temperatures. A mild frost can kill the blossoms, thus destroying the harvest for one year. A harder frost will kill the entire tree. The map below illustrates where and what variety of coffee is grown.



*(*[*https://en.wikipedia.org/wiki/Coffee*](https://en.wikipedia.org/wiki/Coffee)*)*

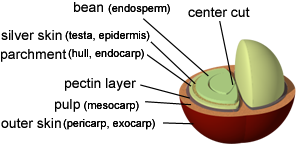
*Coffea arabica* naturally grows to 15 feet (5 m) and is native to the cool highlands of Ethiopia and Sudan. This variety is typically grown at an altitude of 2,000 to 6,000 ft. above sea level. It is self-pollinating and produces seedlings with little variation from the parent. The cherries produced by the arabica trees ripen in 6 to 8 months. Only in Colombia do the coffee plants produce two crops annually, though one is larger than the other. Arabica trees are cultivated in Latin America, East Africa, and Asia.

*Coffea robusta* is a larger tree growing to a height of 33 ft. (10 m) and is native to the lower altitude and hotter, more humid West Africa. This variety is typically grown at an altitude of 600 to 2,400 ft. above sea level. It is not self-pollinating and requires outcrossing (flowers must be fertilized with pollen from another tree). Therefore, the most common method of propagation for this plant is cuttings, grafting, or budding.

The cherries produced by the robusta trees ripen between 9 to 11 months. Robusta trees   
are grown in central Africa, Southeast Asia, and Brazil. These trees are generally more   
disease-resistant than the arabicas. The fruit of these trees has a higher caffeine content, which is toxic to insects. Since the robustas grow in a climate with more insects, it is hypothesized that the varieties with greater concentrations of caffeine were naturally selected. The arabicas grow in higher altitudes where there are fewer insects. There was no environmental push for these plants to be selected for survival due to their caffeine content, so it is lower than the robustas.

The fruit of the coffee tree is referred to as a cherry. They occur in large clusters, which start out green and slowly ripen, turning yellow then red. While some are strip harvested, either by hand or mechanically, the finest coffees are hand-picked when the cherries are red. The seed inside the cherry is what will eventually be processed and roasted for your morning cup of coffee (see illustration below).

The coffee cherry's outer skin is called the *exocarp*. Beneath it is the *mesocarp*, a thin layer of pulp, followed by a slimy layer called the *parenchyma*. The beans themselves are covered in a paper-like envelope named the *endocarp*, more commonly referred to as *the parchment*.



*The coffee “cherry”*

*(*[*http://www.ncausa.org/About-Coffee/What-is-Coffee*](http://www.ncausa.org/About-Coffee/What-is-Coffee)*)*

Inside the parchment, side-by-side, lie two beans, each covered separately by yet another thin membrane. The biological name for this seed skin is the *spermoderm*, but it is generally referred to in the coffee trade as the *silver skin*.

In about 5% of the world's coffee, there is only one bean inside the cherry. This is called a peaberry (or a *caracol,* or "snail" in Spanish), and it is a natural mutation. Some people believe that peaberries are actually sweeter and more flavorful than standard beans, so they are sometimes manually sorted out for special sale.

(<http://www.ncausa.org/About-Coffee/What-is-Coffee>)

After the cherries are harvested, they are either wet processed or dry processed. The wet process involves immediately removing the outer skin and pulp and then washing the beans before they are set out to dry. In the dry process, the pulp and outer skin are dried until they fall off of the bean. In both processes, the parchment hull is removed and the silver skin is left intact before roasting. The same process can be used for either arabica or robusta varieties.

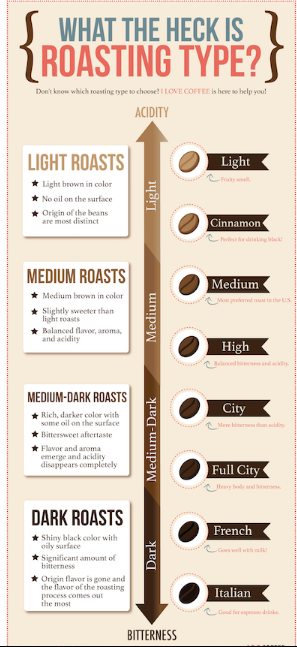
Coffee beans are generally exported green to be roasted on location. Coffee is second only to oil as the most valuable legally traded commodity in the world. Brazil is the world’s top producer of coffee, followed by Viet Nam which produces robusta beans, and third, Colombia, which only grows arabica beans. The world’s top 10 coffee producers are listed in the table below.



*(*[*https://en.wikipedia.org/wiki/Coffee*](https://en.wikipedia.org/wiki/Coffee)*)*

**Roasting** **and its chemical reactions**

Roasting is the processing step of the coffee bean that will determine the flavor and color of the final product, by changing the bean both chemically and physically. Roasting takes place between 375–425 °F, or 190–220 °C. Beans are placed in a preheated roasting oven that gently tumbles the beans as they are being roasted. Beans absorb heat from the oven during the first phase of what is an endothermic stage of roasting. During this phase the internal pressure in the beans increases, as their water content is converted to steam. The beans crack (“first crack”) or pop as they double in volume and lose 5% of their weight. At this stage the beans are light brown or cinnamon colored, as chemical reactions begin to take place within the bean.

 During the next two to three minutes of roasting, the beans will continue to lose weight, due to the formation of gaseous decomposition products formed during pyrolysis. The color changes from sienna to chestnut brown. Light roasts may be stopped at this point.

As roasting continues at higher temperatures, proteins, sugars, carbohydrates, and phenolic compounds fragment and begin reacting with each other in reactions that are exothermic. At this stage the beans suddenly expend heat and emit a crackling sound called the “second crack”. At 205 °C or 401 °F, lots of CO2 is produced, driving oils from inside the bean to the surface and giving the beans an oily sheen. Oils like caffeol, largely responsible for coffee’s aroma and flavor, form as a result of the Maillard and pyrolytic reactions. The bean color turns a rich chestnut. At this stage, the full flavor potential of the bean is reached. Roasting well into the second crack or darker is not favorable since the volatile aromatic compounds are stripped off, and oils on the outside of the bean are more easily oxidized.

Further processing causes the sugars that have been caramelized to burn and turn to carbon. This produces the dark color and charred, smoky flavor that is associated with the Italian and French roasts. In these roasts, you mainly taste the roast and not the chemistry of the bean. As soon as the bean has reached the desired roast, the beans are emptied into a cylindrical cooling tray, where a mechanical sweep keeps them moving so they are evenly exposed to air, in order to stop the roasting process.

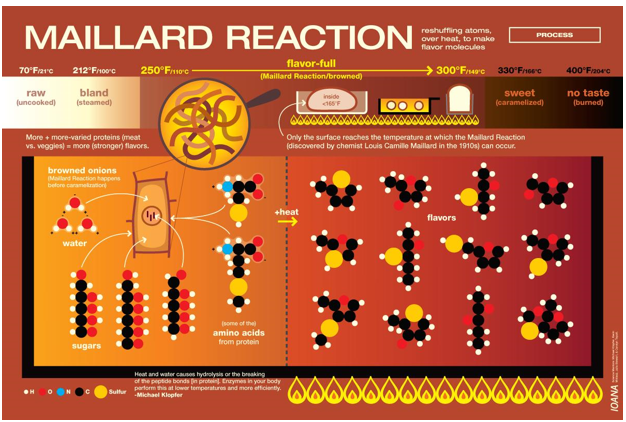
*(*[*https://nationalcoffeeblog.org/2015/11/19/a-guide-to-roasting-types/*](https://nationalcoffeeblog.org/2015/11/19/a-guide-to-roasting-types/)*)*

**The Maillard reaction**

During roasting, carbohydrates and proteins combine in what may be one of the most important reactions for heat processed foods—the Maillard reaction, discovered by a French chemist in 1910. As temperatures reach 150 °C, free proteins or amino acids in coffee combine with sugars, resulting in the formation of hundreds of important aromatic compounds, such as pyrazines and pyridines. These aromatic compounds are responsible for the distinct maize/nutty/roasty aromas found in coffee. The reaction also leads to the formation of the brown-colored melanoidins that are responsible for coffee’s color.

The Maillard reaction can be broken down into three main steps. First, the reactive carbonyl group of the sugar reacts with the amino group of the amino acid, producing   
N-substituted glycosylamine and water. Second, the unstable glycosylamine undergoes Amadori rearrangement forming ketosamines. Third, the ketosamines react further in multiple ways to produce a range of different products, which themselves can react further. Toasty flavored pyrazines, nutty tasting pyroles, caramel tasting furanones, furans with their meaty taste, nutty flavored oxazoles and bitter or burnt tasting alkylpyridines are some of the products of this reaction. Melanoidins, which are responsible for a brown color are also produced. This process is favored in the coffee beans’ alkaline environment, where the amino groups will not be neutralized.

“A Guide to the Maillard Reaction”, using structural formulas, can be viewed here: <http://compoundchem.com/wp-content/uploads/2015/01/The-Maillard-Reaction.pdf>.



*A graphic depiction of the Maillard reaction*

*(*[*http://blog.ioanacolor.com/wp-content/uploads/2011/06/ioana\_top-chef-masters\_science\_maillard-reaction.jpg*](http://blog.ioanacolor.com/wp-content/uploads/2011/06/ioana_top-chef-masters_science_maillard-reaction.jpg)*)*

**Caramelization**

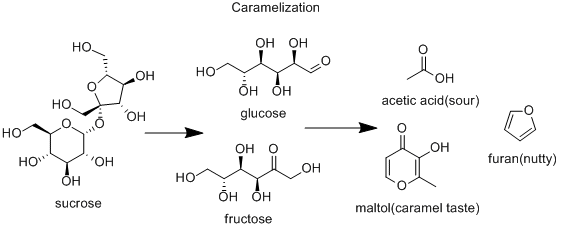
Caramelizationis the decomposition of carbohydrates, such as sucrose, into smaller molecules. In the case of sucrose, the products are fructose and glucose. These sugars further decompose into smaller molecules and fragments that can combine in a variety of different compounds. These compounds give the final product a brown color and a different flavor.

A significant portion of coffee’s acidity comes from the caramelization of carbohydrates, primarily sucrose, to form smaller fragments of acetic, formic, glycolic, and lactic acids. Phytic acid, present in the bean originally, is thermally decomposed to phosphoric acid. The amount of sugar present in the bean originally and the degree of roast help determine the acidity of the final beverage.

Caramelization reactions are sensitive to the chemical environment. By controlling the level of acidity (pH) the reaction rate (or the temperature at which the reaction occurs readily) can be altered. The rate of caramelization is generally lowest at near-neutral acidity (pH around 7), and accelerated under both acidic (especially below 3) and basic (especially pH above 9) conditions.

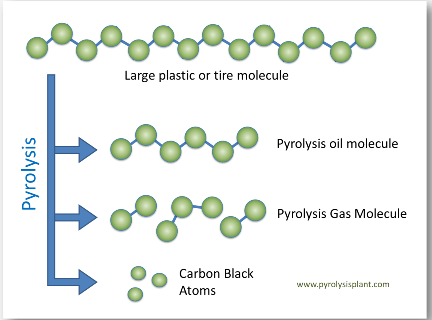
(<https://en.wikipedia.org/wiki/caramelization>)

The flavor of the caramel can change, depending on the combination of products that are formed in the cascade of reactions.

*(*[*https://bondingwithfood.files.wordpress.com/2012/02/chem2.gif*](https://bondingwithfood.files.wordpress.com/2012/02/chem2.gif)*)*

**Pyrolysis**

Pyrolysis is a decomposition reaction that is thermally initiated in the absence of oxygen. Large polymer molecules like lipids and some carbohydrates, when heated, are broken into smaller molecules. An example of this is the pyrolytic cracking of long-chain hydrocarbons in crude oil to produce gasoline and other smaller hydrocarbons. In the coffee bean, some of the fats within the bean are converted to aromatic oils, while the gaseous products like CO, CO2, and water that are formed in these reactions are burnt off during roasting. These new aromatic oils are responsible for much of the flavor and aroma of roasted coffee. An example of a pyrolytic reaction involving an organic polymer is illustrated below.

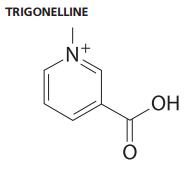
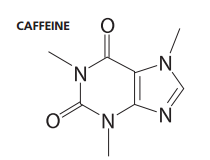


*Pyrolysis products of an organic polymer*

*(*[*http://pyrolysisplant.com/what-is-pyrolysis/*](http://pyrolysisplant.com/what-is-pyrolysis/)*)*

**Compounds found in coffee**

**Alkaloids—caffeine and trigonelline**



*(*[*https://www.coffeechemistry.com/send/6-published-articles/22-the-chemistry-of-coffee*](https://www.coffeechemistry.com/send/6-published-articles/22-the-chemistry-of-coffee)*)*

Though not the most abundant compound in the bean, the alkaloid **caffeine** is the compound that gives coffee its energetic effects. It is extremely soluble, as 95% of caffeine in the coffee grounds is released from the bean during the first minute of brewing. Caffeine sublimes at 178 °C but is able to withstand roasting, due to the other chemicals in the beans with which it is complexed. Some of the effects of caffeine in one or two cups of coffee on the human body are:

* stimulates the central nervous system
* relieves drowsiness and fatigue
* imparts quicker reaction times
* increases energy production in muscles
* improves mood and mental performance
* can produce an abnormally fast heartbeat
* speeds the loss of calcium from bones
* promotes the movement of fluid and solid wastes through the body

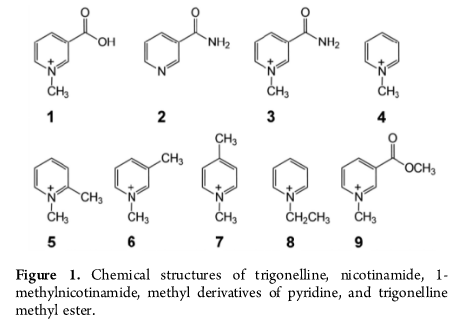
In greater amounts, caffeine can cause chronic anxiety, insomnia, twitching muscles, and diarrhea. Toxic effects appear after about 10 cups of strong coffee, and in enormous doses caffeine is deadly. The lethal dose of caffeine in humans is estimated at about ten grams, or the equivalent of consuming 100 cups of coffee in one sitting.

According to an article in the *Journal of the American Dietetic Association*, coffee has the following caffeine content, depending on how it is prepared:

|  |  |  |
| --- | --- | --- |
|  | **Serving size** | **Caffeine content** |
| Brewed | 7 oz., 207 mL | 80–135 mg |
| Drip | 7 oz., 207 mL | 115–175 mg |
| Espresso | 1.5–2 oz., 45–60 mL | 100 mg |

*(*[*https://en.wikipedia.org/wiki/Coffee*](https://en.wikipedia.org/wiki/Coffee)*)*

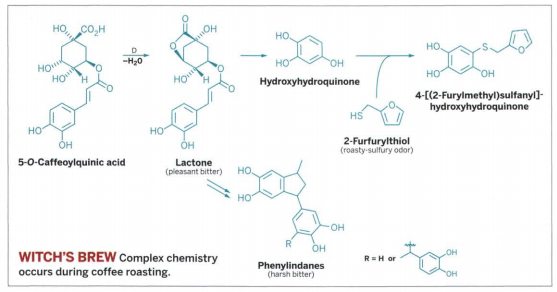
The lesser known alkaloid in coffee is **trigonelline**. Although its concentration is slightly less than that of caffeine, trigonelline is responsible for many of the compounds that give coffee its flavor and aroma. Unlike caffeine, trigonelline readily decomposes during roasting, when the temperatures approach 160 °C. At this temperature, studies have shown that 60% of the initial trigonelline is decomposed during pyrolysis to form carbon dioxide, water and aromatic compounds called pyridines. Pyridines have the greatest aromatic contribution and are responsible for the distinct nutty/roasty aromas found in coffee. Trigonelline and the pyridine products of pyrolysis are included in the figure below.



*(*[*http://pubs.acs.org/doi/pdfplus/10.1021/jf5008538*](http://pubs.acs.org/doi/pdfplus/10.1021/jf5008538)*)*

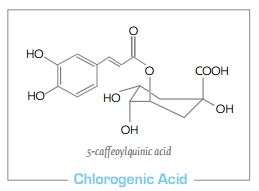
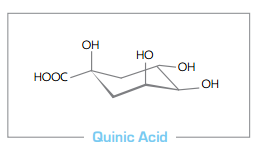
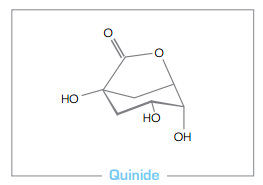
**Chlorogenic acids**

Chlorogenic acid is the major polyphenolic compound in coffee, making up 12% of the weight of the raw bean. This compound, long known as an antioxidant, slows the release of glucose into the bloodstream after a meal. This could be one of the compounds that explains how drinking coffee provides some protection against developing type 2 diabetes. During roasting, unlike caffeine, chlorogenic acids readily hydrolyze to form free phenolic acids like quinic acid and caffeic acid. Chlorogenic acid can also dehydrate to form the bitter tasting chlorogenic lactones. Upon further roasting, these lactones break down through multiple steps to form multiply hydroxylated phenylindanes which yield a lingering, harsh type of bitter sensation in coffee taste. The quinic acid that is formed can isomerise to form quinide. It is this form of quinide that can hydrolyze back into quinic acid as it is exposed to hot water during brewing, increasing the overall acidity of the final beverage. This also explains why coffee becomes more acidic the longer it is held at high temperatures for serving.



*The dehydration of 5-O-Caffeoylquinc acid (chlorogenic acid) to produce lactones and phenylindanes*

*(*[*http://pubs.acs.org/doi/pdf/10.1021/cen-v085n038.p032*](http://pubs.acs.org/doi/pdf/10.1021/cen-v085n038.p032)*)*

*Other products of the roasting of coffee*

*(*[*https://www.coffeechemistry.com/send/6-published-articles/19-organic-acids-revisited*](https://www.coffeechemistry.com/send/6-published-articles/19-organic-acids-revisited)*)*

**Organic acids**

The acid profile of a coffee is like a fingerprint. The origin of the coffee can be confirmed by using its unique acid profile. The specific acids present, as well as their quantity, is part genetics and part environment. *Coffea arabica* beans contain more sugars and less acid than *Coffea robusta*. Arabica beans are grown at higher elevation and cooler temperatures. Coffee scientist Joseph Rivera states that “at cooler temperatures reaction rates decrease and the plant effectively has more ‘time’ to pack nutrients and sugars into the beans”. (<https://www.coffeechemistry.com/send/6-published-articles/20-alchemy-in-the-roasting-lab-part-1>) Altitude, temperature, and humidity all are factors in the acid profile.

Maturity of the bean when it is harvested is also important. Beans that are picked before the fruit is ripe will have more acid and little sugar. With these beans, the best thing to do is make French roast (burn them). The best roast for enjoying a coffee’s unique acid profile is a light or medium roast. In the darker roasts, many of the acids have just been reduced to charred carbon.

Some acids, such as citric, malic, phytic, and chlorogenic, are contained in the raw bean before roasting, while others, such as acetic acid and quinic acid are the product of the pyrolytic reactions that occur during roasting. There are more than 30 organic acids in a cup of coffee. Which ones and their quantities depend of the bean and on the roast. The most abundant acids in coffee, in increasing order, are:

* Phosphoric
* Malic
* Lactic
* Acetic
* Citric
* Quinic
* Chlorogenic

Phosphoric acid is not an organic acid but is still present in coffee. It is formed by the decomposition of phytic acid and withstands further decomposition in the high heat of roasting. In fact, the darker the roast the higher the concentration of phosphoric acid becomes.

(<https://www.coffeechemistry.com/send/6-published-articles/20-alchemy-in-the-roasting-lab-part-1>)

**Brewing coffee for espresso drinks**

Principles of mixtures, solubility, reaction rates, entropy, and gases are all incorporated in brewing a cup of espresso. A cup of coffee is a mixture. If it has been made by a filter method, with no undissolved solids present, then it is a homogeneous mixture, or true solution. It if is like Turkish coffee, with a lot of undissolved solids settled to the bottom of the cup, then your drink is a heterogeneous mixture or a suspension. If you add milk, you are adding a colloid.

In regards to solubility, temperature affects the number of solids that will dissolve, as well as what reactions will occur, and how fast they will happen. The optimum temperature for brewing coffee is between 88–93 °C, or 190–200 °F. Temperatures higher than this extract bitter compounds too quickly. At temperatures lower than 88 °C, fewer of the compounds that give coffee its flavor will be dissolved. Which compounds dissolve and their final concentration depend on the type of coffee, the amount used, the amount of water added, the particle size of the grounds, and the length of time the grounds are in contact with the water.

The best water to use in making coffee is one with a moderate mineral content with a near neutral pH, so that the final brew will have a pH close to 5. Some tap water is alkaline because water treatment plants adjust the pH to a value close to 8 in order to protect the water pipes. To decrease the pH of the alkaline tap water, a pinch of cream of tartar can be added to slightly lower the pH. Distilled water should not be used to brew coffee, because it makes a brew that tastes flat. Hard water also should not be used, as the CaCO3 and MgCO3 slow down flavor extraction. They also clog the pipes of the espresso machine. Softened water over-extracts coffee and imparts a salty flavor.

Once the water is heated, it is forced though very finely ground dark roasted coffee grounds at 9 atm of pressure in 30 seconds. Espresso uses a dark roast, either French or Italian. Lighter roasts have a higher acid content that will lead to a very acidic final product. Three to four times more finely ground coffee is used in making each cup of espresso. Because it is so concentrated, it is served in small portions. The amount of caffeine in one serving of espresso is actually less than that in a serving of regular filtered coffee primarily because a serving of espresso is 45–60 mL while a regular coffee is 210 mL. However, if you compare concentrations, regular coffee has 40 mg/100 g of caffeine while espresso has 212mg/100g of caffeine; plus, espresso contains magnesium, B vitamins, niacin, and riboflavin, due to the coffee solids that are present.

High pressure forces more oils from the beans to form a creamy emulsion of oil droplets that contribute to a slow, prolonged release of coffee flavor in the mouth. Harold McGee, in his book *On Food and Cooking, the Science and Lore of the Kitchen,* describes this *crema.*

Another unique feature of espresso is the crema, the remarkably stable, creamy foam that develops from the brew and covers its surface. It’s the product of carbon dioxide gas still trapped in the ground coffee, and the mixture of dissolved and suspended carbohydrates, proteins, phenolic materials, and large pigment aggregates, all of which bond in one way or another to each other and hold the bubble walls together.

(McGee, H. *On Food and Cooking: The Science and Lore of the Kitchen;* Scribner: New York, NY, 2004; p 447, <http://www.wtf.tw/ref/mcgee.pdf>)

Cappuccinos and lattes start with one or two shots of espresso and add steamed or foamed milk. A cappuccino is made using 1/3 espresso, 1/3 steamed milk, and 1/3 foamed milk, while a latte uses 1/6 espresso, 4/6 steamed milk, and 1/6 foamed milk. The milk provides proteins that bind to the tannic phenolic compounds, which weaken the aroma and overall coffee flavor. This could be why lattes are so popular among the high school set.

Milk adds another sugar and more proteins and fat to the drink. Lactose is a disaccharide (glucose and galactose), but it is not as sweet as sucrose, probably because it is less soluble. On a scale of relative sweetness, sucrose is 100, while lactose is 16. By heating the milk, the lactose is rendered more soluble and the warm milk will taste sweeter than cool milk. Milk is composed of two proteins. Casein comprises 80% of milk protein. The casein helps create walls around the steamed air bubbles. The other 20% of milk protein is whey, which stabilizes the foam. The relationship of fat and protein impacts how easily the milk will foam. Increases in milk fat up to 5% causes a decrease in foam volume. Therefore, skim milk is the easiest to foam, but 2% or whole milk will give the drink a velvety feel in the mouth. Milk fat greater than 5% increases both foam volume and stability. Regardless of which milk is used, it should be cold at the beginning and steamed in a clean cold pitcher.

**Coffee and health**

There have been countless studies to try to determine the long-term effects of drinking coffee. From time to time, a singular study may report on the ill effects of coffee, but the overall research finds that coffee may actually provide protection from various diseases. As there are nearly 1,000 compounds in coffee, it is not safe to assume that the observed effects are due to one single compound like caffeine, but they may actually be due to a combination of compounds. A 2015 article in the *New York Times* reported on several meta-analysis studies on the effects of coffee consumption on various illnesses. *Healthy Fellow*, a Web site that promotes individual wellness by passing along evidence-based natural health information, reported on several studies concerning skeletal health. They used articles published in reputable sources like *PubMed*, *Clinical Chemistry*, and *Journal of Nutrition*. Several studies investigating the health effects of coffee were also cited in an article published in *The Atlantic*. Following is a table that compiles the reports in these resources:

|  |  |  |  |
| --- | --- | --- | --- |
| Date | Disease | Sample Size | Findings |
| 2011 | Stroke | 480,000 | Lower risk of disease for moderate coffee consumption |
| 2012 | Heart Failure | 140,220 | Lower risk of disease for moderate coffee consumption. Lowest for the 4 cups a day group |
|  | Cardiovascular Disease | 1,270,000 | Lowest risk in the group consuming 3-5 cups of coffee a day |
| 2007 | Liver Cancer | 241,410 | Moderate coffee consumption resulted in a 40% lower risk |
| 2010 | Prostate Cancer |  | No effect detected |
|  | Breast Cancer |  | No effect detected |
|  | Lung Cancer |  | Increased risk with more coffee consumption |
|  | Liver Disease |  | Decreased progression to cirrhosis seen among moderate coffee drinkers |
|  | Parkinson’s disease |  | Slower cognitive decline among moderate coffee consumption |
| 2014 | Type II Diabetes | 1,100,000 | 8% lower risk in women coffee drinkers, 4% lower risk in men coffee drinkers, 7% lower risk for decaffeinated coffee drinkers |
|  | Osteoporosis |  | Increased risk of bone degeneration in select populations |
| 2012 | Death | 1,000,000 | Higher coffee consumption was associated with lower risk of death |

*A summary of reports showing findings of studies relating health concerns to drinking coffee*

*(*[*http://www.healthyfellow.com/771/coffee-calcium-controversy/*](http://www.healthyfellow.com/771/coffee-calcium-controversy/)*)*

*(*[*https://www.theatlantic.com/health/archive/2012/11/the-case-for-drinking-as-much-coffee-as-you-like/265693/*](https://www.theatlantic.com/health/archive/2012/11/the-case-for-drinking-as-much-coffee-as-you-like/265693/)*)*

*(*[*https://www.nytimes.com/2015/05/12/upshot/more-consensus-on-coffees-benefits-than-you-might-think.html*](https://www.nytimes.com/2015/05/12/upshot/more-consensus-on-coffees-benefits-than-you-might-think.html)*)*

For the first time, the latest (2015) USDA diet guideline gives the go-ahead on drinking coffee and says it might be good for you. This is an excerpt from the “Scientific Report of the 2015 Dietary Guidelines Advisory Committee”:

Currently, strong evidence shows that consumption of coffee within the moderate range (3 to 5 cups per day or up to 400 mg/d caffeine) is not associated with increased long-term health risks among healthy individuals. In fact, consistent evidence indicates that coffee consumption is associated with reduced risk of type 2 diabetes and cardiovascular disease in healthy adults. Moreover, moderate evidence shows a protective association between coffee/caffeine intake and risk of Parkinson’s disease. Therefore, moderate coffee consumption can be incorporated into a healthy dietary pattern, along with other healthful behaviors.

(<https://health.gov/dietaryguidelines/2015-scientific-report/10-chapter-5/d5-5.asp>)

**Black Ivory coffee**

The side bar in the article mentions some pretty expensive coffee for $70 a serving. This is an average. If you shop around you might be able to find it for $50 for four demitasse servings at The Elephant Story in Comfort, Texas. This is the only place outside of a 5-star hotel in Thailand where you can try it. The coffee is produced at the Golden Triangle Asian Elephant foundation in Thailand. Street rescued elephants are given refuge at the Golden Triangle elephant sanctuary, where they are fed a diet of Thai arabica coffee cherries. Enzymes in the elephant’s digestive system, coupled with fermentation, break down coffee proteins and other bitter compounds in the cherries. After the cherries have passed through the elephants’ digestive systems, local indigenous people named Mahouts, remove the coffee beans from the elephant dung. The beans are then washed and dried in the sun and later roasted. A percentage of the proceeds from the sale of the coffee is used for the elephants’ care. Thirty-three kg of coffee cherries are required for 1 kg of coffee. The elephants do not seem to be harmed by their diet. In fact, elephants in the wild have been killed for invading coffee plantations for the cherries.

Black Ivory coffee probably was inspired by Kopi luwok coffee. Kopi luwok is coffee that is made from coffee beans that have passed through the digestive track of the cat-like palm civet. It, too, is very expensive, and this encouraged the growth of many backyard businesses. However, the industry is not very humane, as the civets are caged and often force-fed. The animals are susceptible to disease, and the wild civet population was threatened. Since the industry is not regulated, the same type of coffee beans is not necessarily used for all civets, giving a broad range of flavors for one specialty product.

The history of Kopi luwok dates back to the 18th century Dutch colonists. Using arabica trees from Yemen, the Dutch started their first coffee plantation. Local natives were used to work the farms, but they were not allowed to take any of the coffee beans. Out of curiosity, the natives wondered about the Dutch beverage. They noticed that the native civets ate the coffee cherries, and the beans were present in their feces. The natives collected the “luwoks” coffee seed droppings, then cleaned, roasted, and ground them to make their own coffee beverage. The fame of the aromatic civet coffee spread to the Dutch plantation owners and soon became their favorite. It was expensive, even then. If you have ever seen “The Bucket List” with Jack Nicholson and Morgan Freeman, Kopi luwok is Jack’s favorite beverage.

**Decaffeinated coffee**

Since 1903, when a boat shipment of coffee beans got soaked by salty seawater in transit to Germany, decaffeinated coffee has met the needs of people who enjoy the flavor of coffee but are sensitive to the effects of caffeine. After the German coffee merchant, Ludwig Roselius received the damaged beans, he went ahead and roasted them anyway and was pleased to find that the flavor of the resulting coffee was still the same, but he tested the coffee and discovered the caffeine was missing. He sold the coffee and marketed it as decaffeinated. He then developed and patented (1906) a method for decaffeinating coffee for future sales.

Today there are three methods that are used to decaffeinate coffee for commercial use. These are the Swiss water method, the solvent extraction method, and the supercritical CO2 method. These processes draw heavily on the concepts of solubility and osmosis to extract the caffeine. All three methods begin with green coffee beans that have been moistened at   
70–100 °C to make the caffeine soluble so it can be drawn out. Caffeine is polar and is extremely soluble in water. The idea behind these processes is to remove the caffeine, while leaving the sucrose, cellulose, proteins, and acids in the coffee beans in their original concentrations.

In the Swiss water processing, a bean solution is prepared by soaking the beans in water until everything that is soluble is drawn out of the bean. Next, this solution is passed through carbohydrate treated activated charcoal designed to selectively absorb caffeine. The caffeine free extract can then be used on a new batch of beans to selectively extract only the caffeine since all the other water soluble compounds in the bean will be in equilibrium with those same compounds present in the bean extract, utilizing the concepts of osmosis. The solution can be decaffeinated and used for multiple batches of beans. This method extracts 94–96% of the caffeine.

The second method of caffeine extraction involves using solvents like methylene chloride or ethyl acetate to specifically extract caffeine. The moistened beans are soaked in the solvent for several hours. After removal from the solvent, the beans are gently steamed to remove the solvent. The solvent can then be decaffeinated by passing through activated charcoal so it can be reused. This process removes 96–97% of the caffeine.

Supercritical CO2 is used to selectively extract caffeine in the third method.

Supercritical carbon dioxide is a fluid state of carbon dioxide where it is held at or above its critical temperature and critical pressure.

Carbon dioxide usually behaves as a gas in air at standard temperature and pressure (STP), or as a solid called dry ice when frozen. If the temperature and pressure are both increased from STP to be at or above the critical point for carbon dioxide, it can adopt properties midway between a gas and a liquid. More specifically, it behaves as a supercritical fluid above its critical temperature (304.25 K, 31.10 °C, 87.98 °F) and critical pressure (72.9 atm, 7.39 MPa, 1,071 psi), expanding to fill its container like a gas but with a density like that of a liquid.

(<https://en.wikipedia.org/wiki/Supercritical_carbon_dioxide>)

A large extraction vessel is used where supercritical CO2 is forced into the coffee at pressures of 1000 pounds per square inch. The caffeine is dissolved in the CO2 which can then be removed from the vessel where it is passed through charcoal filters to remove the caffeine, rendering the CO2 ready for reuse. This process typically removes 96–98% of the caffeine. This is the method that is used by large commercial processors for the decaffeinated coffee that is sold in the grocery stores. The benefit of using supercritical CO2 is its low toxicity, relative to other solvents used for caffeine extraction, and its low environmental impact.

According to an article in *Entrepreneur*, coffee drinkers who prefer decaffeinated coffee may be true connoisseurs of coffee flavor.

… according to industry estimates, the decaf market account[s] for only 15-20% of all coffee sales, but within this small sector lies perhaps one of the most devoted coffee customers available. For this it is this consumer who seeks and consumes coffee, not for its stimulatory effects, but its pure sensorial pleasure. And from a biological perspective, preliminary data may prove that decaf consumers may consume even more coffee (per cup) than regular drinkers. Why? According to medical research, once a certain level of caffeine has been established in the blood, the desire to consume more coffee (ie. caffeine) quickly subsides. In the case of decaf, the reduced caffeine content in decaf coffee would theoretically allow them to consume more coffee than regular. The theory, which has prompted a handful of research institutions to develop varieties of coffee with lower caffeine producing traits, has yet to be seen, but the development does hold a promising future in terms of global coffee consumption.

(<https://www.coffeechemistry.com/news/general/entrepreneur-magazine-covers-decaf-publication?highlight=WyJkZWNhZmZlaW5hdGVkIiwiZGVjYWZmZWluYXRpb24iLCJkZWNhZmZlaW5hdG9yIiwiY29mZmVlIiwiY29mZmVlJ3MiLCInY29mZmVlIiwiY29mZmVlcyIsIidjb2ZmZWUnLCIsImRlY2FmZmVpbmF0ZWQgY29mZmVlIl0>)

# References

**(non-Web-based information sources)**

**The references below can be found on the *ChemMatters* 30-year DVD, which includes all articles   
published from the magazine’s inception in October 1983 through April 2013; all available Teacher’s Guides, beginning February 1990; and 12 *ChemMatters* videos. The DVD is available from the American Chemical Society for $42 (or $135 for a site/school license) at this site:** [**http://ww.acs.org/chemmatters**](http://www.acs.org/chemmatters)**. Click on the “Teacher’s Guide” tab to the left, directly under the “*ChemMatters Online"* logo and, on the new page, click on “Get the past 30 Years of *ChemMatters* on DVD!” (the icon on the right of the screen).**

**Selected articles and the complete set of   
Teacher’s Guides for all issues from the past three   
years are available free online at the same Web site, above. Click on the “Issues” tab just below the logo, *“ChemMatters Online”*.**



***30* Years of *ChemMatters !***

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Three processes used to decaffeinate coffee are explained in this 1999 *ChemMatters* article. (Barstow, K. The Case of the Missing Caffeine. *ChemMatters*, 1999, *17* (2), pp 12–13)

The health effects of a few of the 800+ chemicals found in coffee are presented in a way that would make this article an excellent addition to the current article. Some of the same concepts, such as the chemical reactions and roasting of coffee beans, are discussed, but the primary focus of this article is the effect of caffeine on brain chemistry. (Haines, G. Brain Booster to Go? *ChemMatters*, 2008, *26* (4), pp 7–9)

The Teacher’s Guide to the Haines article above contains further historical information, a list of the chemical compounds found in coffee beans, and multiple ideas for projects and class discussions.

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Harold McGee discusses the history of coffee brewing, coffee beans and their roasting, always bringing out the chemistry involved in each step. There is a good table on page 446 on methods of brewing coffee. (McGee, H. *On Food and Cooking: The Science and Lore of the Kitchen;* Scribner: New York, NY, 2004; pp 441–447, <http://www.wtf.tw/ref/mcgee.pdf>)

# Web Sites for Additional Information

**(Web-based information sources)**

**History of coffee**

A history of coffee can be found here as part of a series on the stories behind the foods we eat. The article ends with some recipes for coffee drinks, as well as a flank steak marinated in coffee. (<http://www.pbs.org/food/the-history-kitchen/history-coffee/>)

More information about the history and development of coffee can be found at this wiki site. Here you will find the words to Bach’s cantata about coffee. (<https://en.wikipedia.org/wiki/Coffee#/media/File:Carte_Coffea_robusta_arabic.svge>)

**Coffee**

This *National Geographic* site is a treasure trove of information about coffee. There is a good world map that highlights the coffee producing countries. (<http://www.nationalgeographic.com/coffee/ax/frame.html>)

Another world map that show where the different varieties of coffee are grown can be found at this site: <https://upload.wikimedia.org/wikipedia/commons/3/3c/Carte_Coffea_robusta_arabic.svg>.

The reference page for Coffee Review has information links provided for every aspect of coffee. For students looking for more information, it would be a good place to start. (<http://www.coffeereview.com/coffee-reference/>)

The National Coffee Association Web site provides general information about coffee production, from farm to table. ([www.ncausa.org](http://www.ncausa.org))

At this site you will find a link to four different published academic articles about coffee chemistry. (<https://www.coffeechemistry.com/category/6-published-articles>)

**Coffee roasting reactions**

The chemistry of roasting reactions, as well as a complete description of the changes occurring in the coffee bean during each minute of roasting are presented at this site. (<https://www.quora.com/What-is-the-science-behind-coffee-roasting>)

Information on the Maillard reaction can be found here: <http://www.scienceofcooking.com/maillard_reaction.htm>.

A comprehensive flow diagram of the Maillard reactions, using the structural formulas of the compounds, is located at this site: <http://compoundchem.com/wp-content/uploads/2015/01/The-Maillard-Reaction.pdf>.

The caramelization reaction is discussed at this Wikipedia Web site: <https://en.wikipedia.org/wiki/caramelization>.

A guide to roasting types can be found at this site. It is an infographic of all 8 roasts of coffee and their respective acidity and roast characteristics. (<https://nationalcoffeeblog.org/2015/11/19/a-guide-to-roasting-types/>)

A two part article about the science of roasting coffee, and the chemistry that is involved, can be found here.

* (<https://www.coffeechemistry.com/send/6-published-articles/20-alchemy-in-the-roasting-lab-part-1>)
* (<https://www.coffeechemistry.com/send/6-published-articles/21-alchemy-in-the-roasting-lab>)

Pyrolysis reactions are presented here: <https://en.wikipedia.org/wiki/pyrolysis>.

Roasting reactions such as pyrolysis and the pyrolytic products of trigonelline are presented in this paper, titled “the antithrombotic effects of pyridinium compounds formed from trigonelline upon coffee roasting.” (<http://pubs.acs.org/doi/ipdf/10.1021/jf5008538>)

**Brewing coffee**

A frothing guide and extensive information about the chemistry of milk in frothing for espresso drinks is available at this coffee geek Web site. (<http://coffeegeek.com/guides/frothingguide/milk>)

More on the science of producing milk foam used in espresso drinks can be found at this site. Discussion about the differences between lattes, cappuccinos and machiatos is also included. (<http://www.thecoffeebrewers.com/article2.html>)

“A chemistry teacher’s guide to brewing the perfect cup of coffee” is the title of this article in *The Guardian*. Most chemistry variables related to the brewing process are discussed. (<https://www.theguardian.com/commentisfree/2015/oct/23/a-chemistry-teachers-guide-to-the-perfect-cup-of-coffee>)

The story of the first espresso machine, complete with a picture of the inventor and his patent sketches, is located here: <http://www.thecoffeebrewers.com/about-demitasse-spoons.html>.

**Caffeine**

A table containing the caffeine content of many popular beverages can be found here: <https://www.math.utah.edu/~yplee/fun/caffeine.html>.

**Compounds in coffee**

Technical information about chlorogenic acid can be found at this data base site: <https://pubchem.ncbi.nlm.nih.gov/compound/chlorogenic_acid#section=Top>.

A hyperlinked list of many of the acids found in coffee is located at this site. The hyperlinks take you to the structural formulas of the acids. Not all acids on the list are hyperlinked. (<http://www.coffeeresearch.org/science/sourmain.htm>)

This scientific article about acids in coffee is a good source of diagrams of chlorogenic acid and the quinides. The article describes the reactions occurring during roasting. (<https://www.coffeechemistry.com/send/6-published-articles/19-organic-acids-revisited>)

“The chemistry of Coffee” is the title of this paper. Caffeine, trigonelline, lipids, pyrazines, and pyridines, and Maillard reactions in coffee are all discussed. Structural diagrams of some of the compounds are used. (<https://www.coffeechemistry.com/send/6-published-articles/22-the-chemistry-of-coffee>)

The aroma compounds like the chlorogenic lactones and the phenylindanes are discussed in this *C&EN* article on coffee aroma, titled “Tweaking Coffee’s Aroma.” (<http://pubs.acs.org/doi/pdf/10.1021.cen-v085n038.p032>)

**Coffee and health**

**“**Chemistry in Every Cup” is the title of this article that addresses the effects coffee has on each major organ system in the body. (<https://www.chemistryworld.com/feature/chemistry-in-every-cup/1012386.article>)

Coffee consumption and how it affects bone density is addressed in this article. Also addressed is whether adding milk to coffee influences how compounds in coffee are absorbed by the body. (<http://www.healthyfellow.com/607/coffee-milk-controversy/>)

This journal article describes a study that correlated coffee consumption and bone loss. (<http://ajcn.nutrition.org/content/74/5/694.full>)

This *New York Times* article reports on the results of numerous meta-analysis studies about the health effects of coffee consumption. (<https://www.nytimes.com/2015/05/12/upshot/more-consensus-on-coffees-benefits-than-you-might-think.html>)

An article in *The Atlantic* discusses the results of several studies into the effects of coffee consumption on human health. A study that links coffee to protection from type II diabetes is included in this article. (<https://www.theatlantic.com/health/archive/2012/11/the-case-for-drinking-as-much-coffee-as-you-like/265693/>)

What are the compounds responsible for the heart-healthy effects of drinking coffee is the focus of this paper, titled “the antithrombotic effects of pyridinium compounds formed from trigonelline upon coffee roasting”. (<http://pubs.acs.org/doi/ipdf/10.1021/jf5008538>)

Studies that investigated if there was any correlation between cancer and coffee consumption are reported in this article: <http://healthyfellow.com/651/coffee-estrogen-link/>.

Calcium depletion, spinal osteopenia and coffee intake is the topic of the paper found at this address: <http://www.healthyfellow.com/771/coffee-calcium-controversy/>.

**Black Ivory coffee**

An NPR interview of the entrepreneur who started the Black Ivory coffee business can be found here: <http://www.npr.org/sections/thesalt/2014/08/20/340154271/no-1-most-expensive-coffee-comes-from-elephants-no-2>.

Links to a variety of articles about Black Ivory coffee are located at this site: (<https://www.blackivorycoffee.com/news>. If you go to the home page from this page you will find more videos and information about Black Ivory coffee.