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Coffee Roasting Chemistry: Chlorogenic Acids

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Chlorogenic Acids: Chemistry & Reality

Coffee roasters and coffee-minded chemistry aficionados, myself included, often speak of chlorogenic acids (also known as caffeoylquinic acids or "CQAs") in coffee. There may be hundreds of scientific studies published on these important constituents of coffee. However, what do we really know about them, in terms of their importance to and impact on our cups? Recently, I realized I myself didn't know much about them, and went in search of more information. In the course of researching the chemistry of coffee roasting, some interesting points have emerged about these compounds, their chemistry, and the "buzz" (please excuse the pun) around them.

What are they?

Many plants besides coffee contain chlorogenic acids. Acids in the chlorogenic group have very similar structures, and make up a family of esters often including caffeic acid and quinic acids as components (Michael N. Clifford, 1999). All of the chlorogenic acids fall into the larger category of phenolic acids (Flament, 2002). In nature, phenolic acids are often used as defense compounds by plants, or a signaling mechanism between plants and soil microbes (Mandal, Chakraborty, & Dey, 2010). They make up four-to-nine percent of green arabica coffee (on a dry-weight basis) and this makes them the most abundant of all acids in coffee (Belitz, Grosch, & Schieberle, 2004; Feldman, Ryder, & Kung, 1969; Jansen, 2006).

Often, you see them referred to by their isomers (individual chemical structure) in abbreviated form, such as 3-CQA instead of 3-caffeoylqunic acid. The most common chlorogenic acid is 5-0-caffeoylquinic acid (5-CQA), which is the one commercially available, and is often used as a placeholder for the larger family of acids (Michael N. Clifford, 2000). We in the coffee industry don't have to worry about the specific chemistry of these molecules, but can lump them together in the larger category of CQAs. The amount in green *Coffea arabica* seeds varies due to genetics, environment, climate, and growing conditions (Hecimovic, Belscak-Cvitanovic, Horzic, & Komes, 2011). In fact, one study found that coffee genetics (species and variety) is the number-one determining factor for the amount of CQAs in roasted coffee (Hecimovic, Belscak-Cvitanovic, Horzic, & Komes, 2011).

Some research has connected the ratio of different CQAs present in green beans to the ripeness of cherries when picked (M. N. Clifford & Kazi, 1987; Menezes, 1994; Ohiopehai, Brumen, & Clifford, 1982). This work suggests that immature green beans have a different ratio of CQAs present, which affects the quality of the roasted coffee. However, there has not been enough follow-up to link this to coffee flavor.

Roasting Chemistry

Chlorogenic acids break down during roasting (Farah, de Paulis, Trugo, & Martin, 2005; Leloup, Louvrier, & Liardon, 1995; Moon, Yoo, & Shibamoto, 2009). Reports vary as to the extent to which they break down, depending on roast temperature and time. Losses of about 60 percent have been observed in medium roasts, and up to 100 percent breakdown in dark roasts (Michael N. Clifford, 1979; Trugo & Macrae, 1984). Other studies report that a “light” roast (230 & 250°C for 12 minutes) ranges from 45-54 percent CQA breakdown, depending on the country of origin and genetics (Moon, Yoo, & Shibamoto, 2009). See figure three below for an example of this from Moon and others, 2009. Perrone and others report that coffee roasted for only six minutes retains on average +/-47 percent of its chlorogenic acids, and they could still be found, primarily non-degraded (44 percent), in the brewed coffee (Perrone, Farah, & Donangelo, 2012).

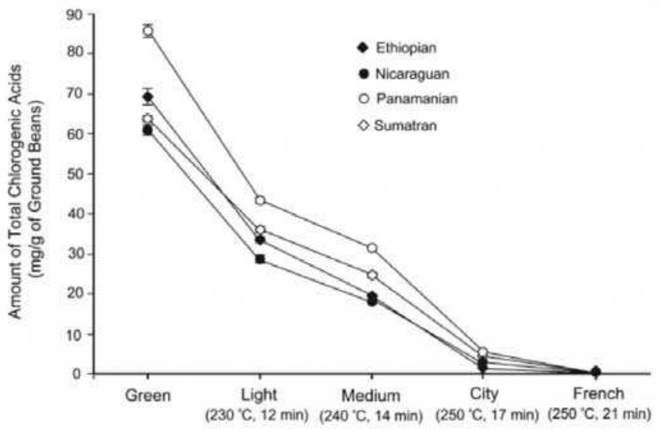

Figure 3. **Total chlorogenic acids found in various green coffee beans and in various roasted coffees treated under different conditions.**

Reprinted with permission from (Moon & Shibamoto). Copyright 2009 American Chemical Society.

Often during the roasting process, as part of the dissolution of these molecules, caffeic and quinic acid components of CQAs split off. Thus, the actual effect of CQAs on the taste of coffee might in fact be from the products of their breakdown. Quinic and caffeic acids are often formed as byproducts of different CQAs, which have been shown to further degrade into phenol and catechols, among almost 30 other chemical compounds (Farah, de Paulis, Trugo, & Martin, 2005; Moon & Shibamoto, 2010). In fact, these may turn into a degraded range of phenols, which participate in other as-yet unquantified reactions (Michael N. Clifford, 2000; Perrone, Farah, & Donangelo, 2012). Some of them will inevitably be transformed into volatile compounds and lost. Moon and others (2010) report about ten percent of the monitored CQAs are lost as volatile compounds. Other scientists have suggested that they react with Maillard-reaction products (Perrone, Farah, & Donangelo, 2012). This means that the breakdown of these CQAs could lead to a myriad of other reactions, which may or may not affect coffee flavor. We do know that eventually, at very high temperatures not often used in coffee roasting (above 482°F) the pyrolysis of chlorogenic acids will lead to char (Sharma, Fisher, & Hajaligol, 2002). Ultimately, the fate of most CQAs degraded during roasting is unknown.

Why do Chlorogenic Acids Matter?

Why we care about this group of molecules stems from much research around the topic of human health and coffee. Coffee is what the medical community calls a "bioactive" substance. This means that it has some sort of biological effect on the human body. Chlorogenic acids, like all polyphenols, are known to be biological antioxidants. The antioxidant effect of coffee is still being researched, but chlorogenic acids and other polyphenols are widely known to be capable of counteracting the damaging effects of excess oxidation in

the human body (Hečimović, Belščak-Cvitanović, Horžić, & Komes, 2011). Research has connected the consumption of these acids in coffee with the slowing of glucose absorption in the human gut, which has potential health implications (Johnston, Clifford, & Morgan, 2003). Most of the scientific research on the topic, in fact, has been focused on understanding the breakdown of CQAs during roasting, due to the interest in potential health benefits. Scientists would like to be able to one day maximize the amount of CQAs in brewed coffee in order to reap potential health benefits. Most of the dozens of studies reviewed for this article had this health-centric focus, perhaps because the most prevalent funding for coffee research is in the medical field.

Do Chlorogenic Acids Affect Coffee Flavor?

There is no consensus in the literature as to the specific impact of CQAs on coffee brew or flavor. A study by Tfouni and others found that brewing method did not impact the amount of CQAs present in the beverage, and that roast level had the strongest relationship with CQA content in brewed coffee (Tfouni, Carreiro, Teles, Furlani, Cipolli, & Camargo, 2014). There is not a lot of evidence as to how chlorogenic acids affect the flavor of coffee. As the SCAA coffee scientist, I was thoroughly disappointed in this research revelation! With all the information available about how CQAs are present in green coffee and broken down during roast, I had honestly expected evidence among it that they affect coffee flavor. It is true that multiple studies have suggested a certain (tasteable) level of CQAs would result in a bitter, astringent, or metallic taste (Farah, Monteiro, Calado, Franca, & Trugo, 2006; Ohiopehai, Brumen, & Clifford, 1982; Variyar, Ahmad, Bhat, Niyas, & Sharma, 2003). However, the evidence presented, in the previously referenced paper by Ohiokpehai (which has been cited many times so far), is anything but conclusive: merely noting "an easily-detected and peculiar lingering metallic taste that can influence the acceptability of coffee brew." These authors have simply reported a non-tested observation in the above statement and paper, and therefore this reference is not adequate upon which to base our assertion that CQAs affect coffee flavor.

So, why do we care so much about these chlorogenic acids? Perhaps the breakdown of chlorogenic acids is very important to the flavor of coffee after all, but research has not yet fully connected these dots. On the other hand, maybe we should be satisfied with the evidence that CQAs may contribute to the potential health benefits of enjoying coffee. The truth is, it is almost impossible to track individual molecules and all of the reactions they participate in during (and after) the roasting process. Like many groups of compounds present in coffee, they are prevalent but fleeting, participating in a myriad of chemical reactions and contributing to the magic combination of chemistry that we know as our favorite beverage. Perhaps it is the mystery of it all that keeps us searching, and perhaps it is that chase that fuels our passion.

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One Response to *Coffee Roasting Chemistry: Chlorogenic Acids*

Mr Nick Jesch *says:*
September 10, 2014 at 5:59 am

This was helpful. I've identified some of the flavours she attributes to the cQA's, particularly when roasted very lightly, and wondered if that was not the result of high levels of chlorogenic acids after roasting. This information seems to confirm this. NOW: the operant question arises: how to assure the roast is sufficient to reduce these acids to the level that allows the sweetness and full flavour to end up in the cup, and without the disagreeable tastes associated with these acids. Roasting to different profiles and cupping is the only way, I suppose.

It was also interesting to note the varying levels in different origins. Any work on the differences being related to varietals?

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