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What is in a "Cup of Joe"? From green beans to spent grounds: a mini-review on coffee composition and health benefits

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Abstract

Coffee is one of the most popular beverages consumed worldwide and is amongst the main dietary sources of bioactive compounds. Recent studies have described a positive association between caffeine ingestion and health, including improvement of exercise performance and enhancement of long-term memories in humans. However, from roasting to extraction, the processing of the coffee beans has a significant impact on the profile of bioactive compounds. For instance, roasting results on the reduction of 5-caffeoylquinic acid and trigonelline, while increases the concentration of melanoidins. Another important component is its lipid fraction (known as coffee oil), which can migrate to the surface of the beans and undergo changes in its composition during roasting. This mini-review presents an overview of the composition of coffee, including changes that occur during processing—from green beans to spent grounds, and recent research on its health benefits, with special focus on their antioxidant properties.

Keywords: Caffeine; Chlorogenic acid; Trigonelline; Roasting, Bioactive compounds.

1. Introduction

Coffee is one of the most popular beverages consumed worldwide and is amongst the main dietary sources of bioactive compounds (Pérez-Jiménez et al., 2010). The continuous increase in coffee demand could be explained by several factors, such as the improvement on the quality of beans, creation and expansion of specialty coffee shops, and dissemination of literature linking its consumption to health benefits. For instance, recent studies have described a positive association between caffeine ingestion and improvement of exercise performance (Grgic et al., 2019) and a new mode of action of this compound at the mitochondrial level with beneficial effects on cardiovascular diseases (Ale-Agha et al., 2018). In addition to the potential role of caffeine as a protective agent on Parkinson's disease, Yan et al. (2018) showed that the co-administration with eicosanoyl-5-hydroxytryptamide (another compound purified from coffee) enhanced the activity of a specific phosphatase that acts on α-synuclein, a characteristic pathogenic protein. However, another study (with more than 340,000 individuals) showed that those who consumed more than 6 cups of coffee a day had 22% more chances of developing cardiovascular diseases than non-drinkers (11%) and drinkers of decaffeinated coffee (7%) (Zhou and Hyppönen, 2019).

Amongst several compounds, caffeine is recognized as the main bioactive substance in coffee. Other examples of bioactive compounds identified in coffee are shown in Table 1. Coffee accounts for approximately two-thirds of the daily intake of caffeine by US population above 10 years old (Barone and Roberts, 1996). Several health benefits have been associated with consumption of caffeine, including increased cognitive performance (Borota et al., 2014), enhancement of anti-inflammatory response (Tauler et al., 2013), hypoalgesic effects (Maridakis et al., 2007), among others shown in Table 2.

Similar to other examples in the literature, the processing

Table 1. Screening of main bioactive compounds of coffee using LC and LC-MS

*[M-H]⁻ or **[M-H]⁺	MS^n	Compound	Feedstock	Reference
195.0877*	137.92	Caffeine	Green coffee, roasted coffee, coffee powder and beverage	Abreu et al. (2011), Angeloni et al. (2019), Caporaso et al. (2014), Liu and Kitts (2011), Priftis et al. (2018)
335.0761*	179.0514, 161.0862, 135.0232	Caffeoylquinic lactone acid	Green coffee, roasted coffee, and beverages	Angeloni et al. (2019), Priftis et al. (2018)
337.0917*	163, 190.8751, 118.9217	3-*p*-coumaroylquinic acid	Green coffee and roasted coffee	Priftis et al. (2018)
337.0917*	163.5239, 190.3598 118.5912	5-*p*-coumaroylquinic acid	Green coffee, roasted coffee, and coffee beverages	Angeloni et al. (2019), Priftis et al. (2018)
353.0867*	191.0208, 179.0095	3-*O*-caffeoylquinic acid	Green coffee, roasted coffee, coffee beverages	Niseteo et al. (2012), Priftis et al. (2018)
353.0867*	191.0518, 173.0086	4-*O*-caffeoylquinic acid	Green coffee, roasted Coffee, coffee beverages	Angeloni et al. (2019), Priftis et al. (2018)
353.0867*	191.0835, 178.9312, 135.0009	5-*O*-caffeoylquinic acid	Green coffee, roasted coffee, coffee beverages	Angeloni et al. (2019), Priftis et al. (2018)
367.1026*	193.1396	3-*O*-feruloylquinic acid	Green coffee and roasted coffee	Priftis et al. (2018)
367.1022*	193.0504	4-*O*-feruloylquinic acid	Green coffee and roasted coffee	Priftis et al. (2018)
367.1024*	193.0502	5-*O*-feruloylquinic acid	Green coffee, roasted coffee, and beverages	Angeloni et al. (2019), Priftis et al. (2018)
417**	151, 123	β-Tocopherol	Green and roasted coffee and coffee beverage	Alves et al. (2009)
431**	165, 137	α-Tocopherol	Green and roasted coffee and coffee beverage	Alves et al. (2009)
515.1188*	353.2199, 335.2577, 173.0377	1,5-dicaffeoylquinic acid	Green coffee and roasted coffee	Priftis et al. (2018)
515.1188*	353.1824, 173.0116 191.0214	3,4-dicaffeoylquinicacid	Green coffee and roasted coffee	Priftis et al. (2018)
515.1188*	353.1999, 172.9495	2,4-dicaffeoylquinic acid	Green coffee and roasted coffee	Priftis et al. (2018)
529.1341*	367.2116, 335.1851, 173.0893	Caffeoyl-feruloylquinic acid	Green coffee and roasted coffee	Priftis et al. (2018)

*Negative mode; **positive mode; LC, liquid chromatography; MS, mass spectrometry, may contemplate tandem mass spectrometry (MS^n)

of the coffee beans has a significant impact on the profile of bioactive compounds, from roasting to extraction. For instance, Vignoli et al. (2014) showed that the levels of 5-caffeoylquinic acid and trigonelline decreased, while melanoidins increased as the roasting progressed. Comparing brewing methods, instant coffee has a higher caffeine level than filtered and Turkish coffee (Samanidou et al., 2012). The serving size also matters: a 25-mL espresso cup has 2.8 times less caffeine and 1.5 times less phenolic compounds than 125 mL of American coffee (Caporaso et al., 2014).

This review aims to present an overview of the composition of coffee, including changes that occur during processing, and recent research on its health properties. First, the chemical profile of green coffee beans is presented. This is followed by a review of the effects of roasting and extraction on the physicochemical properties of the beans. Finally, studies focused on the use of spent coffee ground generated from brewing methods as a source of value-added compounds are presented.

2. Physicochemical properties of coffee

Approximately 99% of the beans of economic importance comes from two species: *Coffeea arabica* L. (or Arabica coffee) and *C. canephora* Pierre ex Froehner (or Robusta coffee), although more than 90 species have been identified (DaMatta and Ramalho, 2006). Some of the differences observed between Arabica and Robusta coffee are the growing requirements (Magrach and Ghazoul, 2015), physical aspects of the beans (Mendonça et al., 2009), sensory characteristics when cupped (Salamanca et al., 2017), and chemical composition before and after roasting, including caffeine content (Perrois et al., 2015), amino acid (Casal et al., 2003), and tocopherol profile (Alves et al., 2009).

Table 2. Potential health benefits of coffee and its main bioactive compounds

Feedstock	Main findings	Reference
Coffee	Lower level of spontaneous DNA strand breaks in peripheral white blood cells	Bakuradze et al. (2015)
Coffee	Increase in the resistance of LDL to oxidative modification and higher concentration of conjugated forms of caffeic, *p*-coumaric, and ferulic acids into LDL	Natella et al. (2007)
Coffee	Reduction of oxidative DNA damage	Bakuradze et al. (2011)
Coffee containing mainly chlorogenic acid isomers and derivatives	Reducing power, scavenging of superoxide and hydroxyl radicals and antimutagenic activity *Salmonella typhimurium*	Priftis et al. (2018)
Coffee and caffeine	Improvement of long-term memory, reduction of lipid peroxidation of brain membranes, and increased activity of glutathione reductase and superoxide dismutase	Abreu et al. (2011)
Caffeine	Enhancement of consolidation of long-term memories in humans	Borota et al. (2014)
Caffeine	Effect is generally greater for aerobic as compared with anaerobic exercise	Grgic et al. (2019)
Caffeine	Attenuation of delayed-onset muscle pain and force loss following eccentric exercise	Maridakis et al. (2007)
Caffeoylquinic and dicaffeoylquinic acid isomers	DNA-protective effects	Xu et al. (2012)

In addition to inter-species differences, the biochemical composition and quality attributes of coffee can be affected by growing conditions, including shading (Somporn et al., 2012), altitude (Worku et al., 2018), and temperature (Bertrand et al., 2012). This section will present the physicochemical and bioactive properties of coffee, from green beans to the cup, including changes that occur during processing. Focus will be given to Arabica coffee, unless otherwise stated.

2.1. Green beans to roasted coffee

One of the main components in green coffee beans is the lipid fraction (or coffee oil), which is comprised of approximately 75% of triacylglycerols (e.g., stearic and oleic acids), up to 20% total free and esterified diterpene alcohols (e.g., kahweol and cafestol, both associated with positive and negative health effects) (Speer and Kölling-Speer, 2006), 5% total free and esterified sterols (e.g., sitosterol and stigmasterol), and a small amount of minor compounds (e.g., tocopherols) (Sunarharum et al. 2014). With roasting, the oil fraction can migrate to the surface of the beans and undergo changes in its composition. Although sterols and most triacylglycerols are mainly unaffected (Speer and Kölling-Speer, 2006; Sunarharum et al., 2014), Kocadağlı et al. (2012) showed that there is a linear increase in lipid oxidation products as the roasting progresses.

Most research on green coffee has focused on their antioxidant capacity and phenolic content, especially in terms of chlorogenic acids (or caffeoylquinic acid derivatives, CQA), which confers a sweet and oily odor to green beans. Green coffee is the main source of CQA in nature (5–12 g/100 g), and more than 30% of the ingested dose is observed in plasma around 0.5 to 8 h (as native compound or metabolites) after consumption of green coffee extract (Farah et al., 2008). According to Zhao et al. (2012), caffeic acid-3-*O*-sulfate, di-hydroferulic acid-4-*O*-sulfate, and di-hydrocaffeic acid-3-*O*-sulfate are the main metabolites of CQA in blood circulation. These compounds have been associated with several health benefits, mostly related to their antioxidant activity (Tajik et al., 2017; Zhao et al., 2012). Therefore, due to their protective effect against DNA damage and LDL-cholesterol oxidation (Bakuradze et al., 2015; Natella et al., 2007), phenolics from coffee may prevent certain types of cancer and decrease the risk of heart disease.

Green coffee beans also have approximately 5% (w/w) total inorganic element content, including potassium (mean 6714.5 µg/g), magnesium (1373.9 µg/g), calcium (560.2 µg/g), phosphorus (559.1 µg/g), aluminum (25.9 µg/g), and copper (12.1 µg/g). It was also noted that preparation of green coffee by the Turkish method was more effective on leaching the elements in comparison to mud coffee (Şemen et al., 2017). In another study, Stelmach et al. (2015) showed that the leachability of calcium and magnesium is higher for green coffee infusions than those prepared with roasted beans possibly due to a stronger binding of these elements to certain compounds formed during roasting.

Roasting of coffee beans occurs at temperatures of 180–250 °C for up to 25 min, depending on the desired characteristics of the final product. During this process, the beans go through several physicochemical changes that can have an impact on its chemical composition and bioactive properties. For instance, a considerable amount of phenolic antioxidants found in green beans is thermally degraded or converted during roasting; however, Maillard reaction results on the formation of certain compounds (e.g., melanoidins) that also exhibit antioxidant activity (Liu and Kitts, 2011). In certain cases, roasting could enhance the antimutagenic activity of coffee (Priftis et al., 2018). Unlike phenolic compounds, caffeine is thermostable, and no significant changes on its concentration during roasting are observed (Vignoli et al., 2014).

In relation to flavor and aroma, more than 1,000 volatile compounds have been identified to date, some of which have biological properties and are responsible for coffee's sensory characteristics. For instance, beans produced from immature cherries or Robusta coffee are often qualified as being of lower sensory quality in parts due to the high levels of phenols, N-heterocyclic compounds (e.g., pyrazines) that confer "earthy" notes, and low amounts of carbohydrate degradation products associated with "sweet" and "caramel" notes (Velásquez et al., 2019).

2.2. Bioactive compounds in coffee brew

Different methods (including variations on coffee/water proportion, grind size, water temperature, pressure, and extraction time) are used for the preparation of coffee beverages. Similar to roasting, they have a significant impact on the physicochemical properties and bioactive compounds extracted from the beans. Rao and Fuller (2018) compared the acidity, antioxidant activity, and concentration of CQA isomers in light roast coffee prepared by hot and cold brew methods. The main difference observed was the higher antioxidant activity of hot brews, possibly due to higher efficiency in extracting non-deprotonated acids than the cold method. In relation to caffeine content, Fuller and Rao (2017) found that its concentration was significantly higher in cold brew prepared with coarse coffee grind (medium and dark roast) than by hot extraction, as the cold extraction occurs for prolonged periods of time.

In another study, Niseteo et al. (2012) evaluated coffee brews prepared by espresso, Turkish/Greek, instant, and filter methods. Overall, instant coffee had the highest total phenolic and flavonoid contents measured as gallic acid equivalents (GAE) (17,307 mg GAE/L and 8,460 mg GAE/L, respectively), whereas the lowest concentration was found in filtered brew (2,967 mg GAE/L and 1,633 mg GAE/L, respectively). These results are in agreement with the antioxidant activity. Niseteo et al. (2012) also investigated the addition of milk to the brews and noted that it decreased the total phenolic content, as a potential result of protein-phenolic interaction. Another factor that Niseteo et al. (2012) investigated was the reheating of Turkish/Greek coffee to a boiling state, which resulted in significant increase of CGA (amount depended on the compound) and caffeine (from 1,942.4 to 2,551.6 mg/L) in comparison to the sample before heat treatment.

Angeloni et al. (2019) also compared different preparation methods, namely Espresso, Moka, French press, and three filter coffee (cold brew, V60, and Aeropress). Coffee brews prepared by the Espresso method had the highest content of caffeine and CGA than Moka and filtered coffees. These authors reported the results in three ways/units: concentration (mg/mL), extraction efficiency (mg/g ground coffee), and content per cup (mg/cup). In relation to caffeine concentration, the highest content was found for samples prepared by the Espresso method (average 4.1 mg/mL), whereas the lowest was obtained with Aeropress (0.78 mg/mL). Espresso samples also presented the highest concentration of CGA (0.2 mg/mL). In terms of extraction efficiency, Espresso coffee had significantly higher concentration of caffeine (17.4 mg/g) and CGA (0.77 mg/g). The content per cup assumes a standard volume established by the authors based on the usual consumption of a given brew. In this case, a 120-mL cup of cold brew coffee had 149.5 mg of caffeine, whereas a 30-mL cup of espresso had 122.4 mg.

These are some examples of reports in the literature that demonstrate the complexity in determining the composition or establishing a method to prepare a cup of coffee. Despite this, studies have demonstrated that the consumption of coffee brew or extracts have positive effects on health. For instance, an animal study carried out by Abreu et al. (2011) showed that the intake of coffee or caffeine for 80 days (20 or 40 mg caffeine/kg/day) improved long-term memory, reduced lipid peroxidation of brain membranes, and increased the concentration of reduced-glutathione.

2.3. Functional value of spent coffee ground

Although brewing methods are efficient in extracting most of the caffeine and CGA from coffee beans, certain compounds are not easily extracted and are discarded as spent grounds. Therefore, similar to other agro-industrial waste (de Camargo et al., 2018; Shahidi et al., 2019), spent coffee could be a valuable source of bioactive compounds. Bravo et al. (2013) investigated different processing conditions on the extraction of bioactive compounds from spent coffee, including different solvent systems, number of extraction cycles, pH, etc. The authors found that extraction with water at neutral pH using a coffee machine at a ratio of 24 g of spent coffee to 400 mL of liquid resulted in the highest antioxidant activity, indicating that this product can still be a source of bioactive compounds (Bravo et al., 2013). Spent coffee obtained from coffee shop have approximately 17.7 mg GAE/g, whereas samples from capsules/pods have around 21.6 mg GAE/g (Zuorro and Lavecchia, 2012).

The production of soluble (or instant) coffee is another process that generates a considerable amount of spent grounds, which can retain approximately 70% of the polysaccharides found in the beans. This is because most of the galactomannans and arabinogalactans present in the coffee are not extracted during various stages of coffee production (roasting and brewing) and remain bound to the spent ground matrix (Campos-Vega et al., 2015). Using an alkali pretreatment, Ballesteros et al. (2015) identified the saccharide moieties present in the spent coffee, as follows: 60.3% mol galactose, 19.9% mol arabinose, 15.4% mol glucose, and 4.4% mol mannose. Overall, the polysaccharides were thermostable, and the extract prepared from spent ground presented antioxidant activity assessed by different methods and high antimicrobial activity against fungi *Phoma violacea* and *Cladosporium cladosporioides* (Ballesteros et al., 2015). Spent ground also contains proteins (average 13.6%), melanoidins (16%), lipids (up to 20%), and minerals (1.6%) (Campos-Vega et al., 2015). The quantities vary depending on the coffee origin, roasting level, brew method, and extraction method used for characterization.

3. Conclusion

Coffee is one of the most important sources of bioactive compounds in modern diet, and its demand continues to grow. Caffeine is the most known bioactive compound from coffee and has been associated with several health benefits beyond energy and performance. Another important class of compounds is chlorogenic acids. Although changes occur during processing of green beans, roasted coffee still contains relevant amounts of CGA. Several reports have been published over the years with conflicting effects of coffee consumption on human health; however, recent studies have highlighted the benefits of moderate consumption (below six cups). This review also showed spent coffee ground can be used for the extraction of value-added compounds which would be otherwise discarded or composted.

Conflict of interest

There are no conflicts to declare.

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