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A Meta-Analysis of Acids in Coffee and a Quantification of Coffee Beverage Color

By

SARA ELIZABETH YEAGER

THESIS

Submitted in partial satisfaction of the requirements for the degree of

MASTER OF SCIENCE

in

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in the

OFFICE OF GRADUATE STUDIES

of the

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DAVIS

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2021

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Obtaining a Master's in Food Science and Technology is a goal of mine that has been in the making since my sophomore year of high school. I have been very blessed to know exactly what I wanted to do when I "grew up", but I fully acknowledge that it could not have been possible without a few key players in my life.

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A Meta-Analysis of Acids in Coffee and a Quantification of Coffee Beverage Color

Abstract

During coffee consumption, acidity and coffee color serve as two facets of quality. The acidity within a cup of coffee must be balanced; the beverage must be "bright", but also not too sour. The key to perfect levels of acidity is to understand not only how different acids can impact the overall sensory quality of the cup, but how the acid concentrations themselves are subject to variation over coffee types and roast levels. The first goal of this research was to elucidate the general trends of acid concentrations in coffee, across all available scientific literature, including multiple coffee types and roast levels. A meta-analysis of 121 publications yielded 7,509 distinct acid concentrations, a wealth of data to serve as a necessary reference for future research pertaining to acid concentration in coffee.

In particular, the acid concentration of cold brew coffee has been an area of great interest brought about by the rise in popularity of cold-brewed coffee beverages. Major coffee retailers purport that cold brew is smoother, sweeter, and more full-bodied than hot coffee; many also believe that cold brew is less acidic and more friendly to the gastro-intestinal tract. In preparation to investigate acid concentrations, we brewed the same coffee across a wide range of temperatures and were met with a stark observation: different brew temperatures resulted in different colored coffee. Thus, the second goal of this research was to explore how roast level and brew temperature affect the color of brewed coffee through a colorimetric analysis of brews prepared across three origins, three roast levels, and three brew temperatures. We find that roast level had the strongest impact on brew color, and that brew temperature had a significant impact on color for light and medium roasts, with less impact on dark roasts.

Qualitatively, the cold brewed coffees tended to be redder, while the hot brewed coffees were blacker. These results suggest that the color of coffee brews might play some role in their perceived sensory qualities and that there is an opportunity to manipulate and brand brewed coffee color through judicious choices of roast level and brewing temperature.

1. Introduction

Within the last five years, cold brew coffee has exploded in popularity. More than half of new ready-to-drink (RTD) product launches in 2017 were a cold brew coffee product (Mintel.com). The National Coffee Association reports that between 2015 and 2017, cold-brewed RTD products retail sales increased by 460%, accounting for over $38 million dollars in sales in 2017 alone (NCA 2018). Increase in sales is further supported by well-known coffee companies crafting their own cold-brew products. Starbucks, which had been creating cold brew products since 2016, claims that their cold brew is "crafted in small batches and slow-steeped for a naturally sweet, smooth flavor" (Starbucks 2016). Dunkin' also markets their cold brew coffee as sweeter, smoother, and more full-bodied than traditionally brewed coffee (Dunkin' n.d.) Moreover, there are many who anecdotally claim that cold brew is less acidic and much easier on the gastrointestinal tract than hot brewed coffee (Brown 2018).

Naturally, the rise in consumption of cold-brew coffee has led to scientific research to investigate the claims in a systematic manner. Notably, Rao and colleagues compared the acidity cold-brew immersion-style coffee to a hot French Press-style coffee across six different types of coffee (Fuller & Rao, 2017). While their research showed that the cold brew had a higher pH and lower titratable acidity than hot brew across the six coffees, it was interpreted by the coffee industry media as there not being a difference. Fuller herself was quoted as saying "I think it's a marketing ploy. Somebody was saying 'It's less acidic! Try cold brew coffee!'… at least by pH measure, there's really no difference, at least in the six coffees we tested" (Betuel

2018). The mismatch of information led to confusion in the coffee industry as to where cold brew truly differed from hot brew in terms of acidity.

While some pioneering research has focused on cold brew coffee, (Ahmed et al. 2019; Angeloni et al. 2019a; Angeloni et al. 2019b; Cordoba et al. 2020; Fuller & Rao 2017; Rao, Fuller, & Grim 2020) many gaps remain in the research. Differences in acidity and individual acid concentrations remains an area of great interest due to the claims about cold brew being less acidic. In addition, the physical appearance of the cold brew itself in comparison to hot brew coffee has not been discussed. Because of the effect color can have on perceived sensory characteristics, it is critical to examine how coffee beverage color can be changed by not only roast level, but brew temperature as well.

This thesis aims to fill in gaps of missing literature by focusing on the differences between cold brew coffee and traditionally brewed coffee. First, Chapter 2 provides a detailed review of sensory measurements and a meta-analysis of the chemical composition of coffee. The data in Chapter 2 serves as necessary background information and a future reference for any research concerning acid concentrations in cold brewed coffee. Chapter 3 then investigates in detail the effect of roast level and brew temperature on the color of the coffee beverage, revealing that some brewing parameters can have some unexpected consequences on the color of the beverage. Together the results presented here shed new light on cold brew coffee.

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2. Acids in Coffee: A Review of Sensory Measurements and Meta-Analysis of Chemical Composition

 Abstract

Coffee contains a variety of organic acids (OAs) and chlorogenic acids (CGAs) that contribute to overall sensory properties like sourness and bitterness. Although much work has characterized particular acid concentrations in various types of coffee, large variations in preparation and measurement methodology complicate interpretation of general trends. Here, we perform a systematic review and meta-analysis of the published literature to elucidate the concentrations of OAs and CGAs in both *Coffea arabica* (arabica) and *Coffea canephora* (robusta), for both green coffee and roasted coffee at multiple roast levels. A total of 121 publications were found to report acid concentration measurements for at least one of 26 different OAs or 23 different CGAs, yielding 7,509 distinct data points. Analysis of the full data set reveals several trends. First, the data indicate that four specific OAs – citric, quinic, malic, and acetic – comprise more than 88% of the total mass fraction of OAs present in roasted arabica coffee. Notably, roasted robusta is much more acidic than arabica with 2 to 5 times as much total OAs, similar amounts of citric, quinic, and malic acid, but larger amounts of formic and acetic acid. As for CGAs, in both arabica and robusta 5-CQA is the major component, and higher roast levels tended to sharply decrease the concentration of all CGAs. The total amount of CGA present was more dependent on roast level than the type of coffee (arabica vs. robusta). Overall, this meta-analysis suggests that the increases in certain OAs with roast level, especially acetic acid, might play more of a role in the sensory profile of dark roast coffees than previously suspected.

2.1 Introduction – Acids in Coffee

Like any other biological material, coffee beans have a complicated chemical composition that includes mixtures of various carbohydrates, lipids, acids, minerals, and proteins, plus other nitrogen-containing compounds like caffeine and trigonelline (Balzer 2008; Poisson 2017). The precise quantities of each depend on the species of coffee and how the coffee was roasted. Generally speaking, green (unroasted) arabica coffee on a dry-weight basis is approximately 50-60% carbohydrates (5-9% of which is sucrose), 15-20% lipids, 10-15% proteins, 3-5% minerals, and 1% caffeine (Trugo 1985; Smith 1985). Robusta coffee (*Coffea canephora*) has a similar breakdown albeit with less carbohydrates and more caffeine.

From a sensory perspective, acids are arguably one of the most important components in coffee. They comprise a large fraction of the total mass, as much as 11% of the green and 6% of the roasted beans. The absolute and relative amounts of specific acids present in the roasted beans strongly affect the final cup quality (Maier 1987; Galli and Barbas 2004). It is widely recognized that acidity and the resulting perceived sourness are key to coffee quality. As well as imparting taste and flavor themselves, acids are generally recognized as flavor precursors for quality descriptors of coffee (Borém et al., 2016). Perceived acidity is one of the main categories that coffee industry professionals use to score coffee quality, and hedonic testing has shown sourness to be a major driver of consumer liking (Cotter et al. 2020, Frost et al. 2019). Seemingly small changes to the pH and titratable acidity of the brew affect the flavor profile and influence consumer liking (Batali et al. 2021).

Acids in coffee are generally divided into two categories: organic acids (OAs) and chlorogenic acids (CGAs). Thirty-eight organic acids have been previously identified and

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quantified in roasted coffees, with citric, malic, and quinic acids as the most prominent in green

coffee (Balzer, 2008; Maier 1999; Poisson 2017). In roasted coffee, an increase in overall acidity

compared to green is attributed to an increase of formic, acetic, glycolic, and lactic acids that

are formed while roasting (Ginz 2000). Sucrose serves as the main precursor to these acids,

meaning a difference in the amount of sucrose in the green coffee will ultimately contribute to

different final amounts of acid (Ginz 2000). Moreover, citric and malic acid, already present in

green coffee, can serve as precursors to other acid breakdown products, such as citraconic,

glutaric, fumaric, and maleic acids (Bahre and Maier 1999). Increasing the amount of any acid

will lower the pH and increase the titratable acidity (Engelhardt and Maier 1985a).

Coffee also contains CGAs, which are naturally occurring bioactive compounds that

accumulate in the bean as the coffee fruit matures (Clifford and Kazi 1987). CGAs are composed

of a variety of different quinic acid esters or series of esters (Clifford 1985); representative

examples of CGA structures are shown in Figure 1. The CGA complex can then be further

divided into subgroups, which contain about three isomers each, based on the number and

composition of the acylating residues. These subgroups include caffeoylquinic acids (CQA),

dicaffeyloquinic acids (diCQA), and feruloylquinic acids (FQA) (Clifford 1985). Within each

subgroup, each isomer is usually labelled with the position of esterification on the quinic acid

ring, such as 4-o-CQA (4-CQA). As CGAs are considered phenolic compounds, they have been

extensively studied in green, roasted, and soluble coffee (Lopez-Gallilea et al. 2007; Vignoil et

al. 2011; Ludwig et al. 2012; Herawati et al. 2019; Rao et al. 2020).
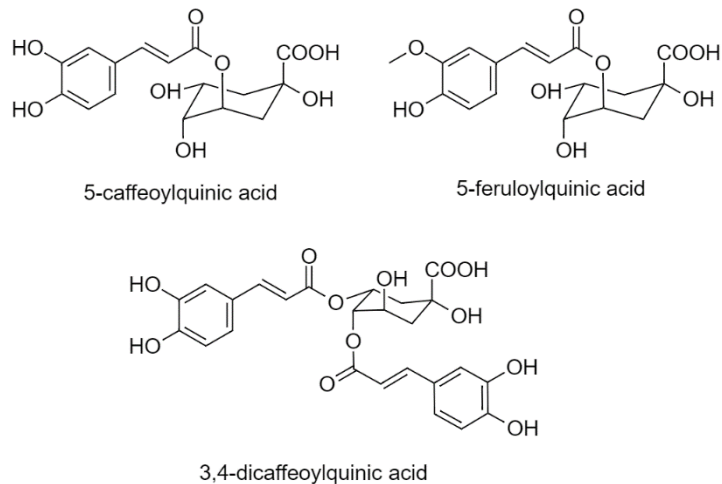
Figure 2.1: Chemical structure of 5-caffeoylquinic acid, 5-feruloylquinic acid, and 3,4-dicaffeoylquinic acid.

Given the prominence of acids in coffee, there are two fundamental questions to ask: how does each acid affect the final sensory profile, and how much of each type of acid is present in the coffee beans? Unfortunately, these questions are easy to ask but difficult to answer in a comprehensive manner. Assessing the sensory impact of individual acids in a complex food matrix like coffee is non-trivial; moreover, the published scientific literature on coffee documents the amounts of acids present in many disparate ways, across multiple coffee species, roast levels, extraction methods, and analytical techniques. As such, research on acids in coffee remains very disjointed – general trends about how acid levels vary in coffee remain unclear and unresolved. To date the most comprehensive attempt to synthesize research on coffee acids was presented by Balzer in 2008, who updated earlier work by Woodman in 1985. Balzer's work summarized individual results from contemporary publications that described changes in acid composition during roasting and consequent impact on sensory characteristics. To date, however, no work has attempted to synthesize general trends in the impact and concentration of individual acids from published work in various disciplines.

The main goal of this article is to present an exhaustive review and meta-analysis of the

scientific literature aimed at identifying the acid compositions of arabica and robusta coffee, for

both green and roasted coffee, to provide insight on the resulting sensory profiles. More than

7,000 distinct acid concentration data points from 121 separate publications were compiled

into a single database, with the roast level for each qualitatively denoted as light, medium, or

dark. The figures presented here, as well as the raw data in the associated database included

as supplemental data, provide an updated, complete resource that documents acid levels in

coffee across a variety of sample types, and is intended to serve as a guide and reference for

future coffee research.

The remainder of this article is organized as follows. In section 2 we begin with a

detailed review of the extant literature on sensory measurements of particular acids in coffee.

In section 3 we describe the methodology for a meta-analysis of the literature for acid

concentrations in coffee, and in section 4 we present the results of that analysis. Section 5

concludes with a discussion of the implications of the meta-analysis and unanswered questions

regarding the role of acids in coffee.

2.2 Coffee Acids and Sensory Quality

2.2.1 Overall Sensory Impressions of Individual Coffee Acids

Beyond just contributing to sourness, individual acids have different inherent sensory

properties. Citric, acetic, formic, malic, quinic, pyruvic, succinic, fumaric, tartaric, and lactic acid

are all sour tasting acids, but some have other aroma qualities such as the characteristic vinegar

aroma of acetic acid, the burnt caramel flavor in pyruvic acid, or the pungent and fermented

aroma in formic acid (The Good Scents Company Information System n.d.; Hartwig and McDaniel 1995; Rubico and McDaniel 1995). In addition to sour taste, many acids such as formic, quinic, succinic, and caffeic also have a perceptibly bitter taste (Frank et al. 2007; The Good Scents Company Information System n.d.; Rubico and McDaniel 1995) Organic acids like quinic and lactic acid also contribute to the mouthfeel and chemesthetic sensation of astringency (Hartwig and McDaniel 1995; Neta, Johanningsmeier, McFeeters 2007; Rubico and McDaniel 1995). Finally, organic acids can be of further benefit to sensory quality by serving as flavor enhancers, a property of fumaric, tartaric, and oxalic acid (The Good Scents Company Information System n.d.; Neta, Johanningsmeier, McFeeters 2007). An overview of all these organic acids and their sensory properties can be found in Table 1.

Table 2.1: Reported sensory properties of organic acids found in coffee.

Acid	Reported Sensory Properties
Citric	Sour, odorless (The Good Scents Company Information System n.d.; Hartwig and McDaniel 1995)
Acetic	Sour (higher intensity than others), salty, vinegar aroma (Hartwig and McDaniel, 1995)
Formic	Sour and bitter taste, Chemical, pungent, fermented aroma (The Good Scents Company Information System n.d.)
Malic	Sour, odorless (The Good Scents Company Information System n.d.; Hartwig and McDaniel 1995)
Quinic	Sour, bitter, astringent but overall lower intensity (Rubico and McDaniel, 1992)
Pyruvic	Sour, vinegar, burnt caramel (The Good Scents Company Information System n.d.)
Succinic	Sour, bitter, odorless (The Good Scents Company Information System n.d.; Rubico and McDaniel 1992)
Oxalic	Bland, caramel, mild, some results suggest it is a flavor enhancer (The Good Scents Company Information System n.d.; Holm, Aston, and Douglas, 1993)
Fumaric	Sour, odorless alone, enhances fruit flavors (The Good Scents Company Information System n.d.; Neta, Johanningsmeier, and McFeeters 2007)
Tartaric	Sour, odorless alone, enhances fruit flavors (The Good Scents Company Information System n.d.; Neta, Johanningsmeier, and McFeeters 2007)
Lactic	Sour, astringent, acrid (Hartwig and McDaniel, 1995, Neta, Johanningsmeier, and McFeeters 2007
Glycolic	Mild buttery aroma (The Good Scents Company Information System n.d.)
Caffeic	Intensely bitter (Frank et al, 2007)

Unlike organic acids, the organoleptic properties of CGAs have been the subject of relatively few studies. Among the limited observations of sensory properties of pure CGAs, 5-caffeoylquinic acid has been characterized as minimally acidic compared to free quinic acid, with a small amount of bitterness, and di-CQA mixtures increase in bitter intensity and have a

metallic taste and astringent quality (Clarke and Macrae 1985; Ohiokpehai n.d.; Upadhyay and Mohan Rao 2013). Similar to several of the organic acids, there is some evidence that 5-CQA can contribute to flavor enhancement, specifically through a mechanism of enhanced volatile flavor solubility (King and Solms 1981). The limited characterization of pure CGAs, as opposed to CGAs in coffee, makes it challenging to draw conclusions about the sensory impact of CGAs without confounding factors.

2.2.2 Effect of Acid Concentrations in Green Coffee on Sensory Quality of Roasted Coffee

Organic acids naturally occur in green coffee as a part of the fruit, so initial acid content can be a marker for quality based on known mechanisms for acid degradation and formation during roasting. Acetic, formic, lactic, and glycolic acid tend to form during roasting from carbohydrates in green coffee, and citric and malic acid degrade into succinic, fumaric, maleic, and others (Balzer 2008). Chlorogenic acids form chlorogenic acid lactones during roasting, which impart bitterness (Frank et al. 2007). Based on this knowledge, a handful of chemosensory studies have investigated acids in green coffee as a predictor for sensory quality.

Green coffee acidity has been a focal point of microbiological studies examining the difference between fermentations, either comparing natural diversity or inoculation. Evangelista et al. used a "temporal dominance of sensation" approach and found that higher lactic, malic, and citric acid in green coffee contributed to more citric and herbaceous perceptions upon roasting, whereas lower acid green coffee samples were perceived as nuttier upon roasting, though there was no overall difference in cupping scores of the roasted coffees (Evangelista et al. 2015). Another study by Ribeiro et al. showed that differences in the

microbiome of spontaneous fermentation did impact flavor as well as cupping scores, with a varietal higher in citric acid scoring higher overall in cupping scores (Ribeiro et al. 2018). As indicated by flavor differences associated with natural microbiological diversity, microbial inoculation has also been shown to contribute to differences in quality. Inoculation with lactic acid bacteria during fermentation increased lactic, citric, acetic, fumaric, and malic acid, which lead to an increase in cupping score and higher perception of fruity, pineapple, and banana flavors (Pereira et al. 2016). Yeast (Saccharomyces Cerevisiae) inoculation during dry processing also increased cupping score with an increase in citric acid (Ribeiro et al 2017).

Chlorogenic acids in green coffee have been studied even more extensively for their role as precursors to the sensory quality of roasted coffee. Foundational work by Farah et al. showed higher concentrations of 5-CQA and FQA in coffees that received poor cupping scores after roasting, particularly with "Rio" off flavor that is often described as musty or medicinal (Farah et al. 2006). However, more recent publications have cast doubt on this interpretation. Some results align with Farah et al., showing that coffees grown at lower altitude have higher overall chlorogenic acids in green coffee and lower cupping scores in roasted coffee (Martins et al. 2020); but other experiments show opposing results of higher chlorogenic acids at higher growing altitudes and a subsequent improved cup score and floral flavor (Worku et al. 2018). In green robusta coffee, FCQA, diCQA, FQA, CQA, ferulic, and caffeic acid were all associated with positive cup quality, and only quinic acid was associated with lower scores (Lemos et al. 2020). With green *Coffea arabica*, one study showed 3,4-diCQA was associated with sweetness and full body while 3,5-diCQA was associated with astringency and immature bean taste (Maria et al. 2020), whereas another study found that concentrations of 3,5-diCQA (along with 5-CQA and

4,5-diCQA) were positively associated with cup quality scores (dos Santos Scholz et al. 2018). Other work found that 5-CQA in stored green coffee was also potentially responsible for sensory perception of coffee freshness (Rendón et al. 2014).

These disparate results indicate that there remains much to be determined about correlations between acid concentrations in green coffee and the resulting sensory qualities. As mentioned previously, the lack of literature on the sensory properties of pure CGAs makes it difficult to draw causal conclusions from reported correlations between concentrations of CGA and sensory quality. Understanding markers of quality in green coffee is of interest to farmers and green buyers, but ultimately there will be a substantial amount of variation from changes during roasting and extraction in brewing.

2.2.3 Correlations between Acid Concentrations and Sensory Quality of Roasted and Brewed Coffee

Because of all of the complex chemical reactions that occur during roasting, a more direct approach is to search for correlations between the chemical composition of the roasted and brewed coffee with the perceived sensory qualities. When looking at the pH and titratable acidity of roasted coffee, some studies showed that an increase in acidity was correlated with an increased perceptible sourness but decreased bitterness (Kim et al. 2018), whereas other studies indicate that a higher acidity is an indicator of higher overall flavor intensity, bitterness included (Cordoba et al. 2019; Voilley et al. 1981). Higher measured acidity (both lower pH and higher titratable acidity) was also associated with lower consumer liking, but when coffee was graded by experts the differences in pH did not necessarily result in difference in sourness (Rodriguez, Guzman, and Hernandez 2020; Manzocco and Lagazio 2009). Recent work by Batali

et al. has shown that titratable acidity correlates with perceived sourness in brewed coffee, but pH only varies meangingfully between coffess at different roast levels (Batali et al. 2021). In contrast, titratable acidity correlates with liking of acidity (Batali et al., 2021), and acidity liking is a major driver of difference between consumer cluster preferences of brewed coffee with some consumers reacting very positively and others negatively (Cotter et al. 2020).

The pH and titratable acidity reflect the totality of all acids present; assessing the impact of specific individual acids is more complicated. Acetic acid is a commonly observed acid in roasted coffee and is associated with more perceptible sourness, as well as rancidity, astringency, and bitterness (Pérez-Martínez et al. 2008a, 2008b; Xu et al. 2019). Acetic acid, as well as propanoic acid, correlate negatively with liking in ranked and paired preference tests of *Coffea canephora* (Kalschne 2020). Increases in acetic acid, as well as caffeic, citric, 5CQA, malic, nicotinic, and tartaric increase overall flavor intensity but not necessarily cupping score (Khamitova et al. 2020a). However, in other studies higher concentrations of acetic acid and 3-methylbutanoic acid were associated with enhanced flowery, fruity, bitter, spicy, and woody characteristics, some of which may be desirable in coffee (Liberto et al. 2019). Sittipod et al. examined the impact of more obscure OAs and found 3-O-caffeoyl-4-O-3-methylbutanoyl quinic acid improved cup quality by flavor modulation, with no flavor activity alone (Sittipod et al. 2019). This result is consistent with the general trend of acids serving as flavor modulators and enhancers, whether or not they have substantial flavor on their own (Hartwig and McDaniel 1995).

Chlorogenic acids were first reported in 1983 by Clifford and Ohiokpehai to contribute towards astringency in foods, specifically di-CQA has perceptible astringency at 0.05-0.1 mg/mL

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(Clifford and Ohiokpehai 1983). A study by Frank et al. on coffee bitterness explored 3-, 4-, and 5-CQA, and found that the acid derived lactones contributed more to the bitterness of coffee than the acid precursors (Frank et al. 2007). Other investigations found that 5-CQA concentration correlated with sourness, though that may have been due to the additional correlation of acetic acid (Pérez-Martínez et al. 2008a). A subsequent study by the same group investigating shelf life in refrigerated coffee beverages found that 5-CQA was associated with "pleasant acidity", replacing the initial "unpleasant sourness" as it broke down over time into caffeic and quinic acid (Pérez-Martínez et al. 2011). Several other studies, however, have reported a relationship between CGAs and bitterness, with Gloess et al. (2013) linking higher overall CGA concentration as measured by near infrared spectroscopy to higher bitterness and higher cupping score. Ribeiro et al. (2011) found that higher 3- and 5 – CQA concentrations correlated positively with both bitterness and astringency (Ribeiro et al. 2011).

These studies only examined CGAs, but it is important to note that other acids potentially could serve as a confounding factor for sensory impressions. For example, quinic acid has been shown to strongly correlate with bitterness, whereas CQAs strongly correlated with sourness (Wei et al. 2014), and these investigators speculate that the degradation of CQAs into quinic acid may actually be a cause of the reports of CQAs causing bitterness in coffee. Further evidence suggests that the type of coffee may also confound chemosensory studies. Comparisons between espresso made with washed arabica, natural process arabica, and robusta showed differing correlations between 5-CQA content and both acidity and bitterness for different coffee types, with 5-CQA highest in ramp-up temperature gradient espressos but bitterness and acidity dependent on type of coffee and processing method (Salamanca et al.

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2017). In other studies, different processing methods showed a high variation of chlorogenic acid content in coffees that were all then cupped with no difference in scores (Zanin et al. 2016).

Finally, there is contravening evidence suggesting that 5-CQA does not contribute as substantially to sensory quality. For example, enzymatic reduction of 98% of the 5-CQA present in brewed coffee did not significantly change the flavor (Sieber, Berger, and Nieter 2018). Hydrolyzing chlorogenic acid lactones into chlorogenic acids reduced bitterness attributed to lactones, but did not increase any other sensory attributes, but when 5-CQA was hydrolyzed to caffeic acid, the coffee was perceived as more sour, bitter, and burnt (Kraehenbuehl et al. 2017; Siebert, Detering, and Berger 2019). These observations suggest chlorogenic acids do not contribute much to coffee flavor, but that their derivatives do. There is still substantial room for targeted and systematic investigation of the contribution of chlorogenic acids to flavor, quality, and consumer liking in coffee.

2.3 Meta-Analysis Methodology

To obtain a more complete picture on the acid composition in coffee, we conducted an extensive review and meta-analysis of the scientific literature. Web of Science, Google Scholar, and the University of California Library catalog were searched between April to December 2020 for any publications that included data about the amounts of acid in coffee samples. This search focused explicitly on measurements of the concentration of individual CGAs and OAs in coffee, not the overall amount of acid in coffee (usually expressed as total titratable acidity). Access

was limited to online versions of publications due to COVID-19 restrictions during the time of the database search. Articles not available directly online were obtained through Interlibrary Loan requests. In the case of articles published in languages other than English, a translating website was used to read the article. Abstracts and full texts were examined for specific data about the absolute amounts of any chlorogenic or organic acids. Articles that only examined the presence, relative amounts, or formation pathways of CGAs or OAs were excluded. Papers that reported CGAs or OAs in units of mg/L without including the original mass of coffee used were excluded due to the fact that amounts in units of mg/L cannot be directly compared with amounts in units of mg/kg (comparing mass in wet basis versus mass in dry basis).

If the publication did contain specific amounts of CGAs or OAs that satisfied the preceding conditions, then all roast levels, extraction types, and coffee species were included, except for decaffeinated and instant coffee. The additional processing on decaffeinated and instant coffee complicates comparison with other coffees. If the publication listed data for store-bought samples, those were included as well. In some cases, roast level and coffee species were not specified, and these data points were categorized as "unspecified". For the purposes of this review, *Coffea arabica* will be referred to as "arabica" coffee and *Coffea canephora* cv. robusta will be referred to as "robusta" coffee.

A tremendous complicating factor is the roast level, which strongly affects acid concentrations but is very challenging to quantify precisely; subjective roast descriptions like "dark roast" have no universally accepted definition. For the purpose of the meta-analysis, we therefore performed a semi-qualitative classification of the reported roast levels into three categories – light, medium, or dark – using the following methodology.

The roast levels for specific data in publications was determined in one of four ways: (1) as the publication's self-described roast level; (2) from the publication's reported amount of water lost during roasting (11-13% = light, 14-16% = medium, 17-20% dark) or organic roast loss percentage (ORL%) (2-4% = light, 4.1-5.5% = medium, 5.6-7% = dark) (Perrone et al. 2008; Weers et al. 1995); (3) the publication's reported L*a*b* color values of the roasted beans where L* of 30, 25, and 20 correspond to light, medium, and dark, respectively (Chindapan, Soydok, and Devahastin 2019); or (4) as "unspecified" if the publication did not mention any of the above. If the publication provided finer demarcations of roast level (e.g., a "light roast" and a "very light" roast), then we grouped their samples as appropriate into just our three broad categories. Lastly, samples that were labelled simply as "roasted" without giving any indication to the degree of roast kept the label of "roasted" and were included when comparing roasted coffee as a whole (Correia, Leitao and Clifford 1995; Agnoletti et al. 2019). We emphasize that because roast level is very qualitative and methods of measuring roast level vary greatly, the roast level labels used in this paper are approximate, based on the information available in the cited publications.

Similarly, extraction of the acids for analysis varied widely among the different publications. If a chemical solvent such as methanol was used, the extraction type was labelled as "solvent"; soaking the coffee grounds in hot water was labelled as "immersion"; extraction types such as "French press" or "espresso" were explicitly mentioned in their respective publications and the labels were kept for data collection.

Lastly, all measurements were converted to mg/kg to simplify comparison. Accordingly, the units reported in the publications often had to be converted, e.g., data reported in units of

g/kg was multiplied by 1000 to match units of mg/kg. In cases, where publications reported concentration in terms of mmol/kg, the molecular weight of the specific acid was used to convert to mg/kg. Lastly, in articles that presented the data in units of mg/L and included the original brew recipe (grams of coffee and liters of water), the data was converted to units of mg/kg using the brew recipe, assuming full extraction from the dry coffee grounds.

Data for 23 different CGAs and 26 different OAs was collected and analyzed While thirty-eight OAs have been quantified in coffee (Maier 1999), many are present in trace amounts and not commonly reported. Those reported in fewer than 2 publications and with amounts less than 0.01/kg were not included, accounting for the difference in total OAs analyzed in this review.

In chlorogenic acids the widely reported acids are total CQA, 5-CQA, 4-CQA, 3-CQA, total diCQA, and total FQA. Some publications would report only total concentrations of one class ("Total diCQA") instead of quantifying each isomer, so three categories were created, "Total CQA", "Total FQA", and "Total di-CQA", to compare across publications (Anthony, Clifford, and Noirot 1993). Each of these categories includes the sum of each isomer in that class; for example, "Total CQA" is a sum of 5-CQA, 4-CQA, and 3-CQA. 27 unique CGAs have been identified in coffee (Clifford et al. 2003; Clifford 2006). The limited recurrences (fewer than 2 publications) of some species led to their exclusion from data collection.

Once the data had been collected, it was imported and analyzed to create box plots and column charts. In all box plots shown here, the bottom and top of the box represent the 25th and 75th percentiles, respectively, and the thick black line indicates the median; the whiskers

represent the highest and lowest values excluding outliers (calculated as 25th percentile -1.5 x interquartile range to 75th percentiles +1.5 x Interquartile range). Each box plot also indicates the respective samples size (denoted as n). For each category (arabica and robusta, OA and CGA), the top six acids in terms of numbers of individual data points were selected for detailed box plots presented here. We emphasize that all data is available in the supplementary database. Further statistical analyses of the OAs and CGAs were carried out using R version 4.0.2 (R Core Team 2020). Two-way ANOVA was used to determine the statistical significance of differences among coffee types and between green and roasted coffee and then differentiated into groups using Fischer's LSD test with package *agricolae.*

2.4 Meta-analysis Results
        The extensive literature search yielded 121 different publications that fit the required criteria. Tables 2.2 and 2.3 list the references included in this meta-analysis, as well as a short summary of each study's experimental design. Beginning with research first conducted in 1959 up through 2020, these publications include a total of 5,929 distinct acid concentration measurements and 7,509 data points for 23 CGAs and 26 OAs. There is a large imbalance in the number of studies performed on OAs versus CGAs: an overwhelming majority of the data comes from CGA analysis, with 6297 measurements (approximately 84% of the total) while the rest pertains to OA analysis, 1212 acid concentrations (16% of the total. When analyzing CGAs, 2683 (43% of total CGAs) of the concentration values came from arabica samples, while only about 1345 (21% of total CGAs) came from robusta. While organic acid research had closer to equal amounts of arabica (511 concentration values; 42% of total OAs) and robusta (363

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concentration values; 30% of total OAs), arabica samples again remained the most common.

Literature includes a wide variety of roasts, extraction types, origins, and other experimental

parameters. However, approximately 40% of both arabica and robusta data comes from green

coffee. Additionally, data is not evenly distributed among roasts, with the least data from light

and dark roasts for both CGAs and OAs. Lastly, there are many OAs for which there is very little

data. Across all literature searched, we found that only 14 OAs for Arabica and only 9 OAs for

robusta have more than 10 reported concentration values.

Table 2.2: List of references used in meta-analysis of chlorogenic acids by coffee type analyzed (arabica, robusta, Other, or Unspecified). A short description of each method of examining chlorogenic acid, analytical method used, total distinct measurements, number of unique samples, and number of samples for each type of coffee is included.

RP: Reverse phase; HPLC: High Performance Liquid Chromatography; DAD: Diode Array Detector; MWD/VWD: Multiple Wavelength Detector/Variable Wavelength Detector; SPE: Solid Phase Extraction; MS: Mass spectrometry; NIRS: Near-Infrared Reflectance Spectrometry; LC-Q-TOF-MS: Liquid Chromatography Quad Time of Flight Mass Spectrometry.

Coffee Type Analyzed	Reference	Examines amount of chlorogenic acids by:	Analytical Method Used	Total Distinct Measurements	Number of Unique Samples	Arabica	Robusta	Unspecified	Other
Arabica and Robusta	Agnoletti et al. (2019)	species (arabica and Conilon), green and roasted (unspecified roast level)	RP HPLC-DAD	58	58	34	24		
	Alonso-Salces et al. (2009)	species (arabica and robusta) from major growing regions (America, Africa, Asia, and Oceania)	RP HPLC-DAD	92	6	3	3		
	Andueza (2003b)	species (arabica and robusta), 50% torrefacto roast, and water temperature (88C, 92C, 96C, 98C)	RP HPLC-DAD	12	12	4	8		
	Andueza (2007)	species, water ratio (6.5g/40mL, 7.5/40mL, 8.5g/40mL), and 50% torrefacto roast	RP HPLC-DAD	9	9	3	6		
	Anthony, Clifford, and Noirot (1993)	species (arabica, robusta, and 23 other spontaneous cultivars) from three regions (central and west Africa, east Africa, and Madagascar)	RP HPLC-UV-Vis	189	68	18	2		48
	Bicho et al. (2011)	species (arabica and robusta) and roast level (light, medium, and dark)	RP HPLC-DAD	48	6	3	3		
	Bicho et al. (2013)	species (arabica and robusta)	RP HPLC-DAD	22	2	1	1		
	Budryn et al. (2009)	species (arabica and robusta), roast (green, light, medium, and dark), and brew method (filter, immersion, immersion under pressure, solvent, and solvent reflux)	RP HPLC-UV-Vis	400	40	20	20		
	Caprioli et al. (2013)	species (arabica and robusta) and espresso machine (Leva and Aurelia)	SPE-RP HPLC-DAD	16	4	2	2		
	Casal (2000)	species and roast (green, light, medium, dark, and very dark as determined by water loss during roasting)	RP HPLC-MWD	14	14	7	7		
	Clifford and Ramirez-Martinez (1991)	species (2 cultivars of arabica, Canephora, and 2 hybrids)and bean vs pulp	RP HPLC-UV-Vis	40	5	2	1		2
	Clifford and Kazi (1987)	species (arabica, robusta, and Liberica)	RP HPLC-UV-Vis	12	4	1	2		1
	Clifford and Wight (1976)	species (arabica from Santos and Sao Paulo and robusta from Ghana and Uganda)	Colorimetric (molybdate reagent at 370 nm and metaperiodate reagent at 423 nm)	24	12	6	6		
	Correia, Leitao and Clifford (1995)	species and origin (arabica from Angola, Amboim, Ambriz, Cazengo, Cabinda; robusta from Cameroon, Ivory Coast, Indonesia, and Zaire)	RP HPLC-UV-Vis	170	20	10	10		
	De Luca et al. (2018)	species and origin (Brazil, Colombia, Costa Rica, Ethiopia, Guatemala, Kenya, Mexico, Nicaragua, Peru, and Tanzania)	RP HPLC-DAD	24	24	12	12		
	Farah et al (2005)	species (2 cultivars of arabica and a robusta) and roast (green, light, medium, dark)	RP HPLC-UV-Vis	184	21	14	7		

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Study	Description	Method						
Food Chemistry (2009)	species (arabica and robusta) and roast level (green, light, medium, and dark)		14	14	10	4		
Gutiérrez Ortiz et al. (2019)	species (arabica, Canephora, Liberica and 7 wild species) and origin (Brazil, Colombia, Ethiopia, India, Yemen, Guatemala and Vietnam)	RP HPLC-DAD	54	26	9	2		15
Khamitova et al. (2020)	species (arabica and robusta), filter basket (standard, small, or unique design), particle size distribution, amount of coffee (12g or 14g), height of perforated disc and keeping either time or volume constant	RP HPLC-VWD	228	76	46	30		
Ky et al. (2001)	species (wild arabica and Canephora cultivars)	RP HPLC-DAD	36	9	3	3	3	
Ludwig (2014b)	species (arabica and unspecified), extraction type (espresso, cappuccino, and instant) and by roast (green, light, medium, dark)	RP HPLC-DAD	16	3			3	
Ludwig et al (2012)	species (arabica and robusta) and brew fraction	RP HPLC-UV-Vis	120	20	10	10		
Mau Tu et al. (2001)	species (arabica and robusta), 50% torrefacto roast	RP HPLC-DAD	3	3	2	1		
Moeenfard, Rocha, and Alves (2014)	species (arabica and robusta) and brew method (immersion, French, mocha, or filter)	RP HPLC-DAD	24	8	4	4		
Moreira et al. (2005)	species (arabica and robusta), and roast (light, medium, and dark)	RP HPLC-UV-Vis	53	8	5	3		
Perrone et al (2008)	species (2 arabica cultivars and 1 Canephora) and roast (greeen, light, medium, dark)	HPLC-MS; quantification with DAD	175	18	12	6		
Poisson et al. (2017)	species (Arabic and robusta)		4	4	2	2		
Purdon and McCamey (1987)	species (arabica and robusta), origin, flavor character, and roast (green and roasted)	RP HPLC-UV-Vis	48	16	10	6		
Salamanca et al. (2016)	species, post-harvest method (natural and washed) and brew temperature (88-93°C, 90°C, 93-88°C)	RP HPLC-UV-Vis	9	9	6	3		
Seruga and Tomac (2014)	species (arabica and robusta) and roast (green and roasted)	Square-wave voltammetry (SWV)	6	6	4	2		
Seruga and Tomac (2017)	species (arabica and robusta) and roast (green and roasted)	Flow-through Chronopotenti ometry (FTCP)	6	6	4	2		
Vignoli, Bassoli, and Benassi (2011)	species (arabica and robusta), roast (light, medium, dark), and extraction method (conventional and double extraction)	RP HPLC-UV-Vis	12	12	6	6		
Trugo, L. C., and Macrae, R. (1984) #1	species and roast (green, light, medium, dark)	RP HPLC-UV-Vis	67	10	5	5		
Angeloni et al. (2019) [#1]	brew method (drip and immersion), temperature (22°C and 5°C), and brew time (3.3h and 6.5h)	RP HPLC-DAD	64	8	8			
Angeloni et al. (2019) [#2}]	extraction (3 Espresso types, Moka, French Press, Cold Brew, Aeropress, and V60)	RP HPLC-DAD	64	8	8			
Avelino et al. (2005)	terrior (different areas in Central America)	NIRS	4	4	4			
Barbosa et al. (2019) [#2]	2012, 2013, and 2015 winners in Coffee Quality Parana` contest	NIRS	3	3	3			
Barbosa et al. (2019) [#1]	roast (green, medium, and dark) and extraction method (solvent and filter)	RP HPLC-UV-Vis	6	6	6			
Bekedam et al. (2008) [#2]	roast (green, light, medium, dark) and brew fraction	RP HPLC-UV-Vis	4	4	4			
Bekedam et al. (2008) [#1]	roast (green and medium) and brew fraction	RP HPLC-UV-Vis	2	2	2			
Buratti et al. (2017)	different espresso brewing thermal profiles (constant, increasing, or	RP HPLC-UV-Vis	7	7	7			

	decreasing at various temperatures)					
Corso et al. (2016)	species (arabica and Canephora) and roast (green, medium, and dark)	RP HPLC-UV-Vis	5	5	2		3
Crozier et al. (2012)	postharvest processing method (washed and unwashed) and roast profile (high temperature, short time and low temperature, long time)	RP HPLC-DAD	6	6	6		
Farah et al. (2006)	cultivar (4 arabica cultivars)	HPLC-MS; quantification with DAD	36	4	4		
Guyot et al. (1996)	by cultivar (Catuai and Bourbon), altitude, and amount of shade	*	6	6	6		
Liang et al. (2016)	origin (Dominican, Peru, Sumatra, Papua New Guinea, and Ethiopia) and roast (green, light, medium, dark)	RP HPLC-UV-Vis	20	20	20		
Ludwig et al. (2013)	effect of sugar addition (0, 5, 10, or 15 g per 100g of coffee) [only samples with 0g of sugar added are included]	RP HPLC-UV-Vis	2	2	2		
Martinez (2013)	effect of zinc supplementation on the coffee plant	HPLC-MS; quantification with DAD	2	2	2		
Mehari et al (2016)	region in Ethiopia (East, Northwest, South and West)	RP UPLC-MS	96	12	12		
Monteiro and Farah (2012)	cultivar (4 arabica cultivars)	HPLC-MS; quantification with DAD	96	12	12		
Monente et al. (2015)	amount in coffee brew and in spent coffee after various chemical treatments [only non treated coffee brew included]	RP HPLC-UV-Vis	6	1	1		
Muller and Hoffman (2005)	amount in green coffee bean extract and reconstituted extract [not included]	HPLC-MS; quantification with DAD	1	1	1		
Pilipczuk, Kusznierewicz et al. (2015)	roast (green and medium) and brew fraction	HPLC-MS; quantification with DAD	49	7	7		
Rao and Fuller (2017)	roast (medium and dark), brew time (6, 400, 1400 min) and brew temperature (hot and cold)	RP HPLC-UV-Vis	12	12	12		
Ribeiro et al. (2016)	cultivar (Acaia` and Yellow Bourbon), postharvest processing (wet or dry process) and slope exposure (sun or shade)	RP HPLC-UV-Vis	72	24	24		
Scholz et al. (2011)	cultivar (Itaguaje` and Paranavai)	Colorimetric (molybdate reagent at 370 nm and metaperiodate reagent at 423 nm)	2	2	2		
Scholz et al. (2014)	average of many Ethiopian acessions in validation of analytical method	Spectrophotometric (abs at 530 nm) and NIRS	3	3	3		
Scholz et al. (2016)	region in Ethiopia (Harar, Sidamo, Shoa, Kaffa Jimma, and Illubabor provinces)	Spectrophotometric (abs at 539 nm) and NIRS	3	3	3		
Smrke et al. (2013)	origin (Guatemala or Costa Rica) and roast (Light, Medium, Dark)	Size exclusion HPLC with DAD	7	7	7		
Smrke et al. (2015)	cultivar (Catuai and Tipica), degree of ripeness (unripe, half-ripe, and ripe), and water content	RP HPLC-UV-Vis	30	6	6		
Suarez-Quiroz et al. (2014)	extraction (water or solvent) and isolation method (ethyl acetate or activated charcoal)	RP HPLC-UV-Vis	6	6	6		
Tfouni et al. (2014)	cultivar (Catuai Amarelo and C. canephora cv. Apoata~), roast (light, medium, dark) and extraction (filter or immersion)	RP HPLC-UV-Vis	24	12	6		6
Trugo and De Maria (1991)	analysis method (isocratic HPLC, gradient HPLC or AOAC method)	RP HPLC-UV-Vis	24	24	3	21	

Category	Study	Description	Method					
	Xu et al. (2019)	various pressurized liquid extraction (PLE) conditions: temperature, time, and pressure	LC-Q-TOF-MS	15	15	15		
	Zanin et al (2016)	cup quality (minor, intermediate, good, very good, superior), region in Brazil (south, southeast), and postharvest method (natural, pulped natural)	RP HPLC-UV-Vis	64	32	32		
Robusta	Andueza (2003b)	grind size and inclusion of torrefacto roast (50%)	RP HPLC-DAD	6	6		6	
	Balyaya and Clifford (1995)	processing method (wet processing and dry processing), bean shape (flat and pea) and maturity	RP HPLC-UV-Vis	70	5		5	
	Cheng et al. (2019)	different drying methods (room temperature drying, heat pump drying, freeze drying, microwave vacuum drying, and combined microwave power vacuum drying) and green beans	RP HPLC-UV-Vis	40	9		9	
	Clifford (1988)	origin (Non-Anglon and Angolan)	RP HPLC-UV-Vis	9	2		2	
	Herawati et al. (2019)	roast (green, light, medium, and dark)* [more specific roast levels are listed in the paper]	RP HPLC-UV-Vis	8	8		8	
	Lopez-Galilea (2007)	extraction method (filter, French, mocha, and espresso) and torrefacto roast (0%, 30% and 100%)	RP HPLC-UV-Vis	12	12		12	
Other	Campa et al. (2005)	species (15 species and 6 taxa; not arabica or robusta)	RP HPLC-DAD	57	19			19
	Duarte, Pereira, and Farah (2010)	species (13 hybrids and 4 arabica cultivars) and post-harvesting method (semi-dry and wet)	HPLC-MS; quantification with DAD	272	34	8		26
	Ky et al. (1999)	species (C. pseudozanguebariae, C. liberica, and its F1 and backcross hybrids)	RP HPLC-DAD	155	5			5
	Mori et al. (2020)	cultivar (Diamante, Jequitiba`, and Centena`ria), genotype, and farm site	RP HPLC-UV-Vis	31	31			31
	Risso, Pe`res,andAmaya-Farfan	cultivar (Mundo Novo, Acaia`, Icatu Vermelho, Icatu Amarelo, Catuai` Vermelho, Catuai` Amarelo, Obata:,) and Tupi	Capillary Electrophoresis	36	12			12
	Ribeiro et al. (2018)	species (Bourbon Amarelo and Acaia`) and processing method (wet processing and dry processing)	RP HPLC-DAD	12	2			2
Unspecified	Gloess et al. (2013)	extraction method (semi-automatic and fully-automatic espresso, Nesprossso, Bialetti, French Press, Karlsbader Kanne, and filter)	RP HPLC-UV-Vis	4	2		2	
	Bennat et al. (1994)	compare commercial samples with roasted arabica, and by roast	RP HPLC-UV-Vis	11	11	6	5	
	Fujioka and Shibamoto (2008)	various commercial samples (regular and decaf)	RP HPLC-UV-Vis	108	12		12	
	Jeon et al. (2017)	origin (Brazil, Colombia, Guatemala, Indonesia, Kenya, Papua New Guinea, Tazania, and Ethiopia), grind size (fine, medium, coarse), and roast (medium)	RP HPLC-DAD	126				
	Jeon et al. (2019)	roast (light, medium, and dark), comparison with instant coffee	RP HPLC-DAD	144	36	15	2	19
	Lopes et al. (2019)	brew time (10, 185, or 360 minutes), temperature (20°C, 50°C, or 80°C), mass to volume ratio (1, 3.5, or 6), and grind level (1, 2, or 3)	RP HPLC-DAD	20	20		20	
	Lopes et al. (2020)	brew ratio (1:30, 1:15, 1:10), brew temperature (120°C, 150°C, 180°C), and brew time (1, 5.5, 10 minutes)	RP HPLC-DAD	2	2		2	
	Merritt and Proctor (1959)	brew temperature (100°F, 120°F, 140°F, 160°F, 180°F, 200°F) and brew time (0.5, 1, 2, 5, 10 min)	Spectrophotometric	30	30		30	
	Mills (2013)	roast (light, medium dark, very dark), comparison with instant coffee, and caffienation level (regular and decaf)	RP HPLC-DAD	138	18		18	

Monteiro and Trugo (2005)	brand and roast (traditional and extra strong)	RP HPLC-UV-Vis	78	10		10		
Moon, Yoo, and Shibamoto (2009)	origin (Colombia, Ehtiopia, Guatemala, Nicaragua, Papua New Guiniea, Sumatra), roast (green, roasted, light, medium, dark)	RP HPLC-UV-Vis	126	20		20		
Parenti (2014)	espresso brewing parameters (bar machine, hyper espresso method, I-espresso system)	HPLC-MS; quantification with DAD	12	3		3		
Rao and Fuller (2018)	origin (Brazil, Ethiopia, Myanmar, Colombia, Mexico) and temperature (hot and room temperature)	RP HPLC-DAD	36	12		12		
Rao, Fuller, and Grim (2020)	roast (light, medium, and dark) and temperature (hot and cold brew)	RP HPLC-DAD	24	6		6		
Rodrigues and Bragagnolo (2013)	brew method (drip and instant) and regular versus decaf	HPLC-MS; quantification with DAD	16	4		4		
Schrader et al. (1996)	roast (light, medium, dark), and pre-brewing steam treatment	RP HPLC-DAD	80	10		10		
Trugo, L. C., and Macrae, R. (1984) #2	comparison of different isomers of the cholorogenic acids in instant coffee	RP HPLC-UV-Vis	117	13		13		
Mabrouk and Deatherage (1956)	fraction number [only first fraction is included]	Liquid Chromatography	1	1		1		
SUM:			4653	1116	509	223	214	170

Table 2.3: List of references used in meta-analysis of organic acids by coffee type analyzed (arabica, robusta, Other, or Unspecified). A short description of each method of examining organic acid, analytical method used, total distinct measurements, number of unique samples, and number of samples for each type of coffee is included.

(HR)GC: (High Resolution) Gas chromatography; FID: Flame ionization detector; HPLC: High Performance Liquid Chromatography; MS: Mass spectrometry; MWD/VWD: Multiple Wavelength Detector/Variable Wavelength Detector; CE: Capillary electrophoresis; ECD: Electrochemical detector; RP: Reverse phase; DAD: Diode Array Detector

Coffee Type Analyzed	Reference	Examines aliphatic acids by:	Analytical Method Used	Total Distinct Measurements	Number of Unique Samples	Arabica	Robusta	Unspecified	Other
Arabica and Robusta	Alcazar (2003)	species (arabica and robusta), roast level (green and roasted)	Anion-exchange column with conductivity detector	14	4	2	2		
	Feldman, Ryder, and Kung (1969)	species (arabica and robusta), roast level (medium and dark)	Anion-exchange column with analysis by GC (after methyl esterification)	60	6	4	2		
	Hucke and Maier (1985)	species, roast (Green, steamed, light and dark), caffeination level (regular and decaf), and by commercial samples	GC-FID	53	53	8	21	24	
	Jham et al. (2002)	development of coffee beans (random mixture, immature, mature cherries, and cherry coffee beans dried on cement patio)	both ion-exclusion HPLC-UV Vis and GC-FID	18	14	2	12		
	Poisson et al. (2017)	species (arabica and robusta)	*	4	4	2	2		
	Verardo et al (2002)	species (arabica and Blend), fresh vs aged (72h), roast (green, light, medium, dark), compare regular vs decaf	GC-MS	215	14	2	12		
	Kampmann and Maier (1982)	species and origin (arabica from Burundi, Santos, Colombia, and Keyna; and robusta from Guinea, Burundi, and Togo)	GC-FID	7	7	4	3		
	Khamitova et al. (2020) [#1]	species (arabica and robusta) and espresso machine parameters (12g or 14g of grounds, filter baskets, or perforated disk heights)	HPLC-VWD	160	16	8	8		
	Scholze and Maier (1984)	species (arabica from Santos, Burundi, Kenya, and Mocha; robusta from Burundi, Angola, and Togo; and 4 other species)	isotachophoresis	11	11	4	3		4
	Scholze and Maier (1983)	species (arabica from Santos, Burundi, Kenya, and Mocha; robusta from Burundi, Angola, and Togo; and 4 other species)	isotachophoresis	22	11	4	3		4
	Van der Stegen and Van Duijin (1987)	species (arabica and robusta), roast (green and roasted), commercial samples, and coffee that had been held [only green and roasted data used]	HPLC-UV	36	6	3	3		
	Weers et al. (1995)	species, and roast (Green, light, medium, dark)	CE	83	10	5	5		
Arabica	Ahmed et al. (2019)	cold brewed coffee extraction techniques (conventional, ultrasonication, water bath agitation, agitation with a stirrer, or a combination of the aforementioned methods)	ion exclusion HPLC	42	7	7			
	Bahre and Maier (1999)	treatment (unsteamed, steamed, and lightly roasted) and origin (Kenya and Colombia)	HRGC-MS	65	6	6			
	Blanc (1977)	roast level (light, medium, and dark)	*	35	7	7			
	Bore`m et al. (2016)	genotype (Mundo Novo and Yellow Bourbon from 3 origins) and environment (3 different sites)	HPLC-ECD	35	7	7			

	Study	Description	Method					
	Galli and Barbas (2004)	roast (roasted and green)	CE with UV-Vis	32	2	2		
	International Coffee Organization (1991)	grind (fine, extra fine, or coarse), brew temperature (70°C, 94°C, or 100°C), contact time (1, 5, 6, or 14 min)	enzymatic methods	42	7	7		
	Muller and Hoffman (2005)	amount in green coffee bean extract and reconstituted extract [not included]	HPLC-MS; quantification with DAD	8	1	1		
	Ribeiro et al. (2018)	species (Bourbon Amarelo and Acaia`) and processing method (wet processing and dry processing)	RP HPLC-DAD	28	4	4		
Robusta	Chindapan, Soydok, and Devahastin (2019)	roast (green, light, medium, and dark as determined by L* value), roast method (hot air or super-heated steam), and roast temperature (190°C, 210°C, 230°C, or 250°C)	RP HPLC-DAD	193	48		48	
	Dong et al (2017)	drying technique (Room-temperature, solar, heat-pump, hot-air, and freeze drying)	RP HPLC-DAD	31	5		5	
	Scholz and Maier (1990)	roast (green, light, medium)	GC-FID	3	3		3	
Unspecified	Mabroul and Deatherage (1959)	fraction number [only first fraction is included]	Liquid Chromatography	7	1			1
	Marrubini et al. (2015)	extraction type (espresso and decaf instant)	HPLC-DAD	6	6			6
	Engelhardt and Maier (1985)	comparison of roasted commercial samples and commercial instant coffee samples	GC-FID	34	2			2
	Van der Stegen and Van duijin (1987)	commercial roasted samples	HPLC-UV	32	4			4
	SUM:			1276	95	20	51	24

The compiled database allows for detailed analysis of trends in coffee acid concentrations. Beginning with OAs, citric and malic acid decrease with roasting in arabica, especially when comparing green coffee to medium roasted coffee (Figure 2.2). Due to the small sample size, it remains unclear whether the progression from medium roast to dark roast further decreases the levels of citric acid and malic acid (Figures 2.2A-B). Acetic acid increases proportionally with roast level; dark roasts contain the highest amounts of acetic acid (Figure 2.2C). Notably, even light roasting increased acetic acid, as light roasts contain significantly more acetic acid than green coffee. Lactic acid remains relatively constant as roast progresses, with roasted coffee having only slightly higher levels of lactic acid than green coffee (Figure 2.2D). The small amount of data for quinic acid in roasted arabica coffee prevents any insights

to how roast affects the acid concentration, or even a comparison between green and roasted coffee (Figure 2.2E). Lastly, roasted coffee has a higher amount of tartaric acid than green coffee and may even decrease as roasting progresses (Figure 2.2F).
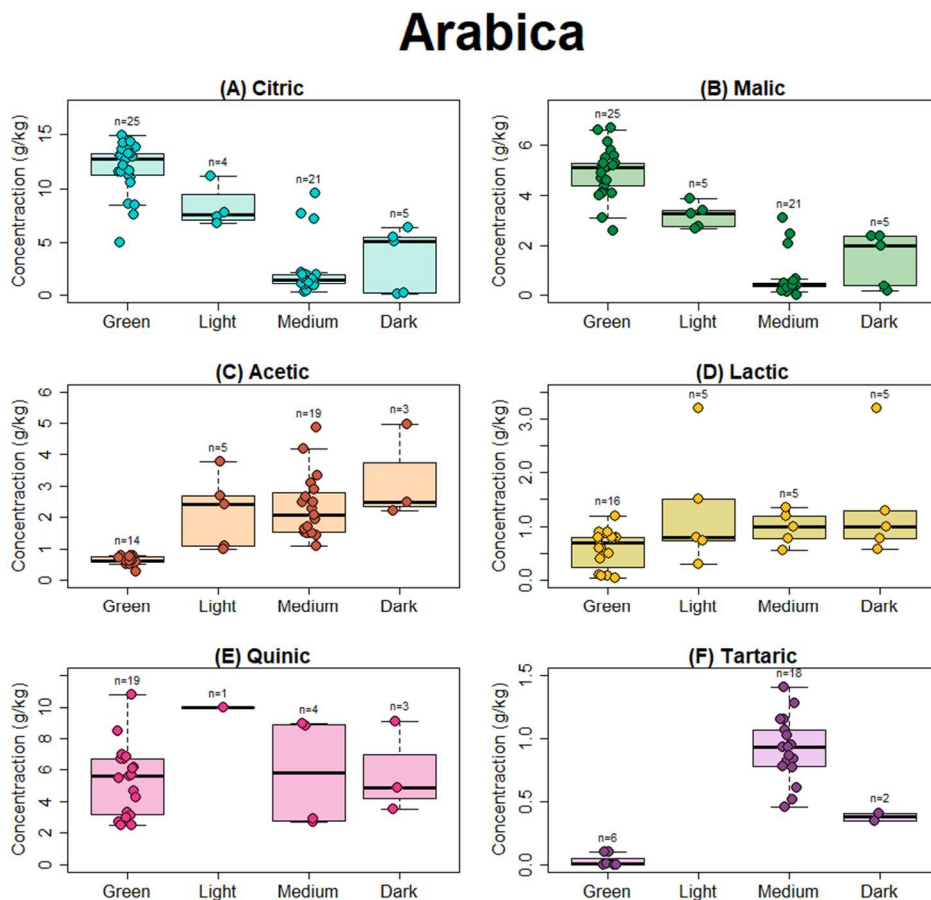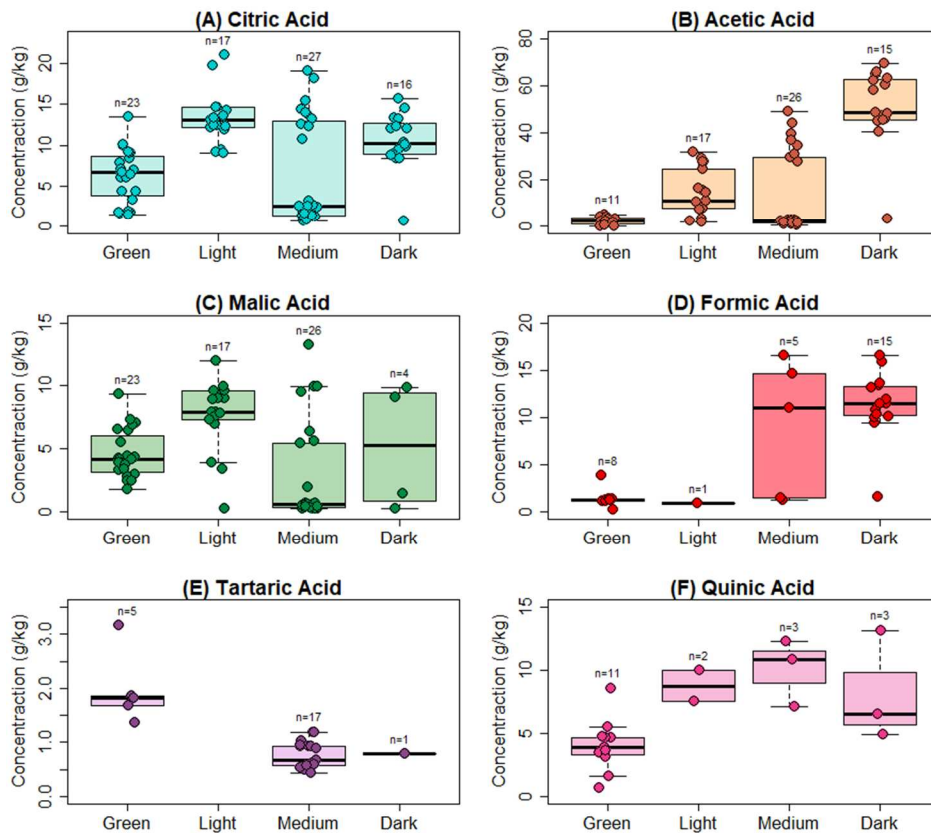

Figure 2.2: Reported amounts of organic acids (g/kg) by roast level in arabica coffee. Each plot is not to the same scale.

In robusta, roasting green coffee increases the amount of citric, acetic, malic, formic, and quinic acid, and decreases the amount of tartaric acid (Fig. 2.3). Most notably, roasting strongly increases the amount of acetic acid, and progressive roasting further increases acetic acid levels, with dark roasts containing the highest concentrations. Dark roasted robusta coffee

contains approximately ten times more acetic acid than green coffee (Figure 2.3B). Roasted

coffee can contain more citric and malic acid than green coffee (Figure 2.3A and Figure 2.3C),

but it is unclear how progressive roasting affects the concentration of these acids. Medium and

dark roasted robusta contains more formic acid than green robusta (Figure 2.3D), however, due

to the small sample size for light roast robusta, it remains to be seen how formic acid differs

with roast level. Green robusta has more tartaric acid than roasted; how progressive roasting

affects the amount of tartaric acid is severely limited by the small number of samples for light

and dark roasts (Figure 2.3E). Finally, while the overall number of samples are small, quinic acid

is lower in green coffee than roasted, and seems to maximize in medium roasts (Figure 2.3F).

Robusta

Figure 2.3: Reported amounts of organic acids (g/kg) by roast level in robusta coffee. Each plot is not to the same scale.

Because the roast levels in Figures 2.2 and 2.3 are qualitative, we also directly compared green versus roasted coffee (Figure 2.4).   Roasting decreases the amount of citric acid in arabica coffee but increases the amount of citric acid in robusta coffee (Fig. 2.4A). Green arabica has a higher amount of citric acid than green robusta, while the reverse is true for roasted coffee – roasted arabica has a lower concentration of citric acid than roasted robusta. Similar behavior is observed with malic acid: roasting decreases the amount of malic acid in arabica, while green robusta and roasted robusta have similar levels (Figure 2.4B). When roasted, robusta has more malic acid on average than arabica.

Very different behavior is observed with acetic acid. Although green arabica and green robusta have comparable amounts of acetic acid, roasting of robusta coffee leads to a tenfold increase (Figure 2.4C). As such, roasted arabica has much lower amounts of acetic acid than roasted robusta.

As for tartaric acid, green arabica contains only trace amounts, whereas green robusta has much higher levels (Figure 2.4D). Roasted arabica and robusta have similar amounts of tartaric acid; in other words, roasting increases the amount of tartaric acid in arabica but decreases the amount of tartaric acid in robusta. Finally, quinic acid is present in roasted robusta at a higher concentration than roasted arabica, even though green robusta and arabica have similar levels of quinic acid (Figure 2.4E).
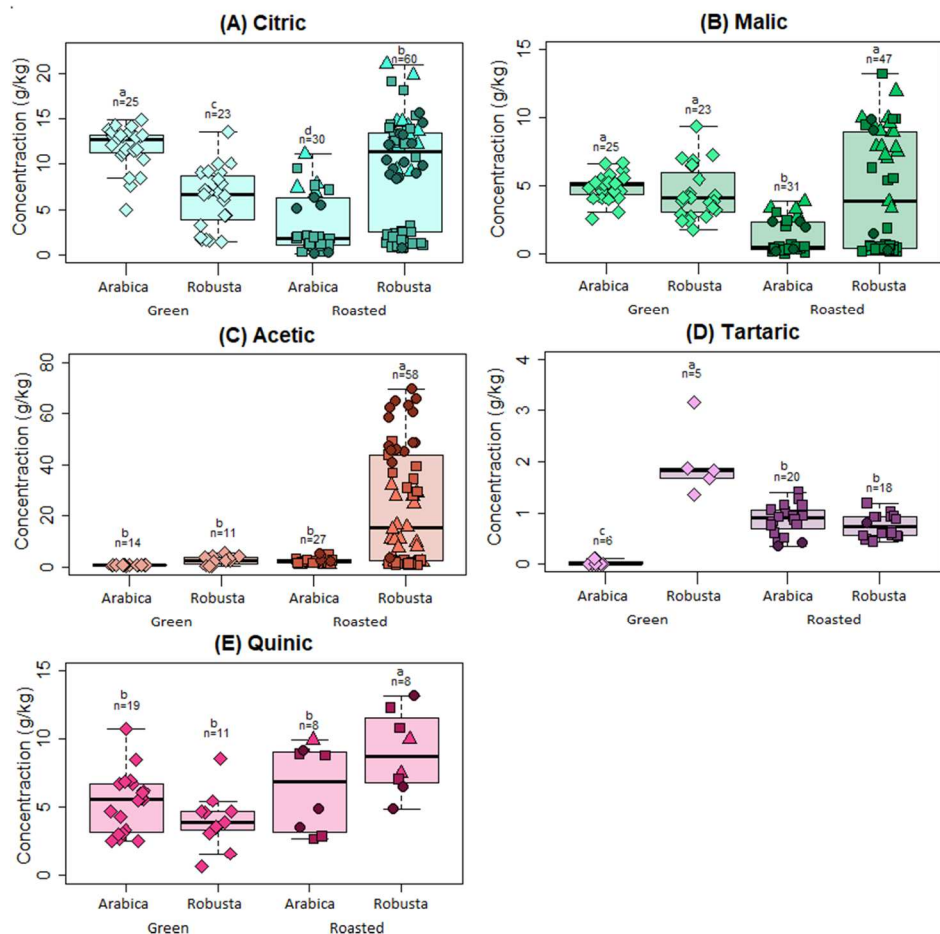
Figure 2.4: Amounts of organic acids (g/kg) for arabica and robusta coffee, either green (unroasted) or roasted (light, medium, dark roast, or roasted). Each plot is not to the same scale. Lowercase letters (a-d) indicate statistically significant differences among groups according to Fischer's LSD test.

Diamond – green; square – light roast; triangle – medium roast; circle – dark roast.

Examination of CGAs also yielded interesting results. The concentrations of the most commonly reported CGAs in arabica and robusta are shown in Figures 2.5 and 2.6, respectively. The general trend observed for total CQA, 5-CQA, total diCQA, and total FQA is that the CGA concentration is highest in the green coffee and decreases progressively with roasting, for both arabica and robusta. In contrast, 4-CQA and 3-CQA exhibit slightly non-monotonic behavior, where a light roast on average has slightly higher concentration than green and progressing to a medium or dark roast decreases the concentration. Note that 5-CQA makes up the majority of

total chlorogenic acids in coffee, being present in amounts as high as 157 g/kg (Figure 2.5B and

2.6B).
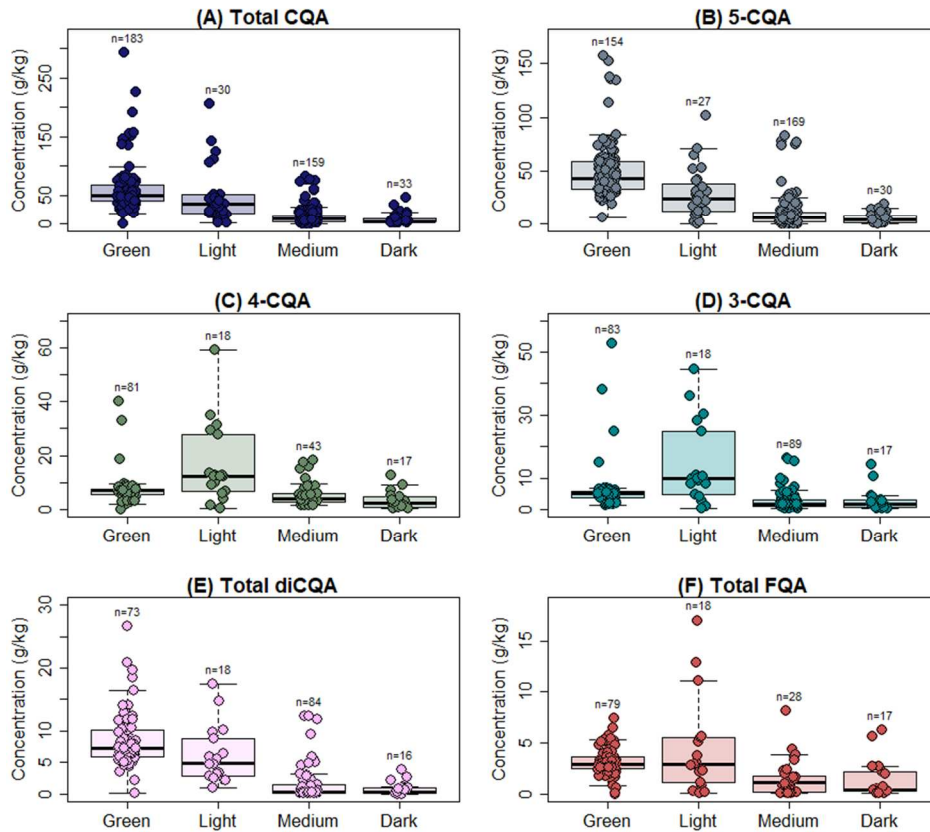
Figure 2.5: Reported amounts of chlorogenic acids (g/kg) in arabica coffee by roast level. Each plot is not to the same scale.

CQA -- caffeoylquinic acid; 5-CQA -- 5-o-caffeoylquinic acid, 4-CQA -- 4-o-caffeoylquinic acid; 3-CQA -- 3-o-caffeoylquinic acid; diCQA -- dicaffeoylquinic acid; FQA -- feruloylquinic acid
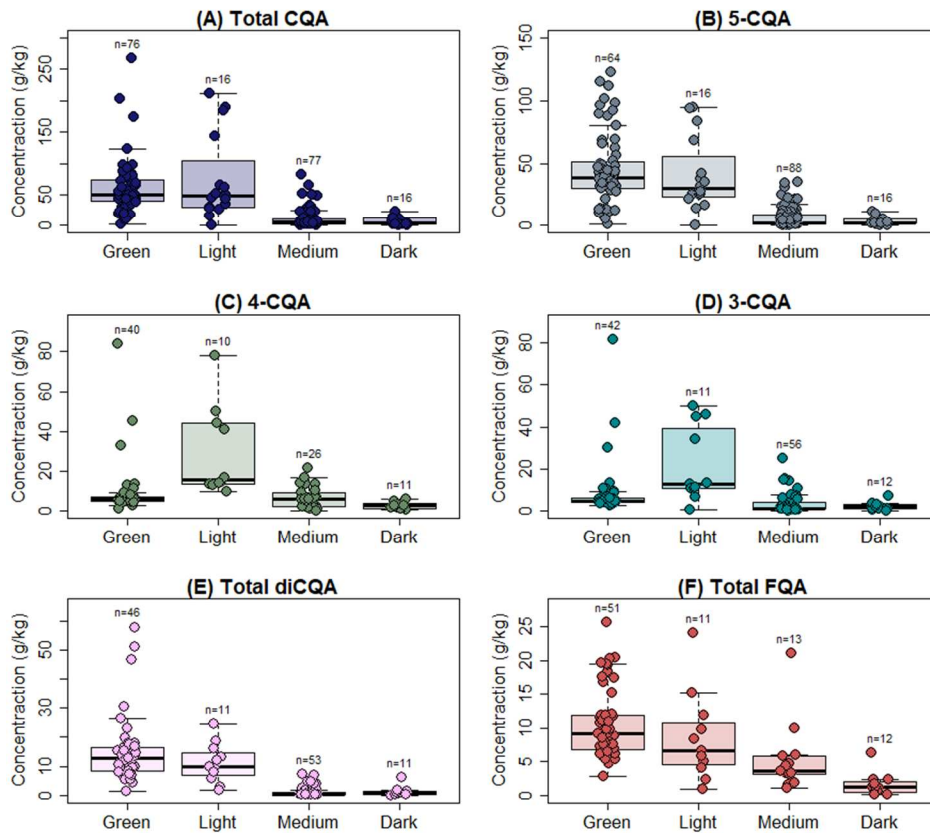
Robusta

Figure 2.6: Reported amounts of chlorogenic acids (g/kg) in robusta coffee by roast level. Each plot is not to the same scale.

CQA -- caffeoylquinic acid; 5-CQA -- 5-o-caffeoylquinic acid, 4-CQA -- 4-o-caffeoylquinic acid; 3-CQA -- 3-o-caffeoylquinic acid; diCQA -- dicaffeoylquinic acid; FQA -- feruloylquinic acid

Again, because the roast levels are qualitative, we also directly compared the two types of coffee (Figure 2.7). Green arabica and green robusta, as well as roasted arabica and roasted robusta, have similar levels of the three CQA isomers, and subsequently the total amount of CQAs (Figures 2.7A-D). As mentioned above, dark roasted coffee has lower levels of all CGAs than green coffee, but the difference between green and roasted coffee becomes smaller as all roast levels are grouped together. The coffee roast level affects CGA concentrations more than the type of coffee, except for total FQA and total diCQA. Oddly, among both green and roasted

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arabica and robusta, the amount of 4-CQA is the same (Figure 2.7C). Green robusta has the

highest levels of total FQA and total diCQA, which decreases with roast (Figures 2.7E-F).
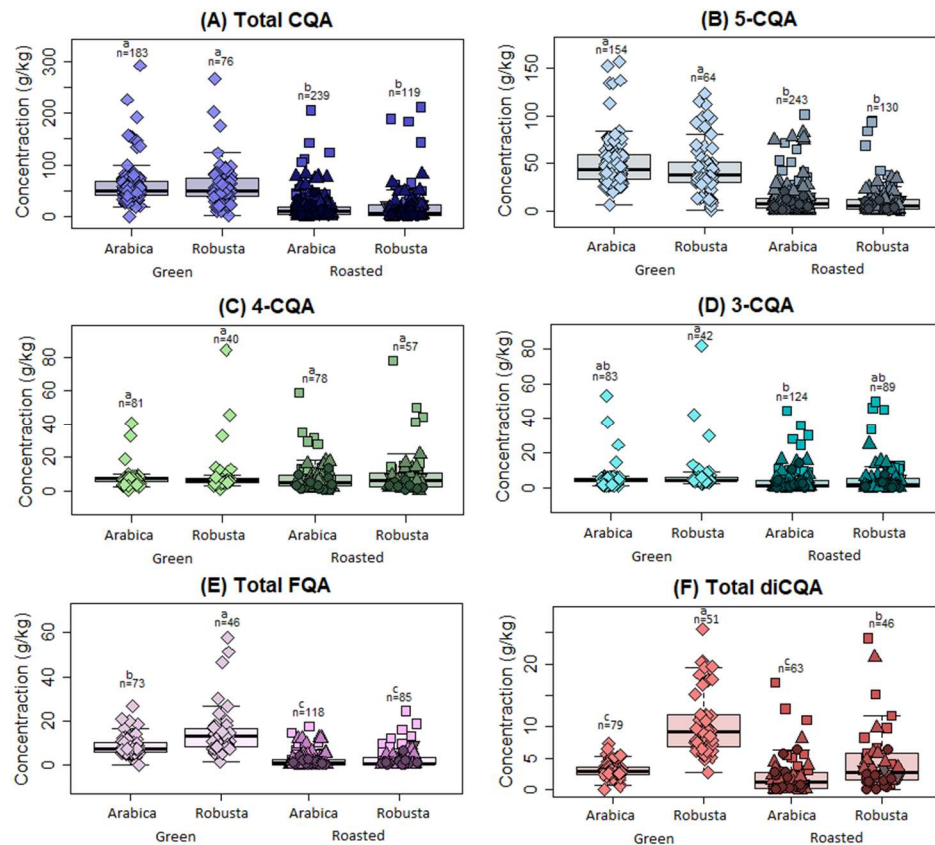

Figure 2.7: Amounts of CGAs (g/kg) for arabica and robusta coffee, either green (unroasted) or roasted (light, medium, dark roast, or roasted). Each plot is not to the same scale. Lowercase letters (a-d) indicate statistically significant differences among groups according to Fischer's LSD test.

Diamond – green; square – light roast; triangle – medium roast; circle – dark roast; upside down triangle – roasted.

CQA -- caffeoylquinic acid; 5-CQA -- 5-o-caffeoylquinic acid, 4-CQA -- 4-o-caffeoylquinic acid; 3-CQA -- 3-o-caffeoylquinic acid; diCQA -- dicaffeoylquinic acid; FQA -- feruloylquinic acid

The preceding figures focus on the statistical distribution of each acid for each type of

coffee. To directly compare the average concentrations, we generated a stacked column plot

of the median concentrations for each roast level in arabica and robusta (Figure 2.8). Here the

different colors indicate the relative amount of each acid, while the total stack height indicates

the total concentration on average of that that category of acids in that coffee type. Both green

arabica and green robusta have similar total OAs, near 20 to 25 g/kg, with the vast majority quinic acid, malic acid, and citric acid. At all roast levels except green, robusta coffee has a higher total amount of organic acids, due to increases in the amount of citric, malic, formic, and acetic acids (Figures 2.8A-B). Roasting increases the total amount of acid in robusta coffee, while further roasting decreases the amount of acid in arabica coffee, minimizing at medium level roasts (Figure 2.8A-B). Arabica's total acid content is mainly comprised of citric, quinic, and malic acids (Figure 2.8A). Dark roast robusta coffee has a higher amount of total acid than dark roast arabica and is mostly comprised of acetic acid (Figure 2.8B). Formic acid also constitutes a large portion of the total acids in robusta coffee at medium and dark roasts (Figure 2.8B).
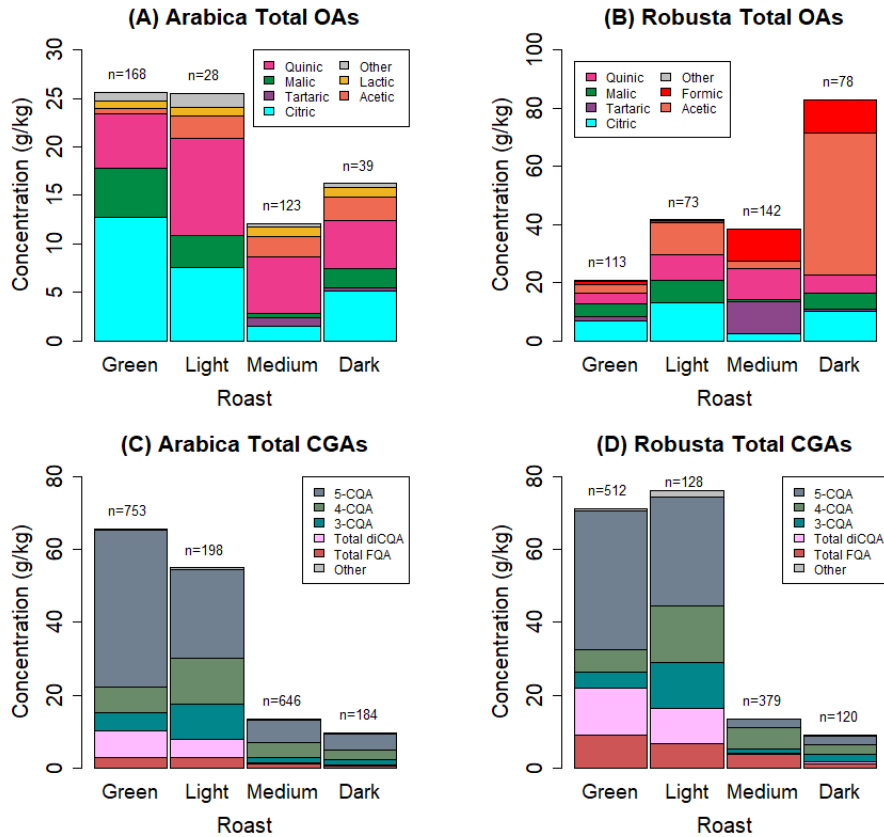
Figure 2.8: Comparison of arabica and robusta coffees for organic acids (g/kg) and chlorogenic acids (g/kg) by the sum of each median for each acid at that roast level. Subplot A and B are on different scales

Surprisingly, the profiles for CGAs are extremely similar between arabica and robusta coffee, (Figures 8C-D). The initial CGA concentrations on average are near 60 to 70 g/kg and roasting to medium or dark decreases them sharply to comparable values. In other words, roast level affects the amount of CGAs more than type of coffee. Light roast robusta coffee has a slightly higher amount of total CGAs due to the increase in both 3-CQA and 4-CQA (Figure 8D). Among both arabica and robusta coffee, 5-CQA comprises by far the largest fraction of total CGAs (Figures 8C-D).

2.5 Discussion

Our meta-analysis provides several new insights on acids in coffee. First, the data indicates that concentrations of citric and malic acid decrease with roast while acetic acid

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increases. In contrast, lactic and quinic acids remained relatively stable throughout progressive roasting. These two acids are thought to increase due to the breakdown of carbohydrates and CGAs (Blanc 1977; Weers et al. 1995; Ginz et al. 2000). However, the relatively small sample size for lactic and quinic acid in roasted arabica as well as some bimodal distributions may affect the ultimate conclusions from Figures 2.1D and 2.1E. More data would need to be collected to fully understand how roasting affects lactic and quinic acid in arabica coffee.

While roasting robusta coffee, the amount of citric and malic acid initially increases, but then decreases as roasting progresses. Yodkaew et al. propose that this behavior is due to the disruption of plant tissues, resulting in the release of this acids, rather than the acids being formed in some sort of reaction (Yodkaew et al. 2017). At medium-level roasts, continued thermal degradation leads to a decrease in citric and malic acid; in some cases, it led to a disappearance of malic acid entirely (Chindapan, Soydok and Devahastin 2019). The nearly 10-fold increase in acetic acid is also consistent with work published by Chindapan et al. 2019, but it is inconsistent with the current theory that acetic acid is formed from the breakdown of sucrose. Because green robusta has a lower sucrose content than arabica, if this were the sole pathway it should have a lower amount of acetic acid at all roast levels (Balzer, 2008).

Additionally, it is thought that acetic acid concentrations should decrease from medium to dark level roasts due to the volatility of the acid (Balzer, 2008). The sensory impacts of acetic acid in robusta are likely similar to those speculated for arabica, and one study has shown acetic acid, as well as propanoic acid, correlate negatively with liking in ranked and paired preference tests of Coffea canephora (Kalschne, Viegas, De Conti, Corso, and Benassi, 2018). To minimize the levels of acetic acid, and any unfavorable sour, bitter, or rancid tastes in the

roasted robusta beans, Chindapan suggests using superheated steam to roast, instead of hot air roasting due to a shorter roasting time (Chindapan, Soydok, and Devahastin 2019). Formic acid also increased with roast, most likely because of Maillard reactions occurring while roasting (Weers et al. 1995; Poisson et al. 2017; Chindapan 2019).

When comparing green and roasted arabica or robusta coffee, the type of coffee will influence how particular OAs change with roasting. The different ratios of OAs could lead to different flavor profiles, so considering which type of coffee to use is important when crafting roasted coffee. Additionally, roasting profiles can be optimized based on the type of coffee (Eggers and Pietsch 2001). The comparatively higher amounts of citric and malic acid in roasted robusta may be attributed to the anomalously high data provided by Chindapan et al. (2019). The small availability of data in general on OAs in roasted robusta coffee allows for the data to be displayed very prominently. However, due to differences in determination of roast level, as mentioned in the methods section, and differences in extraction and experimental design, these anomalously high data may be skewing the overall trends. Previously published data all indicate that progressive roasting ultimately leads to a decrease in citric and malic acid in robusta coffee (Scholz and Maier 1990; Weers et al. 1995; Dong et al. 2017).

As is consistent with literature, roasting either arabica or robusta coffee will decrease the overall amount of CGAs. As CGAs are subjected to thermal degradation, many aromatic compounds are created because of acyl migration, hydrolysis, oxidation, fragmentation, and polymerization reactions (Clifford 1985; Bicho et al. 2011). These aromatic compounds ultimately affect the sensory profile of the brewed coffee. Additionally, CGA lactones are formed, which contribute to bitterness in roasted coffee (Frank et al. 2007). While levels of 5-

CQA may have decreased due to progressive roasting, Vignoli et al. posits that the antioxidant activity of the coffee remains relatively stable, due to an increase in the amount of melanoidins, which are generated in Maillard reactions during roasting (Vignoli et al. 2011). Interestingly, it seems that a light roast, the amount of 3-CQA and 4-CQA increase, possibly explained again by the disruption of plant tissues during the earliest stages of roasting (Yodkaew et al. 2017). 3-CQA has been shown correlating to higher observed bitterness and astringency (Gloess et al. 2013). Additionally, the slightly bimodal distribution of data for this qualitatively described roast level could be affecting the median for these two acids. Higher overall CGA has been shown to increase perceived bitterness as well as increase cupping score of coffee (Ribeiro et al. 2011).

While it has generally been reported that green robusta coffee has higher levels of CGAS than arabica (Clarke and Macrae 1985; Bicho et al. 2013a; Poisson et al. 2017), the most important factor in determining the amount of CGAs in the final coffee product is dependent on roast level rather than type of coffee. Figure 2.6 shows how 5-CQA, the majority component of CGAs, differs significantly when comparing green and roasted coffee rather than arabica and robusta coffee. Because of how 5-CQA can ultimately contribute to the overall flavor of the beverage, this may have implications for how the coffee should be brewed – meaning that choice of coffee type may not matter in terms of contribution of 5-CQA to sensory quality. Similarly, total FQA levels between roasted arabica and robusta coffee are hardly distinguishable even though green robusta coffee had higher levels. Regardless of what causes 5-CQA and FQA levels to increase, the sensory literature strongly indicates that these acids have a substantial impact on coffee taste and flavor. CGAs in green coffee are clearly a marker of

roasted coffee quality (Farah et al. 2006; Lemos et al. 2020; (Rendón, De Jesus Garcia Salva, and

Bragagnolo, 2014), though what is perceived in the roasted coffee is not always the acids

themselves.

Lastly, when looking at the relative proportions of acids in each coffee type, in both

arabica and robusta coffee, OAs are minimized at a medium-level roast. Roasting too lightly or

too darkly leads to an increase in particular OAs, which may affect the overall sensory profile of

the beverage. An increase in overall acidity will increase perceptible sourness, potentially

decrease bitterness, but increase overall flavor intensity (Kim et al. 2018, Cordoba et al. 2019,

Voilley et al. 1981). In general, higher acidity is associated with lower consumer liking

(Manzocco et al. 2009, Batali et al. 2021), which indicates that medium roast coffee might be

overall more acceptable to a wide variety of consumers than light or dark roast. Dark roast

robusta undergoes the greatest increase in acid, primarily acetic acid, nearly double the amount

of total acid at other roast levels. While robusta contains more OAs than arabica after roasting,

the amount of CGAs between arabica and robusta are relatively equal at each roast level,

further supporting the conclusion that roast level affects the amount of CGAs more than type of

coffee. Therefore, chemical drivers of flavor difference between arabica and robusta of the

same roast level are not due to CGA concentrations, but possibly due to OA concentrations and

other non-acid compounds.

2.6 Conclusions

The meta-analysis presented here shines new light on how the concentration of each

coffee acid is dependent on type of coffee and roast level. Arabica coffee tends to have lower

amounts of OAs, which decrease with roast level, plateauing at a medium roast. Progressive

roasting leads to an increase in OAs in robusta coffee – most notably a large increase in acetic acid. From a sensory perspective, acetic acid and overall coffee acidity are in general negatively associated with roasted coffee quality, which could explain why arabica is more popular than robusta. When comparing CGAs, arabica and robusta have similar concentrations, but these concentrations vary greatly with roast level. CGAs, particularly 5-CQA and FQA, impact the sensory quality of coffee but the specific impact (i.e. negative or positive on cupping score) is still coffee dependent so there likely are some interactions between these compounds and other chemical components of coffee.

One overarching conclusion is that relatively little research has been performed on OAs in coffee, despite their important role in sensory quality. Data for the less abundant acids in coffee, such as lactic, formic, and tartaric acid, was notably sparse compared to CGAs. Our hope is that the data presented here help illustrate the need for future research to focus on acid concentrations across varying roast levels to help understand their role in consumer appreciation of coffee.

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3. Roast Level and Brew Temperature Significantly Affect the Color of Brewed Coffee

Abstract: Beverage color significantly affects perceived sensory quality and consumer preference. Although the color of coffee beans is well known to vary strongly with roast level, little work has examined how roast level and brewing conditions affect the color of the final beverage. Here, we report that the color of full immersion brewed coffee is significantly affected by both roast level and brewing temperature. Coffees from three different origins were each roasted to three different levels (light, medium, and dark) and then brewed at three different temperatures (4°C, 22°C, and 92°C). Each sample was brewed towards full extraction and then diluted to precisely 2% total dissolved solids (TDS) so that differences in concentration would not confound color measurements. Absorbance spectra (UV-vis) and color tristimulus values (L*a*b*) were then collected and analyzed. We find that roast level had the strongest impact on brew color, and that brew temperature had a significant impact on color for light and medium roasts, with less impact on dark roasts. Qualitatively, the cold brewed coffees tended to be redder, while the hot brewed coffees were blacker. The results suggest that there is an opportunity to manipulate and brand brewed coffee color through judicious choices of roast level and brewing temperature.

3.1 Introduction

Coffee bean color serves as a robust and valuable indicator of roast level in the coffee industry (Da Porto 1991). Color measurements, whether on the Agtron Gourmet (Staub 1995) scale or in the form of tristimulus color values such as the C.I.E. (International Commission on

Illumination) L*a*b* (Lawless and Heymann 2010), are often included alongside qualitative roast determinations ("light", "medium", "dark", etc.) as a means of quantifying the color of the roast (Bicho et al. 2012; Da Porto 1991; Nicoli et al. 1997; Sacchetti et al. 2009). Da Porto et al. examined how color of whole and ground coffee beans changes with roast in the C.I.E. L*a*b* color space - as roast level increased, L*a*b* values increased up until a light-medium level roast, and then began to rapidly decrease (Da Porto 1991). Similar findings were reported by Nicoli et al., who quantified how increased roasting times led to increased degrees of browning (Nicoli et al. 1997). The color of the grounds remains an important quantitative measure of roast even when examining other physicochemical aspects of coffee, such as antioxidant activity and volatile compounds (Cangussu et al. 2020; Lee et al. 2013; Nicoli et al. 1997; Sacchetti et al. 2009).

Qualitatively, color can affect perceived sensory characteristics (Lawless and Heymann 2010). Color is typically the first assessment of quality a consumer makes, making color a primary indicator of perceived quality (Ferreira, Bassotto, and Castro 2020; Lawless and Heymann 2010; Mazzafera et al. 1988). Moreover, the color and appearance of the product serves as a cue for changes in aroma and flavor, such as the browning that occurs during the coffee roasting process (Cangussu et al. 2020; Lawless and Heymann 2010).

While the color of coffee beans versus roast level has been measured extensively, the color of the resulting brew has received less attention. In early work, Pangborn tested how visual attributes, such as color intensity, turbidity, iridescence, and sediment, can vary alongside flavor attributes, such as strength, bitterness, or burnt flavor, and revealed that across different brew temperatures and holding times, color intensity and strength were rated proportionally

(Pangborn 1982). Kalschne reported that across different types of coffee, color was the most appreciated attribute, solidifying subjective judgements of color as central to consumers' perception of their beverage (Kalschne et al. 2019). Moreover, color has been labelled a defining characteristic during Free-Choice Profiling of brews made from beans grown in different planting designs (dos Santos Scholz 2018), emphasizing its role in the perceived quality of the beverage.

Notably, this prior work focused on subjective perceptions of coffee brew color. To date there is no published work that quantitatively and systematically focuses on the actual color of the brew. It is unclear how roast level translates to the coffee brew itself, nor how brew temperature can further impact the color of the final cup.

In this study, we measured the color of Toddy-style full immersion brewed coffee across multiple origins, roast levels, and brew temperatures. Color was examined both qualitatively, using photography and absorbance spectra, and quantitatively using the Agtron Gourmet scale and C.I.E. L*a*b* color measures. The experiments were designed to elucidate how the color of the coffee brew is influenced by roast level and brew temperature for coffees from different, representative origins.

3.2 Materials and Methods

3.2.1 Coffee

To systematically examine how brew temperature can affect the color of the coffee brew, a wide range of parameters were examined with a 3x3x3 factorial design. Green coffee beans from three different origin coffee beans were used: El Salvador Cerro Las Ranas Honey (ELS), Ethiopia Guji Washed organic (ETH), and Sumatra Fair-Trade Organic Takengon (SUM).

These three origins were chosen to be representative of three important classes of post-harvest processing. The ETH was "washed," where the mucilage is removed via fermentation immediately after depulping; the ELS was "honey processed", where some fruit pulp and mucilage remains on the parchment during drying; and the SUM was 'wet-hulled' as typical in Sumatra where the parchment is stripped from the bean prior to drying. These types of coffees are widely recognized to have very distinct flavor profiles (Illy 1995).

The green coffees were roasted over the course of three days in January 2021, one origin per day, on a Probatino P5 (Probat-Werkevon Gimborn Maschinenfabrik GmbH, Emmerich am Rhein, Germany). Each coffee was roasted to three different levels, representing a typical "light", "medium", or "dark" roast as represented by percent weight loss from the green coffee as well as target score on the Agtron Gourmet Scale published by the SCA (Staub 1995). Representative roast profiles and detailed roast metrics are provided in the supplementary material (Fig. S3.1 and Table S3.1, respectively.) After roasting, the beans were degassed for a week before being packed into vacuum-sealed bags of 300g each. The sealed bags were stored in a freezer at –20 °C. Bags were removed and allowed to defrost 24 hours in advance of brewing.

3.2.2 Brewing procedure

Coffee was ground immediately before each brew using a Mahlkönig Guatemala Lab Grinder (Mahlkönig USA, Durham, NC, USA) at grind size setting 4 with a median particle size of 972.01 ± 18.56 µm (see Liang et al. 2021 for grind size distribution). Nestlé Pure Life Purified Water with pH 7.46 was used for all brews (Nestlé 2019). Prior to brewing, the water was either

brought to room temperature (22°C) for the 4°C and 22°C brews or water was heated to 92°C

using a Bonavita 1.7-L Variable Temperature Electric Kettle (Bonavita World, Woodinville, WA).

A brew ratio of 5 was used for all brews, with 100 g of coffee grounds to 500 g of water.

Each brew was carried out in a Toddy Cupping Kit using the supplied traditional paper

filters (Toddy LLC., Loveland CO, USA). Three Toddy Cupping kits were used for each sample to

brew a sufficient volume of coffee for analysis using a standard full-immersion brew
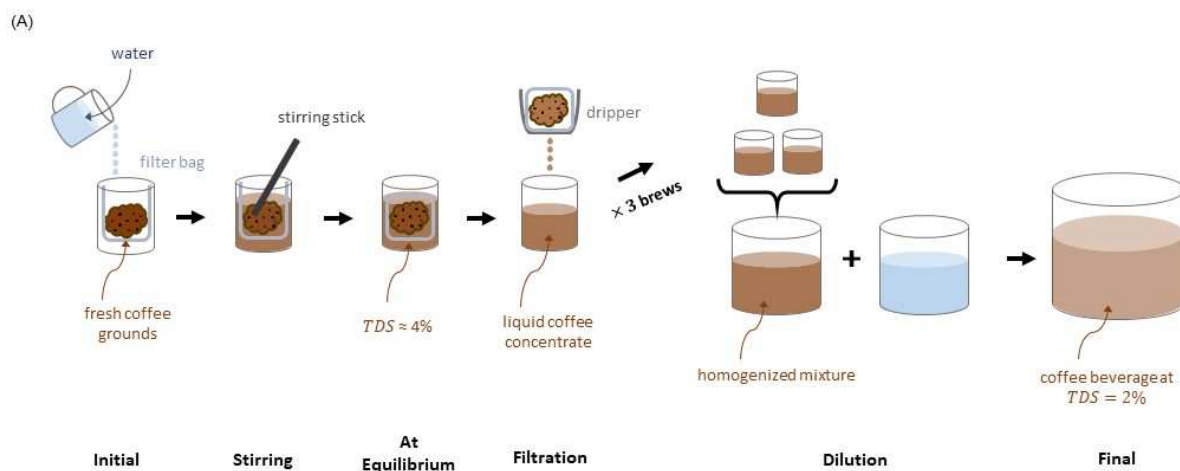
methodology (Fig. 3.1).

Figure 3.1: (A) Representative diagram of Toddy-style full immersion brew process. (B) Photo of Toddy Cupping System

The paper filters were filled with 100 g of room-temperature ground coffee, and the water of appropriate temperature was poured into the open filter bag. Then, the coffee grounds immersed in water were stirred for thirty seconds to fully wet the grounds. Each brew continued, without further agitation, until an equilibrium concentration was reached as measured by sampling the total dissolved solids (TDS) of the brew. For the hot brew, equilibrium was reached after about 1 hour; for the room-temperature brew, equilibrium was reached after approximately 12 hours; for the fridge temperature brew, equilibrium was reached after approximately 36 hours. After reaching equilibrium the filter bag of coffee grounds was removed and allowed to drain by gravity through a dripper back into the brew until it stopped dripping.

Each of the three cupping kits were then homogenized into one larger sample (to provide enough coffee for complementary sensory experiments not described here). The homogenized mixture was then diluted to 2% TDS for uniform analysis. The mass of the coffee liquid and the TDS were measured before and after dilution. The procedure was carried out in triplicate for each sample type, for a total of 3 origins × 3 roasts × 3 brew temperatures × 3 trial replicates = 81 samples (comprising 243 individual brews, homogenized across sets of three). Samples were stored in the refrigerator for approximately 48 hours until colorimetric analysis.

3.2.3 TDS, pH, and Titratable Acidity Measurements

The TDS of the coffee brew was measured at room temperature using a digital refractometer (VST, Inc). Prior to experimental measurements, the refractometer was zeroed with distilled water. Calibration of the refractometer was carried out according to the

procedure described by Liang et al. (2021). The pH of the brewed coffees samples after dilution was measured with a Mettler Toledo SevenCompact Duo S213 pH/Conductivity Meter (Mettler-Toledo LLC, from a buret while 50 mL of the coffee sample was stirred, until reaching a pH of 8.24 ± 0.06. Titratable acidity is expressed in mL NaOH/50 mL coffee.

3.2.4 L*a*b* Measurements

Colorimetric analysis was performed on each brew once it reached ambient temperature (22°C) after being stored in the refrigerator for approximately 48 hours. Results are expressed on the C.I.E. L*a*b* scale L* (lightness), a* (red-green value), and b* (yellow-blue value) (Lawless and Heymann 2010). A 50 mL aliquot of each sample was transferred into a glass petri dish placed on top of white printer paper, and the L*a*b* values were measured. The L*a*b* values of the coffee beans and grounds were also measured. Color analyses were carried out on the brew using a tristimulus colorimeter (Konica Minolta CR 400 Chroma Meter, Minolta, Osaka, Japan). The instrument was standardized against a white tile before each measurement. Color was expressed on the C.I.E. L*a*b* scale. Three measurement replicates were carried out for each sample.

3.2.5 UV-Vis Measurements

To obtain the entire absorbance spectrum for each coffee sample, 1.5 mL of the brew was analyzed in a Shimazdu PharmaSpec UV-1700 spectrophotometer (Shimadzu, Kyoto, Kyoto, Japan). The instrument was calibrated and baselined prior to measurements. The absorbance

spectrum was measured for each sample over the visible range (350 nm-750 nm) of the electromagnetic spectrum. Three measurement replicates were carried out for each sample.

3.2.6 Data Analysis

The L*a*b* values and UV-Vis absorbance spectra were averaged over three measurement replicates within each trial replicate for a total of 9 measurements for each sample type. Variability between measurement replicates was very small – the coefficient of variation was less than 10%. Further statistical analyses of the three trial replicates were carried out using R version 4.0.2 (R Core Team 2020). The L*a*b* values were analyzed using ANOVA, and then differentiated into groups using Fischer's LSD test with package agricolae. Additionally, the values for each sample were plotted in a 3D space using the package plot3Drgl and plot3d. The regression line in the 3D plot was calculated based on the principle axis of the point cloud using function prcomp(). The line was plotted as extending from the center of the principle component (PC) to either the minimum or maximum PC value times the loadings of the PC. The equation of the regression line is presented in cartesian, two-point format along with the direction vector. Package ggplot2 was used to graphically represent the L*a*b* values and absorbance spectra. Lastly, the L*a*b* values were converted to hexadecimal codes (Loncar n.d.) to visually represent the tristimulus values.

3.3 Results

Photos of the coffee grounds showcase the difference in color among the three roast levels (Fig. 3.2). Between the three origins (El Salvador, Ethiopia, and Sumatra) the color remained

similar within the same roast level. The biggest variation of color came from the roast; as expected, light roasts were the lightest in color and dark roasts were the darkest.

Figure 3.2: True-color image of the coffee grounds used in this experiment, using a natural white balance. From left to right: El Salvador, Ethiopia, Sumatra. From top to bottom: light roast, medium roast, dark roast.   Each sample of grounds is placed in a 4-cm diameter glass petri dish.

Quantification of the colors corroborates these qualitative impressions (Table 3.1). The Agtron Gourmet scores for whole beans were approximately 38 for dark roast, 48 for medium roast, and 58 for light roast, regardless of origin. Both the whole bean and the grounds were measured in the L*a*b* color space, and a representative hexadecimal swatch is included in Table 3.1 next to the tristimulus values; this swatch is a visual representation of the L*a*b* values, and we emphasize that the visual representation might differ on different computer monitors or printouts. Consistent with the qualitative impressions, the light roast for each origin had the highest L*a*b* values, with L* near 31 for light roasts, near 28 for medium roasts, and near 23 for dark roasts, again regardless of origin. Similar decreases in a* and b* are

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observed with roast level. Separate measurements of the ground coffee exhibited qualitatively similar trends as the whole beans, albeit with significantly higher values than in the whole beans ($p < 0.1$, $p < 0.001$, $p < .01$ for L*, a*, and b* respectively), except for dark roasts which tended to be more uniform.

Table 3.1: Agtron and L*a*b* values of whole roasted beans and coffee grounds. Values reported as mean ± one standard

Origin	Roast	Agtron Gourmet Score		Whole Bean				Ground			
		Whole Bean	Ground	L*	a*	b*	Hexadecimal Swatch	L*	a*	b*	Hexadecimal Swatch
ELS	Light	58.74 ± 1.40	68.18 ± 0.88	31.05 ± 1.94	9.26 ± 0.42	13.06 ± 0.92		31.10 ± 0.41	12.10 ± 0.10	19.06 ± 0.28	
ELS	Medium	49.64 ± 1.15	53.40 ± 1.15	28.22 ± 0.05	8.48 ± 0.31	10.60 ± 0.08		29.95 ± 0.63	11.46 ± 0.20	17.07 ± 0.36	
ELS	Dark	36.78 ± 1.49	35.92 ± 1.58	23.99 ± 0.69	6.64 ± 0.11	6.32 ± 0.20		23.72 ± 0.32	9.36 ± 0.04	10.22 ± 0.04	
ETH	Light	56.96 ± 0.79	68.20 ± 0.72	33.28 ± 0.36	8.55 ± 0.03	13.83 ± 0.21		34.38 ± 0.74	10.98 ± 0.08	19.59 ± 0.32	
ETH	Medium	49.46 ± 1.33	54.16 ± 1.11	29.16 ± 0.19	8.04 ± 0.14	11.21 ± 0.02		29.10 ± 0.71	10.69 ± 0.25	15.32 ± 0.33	
ETH	Dark	36.82 ± 1.93	34.98 ± 1.94	23.43 ± 0.10	6.89 ± 0.05	6.55 ± 0.12		22.48 ± 0.52	8.94 ± 0.27	9.42 ± 0.35	
SUM	Light	56.14 ± 0.74	66.96 ± 1.34	31.89 ± 0.26	8.91 ± 0.24	13.46 ± 0.36		31.70 ± 1.20	12.06 ± 0.08	18.36 ± 0.39	
SUM	Medium	49.24 ± 0.93	53.48 ± 1.28	28.48 ± 0.35	7.88 ± 0.14	10.52 ± 0.37		29.39 ± 1.12	11.26 ± 0.05	15.36 ± 0.33	
SUM	Dark	38.12 ± 0.69	35.62 ± 0.46	23.48 ± 0.74	6.44 ± 0.22	6.41 ± 0.23		21.06 ± 0.22	8.24 ± 0.14	8.18 ± 0.14	

deviation, with n=5 measurement replicates for Agtron Gourmet Score and n=3 measurement replicates for L*a*b* values. Colors in "Roast" column are only illustrative; colors in "Hexadecimal Swatch" columns correspond to the equivalent L*a*b* values.

Turning attention to the brewed coffee, the physical characteristics of each brew are outlined in Table 3.2, including the equilibrium TDS, the brew mass (i.e., the mass of brewed coffee obtained following filtration), the equilibrium pH, and the equilibrium titratable acidity.

Also tabulated are the measured TDS following dilution to a target of 2% TDS and the final brew mass after dilution.

Table 3.2: Physical and chemical measurements for each of the brews, shown as mean ± one standard deviation for n=3 trial replicates. Color values in "Roast" and "Brew Temperature" columns are illustrative only.

Origin	Roast	Brew Temperature	Equilibrium TDS (%)	Initial Brew Mass (g)	Diluted TDS (%)	Diluted Brew Mass (g)	Diluted pH	Diluted Titratable Acidity (mL NaOH)
ELS	Light	92°C	4.30 ± 0.02	922.57 ± 5.14	1.97 ± 0.05	1988.73 ± 45.67	4.88 ± 0.02	10.03 ± 0.45
		22°C	4.01 ± 0.04	934.10 ± 16.85	1.97 ± 0.06	1916.83 ± 79.55	4.93 ± 0.02	10.00 ± 0.36
		4°C	3.78 ± 0.04	886.70 ± 31.87	2.00 ± 0.03	1670.20 ± 73.52	4.97 ± 0.02	11.03 ± 0.45
	Medium	92°C	4.20 ± 0.06	910.50 ± 33.05	2.04 ± 0.04	1252.73 ± 45.92	5.01 ± 0.01	8.40 ± 0.87
		22°C	3.90 ± 0.05	924.67 ± 22.43	1.97 ± 0.06	1819.87 ± 40.58	5.10 ± 0.01	9.47 ± 0.68
		4°C	3.81 ± 0.15	914.27 ± 38.05	1.91 ± 0.06	569.50 ± 183.58	5.15 ± 0.02	9.00 ± 0.79
	Dark	92°C	4.13 ± 0.07	844.23 ± 13.62	2.00 ± 0.06	1762.83 ± 46.86	5.40 ± 0.02	6.20 ± 0.20
		22°C	3.74 ± 0.04	859.53 ± 13.92	1.99 ± 0.04	1682.00 ± 220.19	5.59 ± 0.01	6.75 ± 0.78
		4°C	3.50 ± 0.04	803.87 ± 22.04	1.97 ± 0.03	1375.17 ± 55.30	5.66 ± 0.03	6.70 ± 0.61
ETH	Light	92°C	4.45 ± 018	978.27 ± 10.90	1.99 ± 0.05	1438.43 ± 23.16	4.81 ± 0.02	10.10 ± 0.00
		22°C	4.21 ± 0.05	974.63 ± 29.84	2.00 ± 0.07	2061.47 ± 79.13	4.87 ± 0.01	10.17 ± 0.91
		4°C	4.06 ± 0.11	976.67 ± 11.21	2.00 ± 0.08	1976.87 ± 79.10	4.91 ± 0.03	10.37 ± 0.57
	Medium	92°C	4.31 ± 0.02	957.97 ± 15.63	2.02 ± 0.06	1355.56 ± 46.43	4.95 ± 0.01	9.43 ± 0.50
		22°C	4.08 ± 0.08	970.47 ± 19.05	1.99 ± 0.06	1916.55 ± 5.44	5.04 ± 0.01	9.13 ± 0.71
		4°C	3.89 ± 0.13	940.57 ± 56.19	1.97 ± 0.01	1829.00 ± 133.72	5.07 ± 0.02	10.00 ± 0.35
	Dark	92°C	4.06 ± 0.16	909.77 ± 8.45	2.02 ± 0.03	1235.03 ± 114.19	5.38 ± 0.06	6.40 ± 0.66
		22°C	3.73 ± 0.08	897.20 ± 28.35	1.96 ± 0.04	1642.27 ± 75.32	5.52 ± 0.02	7.17 ± 0.32
		4°C	3.46 ± 0.04	842.63 ± 44.74	1.99 ± 0.01	1436.37 ± 81.69	5.60 ± 0.02	6.80 ± 0.30
SUM	Light	92°C	4.42 ± 0.04	951.43 ± 18.96	1.97 ± 0.01	2069.60 ± 46.44	4.94 ± 0.02	9.25 ± 0.21
		22°C	4.23 ± 0.09	965.83 ± 17.85	2.01 ± 0.05	2027.80 ± 90.72	5.00 ± 0.01	9.97 ± 0.91
		4°C	4.00 ± 0.11	916.27 ± 36.11	1.97 ± 0.03	1816.33 ± 129.27	5.07 ± 0.10	9.23 ± 0.59
	Medium	92°C	4.30 ± 0.03	925.17 ± 10.80	1.97 ± 0.04	2014.93 ± 77.48	5.08 ± 0.02	8.67 ± 0.38
		22°C	4.11 ± 0.13	938.80 ± 20.66	1.98 ± 0.06	1274.60 ± 26.91	5.17 ± 0.02	8.80 ± 0.40
		4°C	3.78 ± 0.03	892.07 ± 26.31	1.99 ± 0.01	1126.76 ± 55.05	5.21 ± 0.04	9.03 ± 0.15
	Dark	92°C	4.23 ± 0.06	878.37 ± 31.17	1.98 ± 0.04	1846.73 ± 80.59	5.48 ± 0.02	5.60 ± 0.36
		22°C	3.83 ± 0.05	867.60 ± 4.96	1.95 ± 0.00	1680.97 ± 65.24	5.72 ± 0.01	5.57 ± 0.40
		4°C	3.58 ± 0.05	816.40 ± 46.90	1.99 ± 0.02	1445.57 ± 81.41	5.81 ± 0.03	6.23 ± 0.25

In general, hot temperature brews tended to have higher equilibrium TDS than their room or fridge temperature counterparts (Fig. 3.3). The roast level also strongly influenced equilibrium TDS; dark roasts had slightly lower TDS values than light or medium roast at all temperatures (Fig. 3.3A). Brew temperature had less impact on the delivered mass (Fig. 3.3B), with the darker roast levels yielding less brew, presumably because of increased retention of liquid within the spent grounds. Consistent with prior observations (Batali et al., 2021), roast level also strongly influenced the pH and titratable acidity, where brews of the same roast had similar pH levels and total titratable acidity regardless of origin. Dark roasts were the least acidic, and light roasts were the most acidic (Fig. 3.3C-D). To control for any effect differing levels of TDS on the color, all brews were diluted to a target of 2% TDS; as indicated in Table 3.2, when averaged over all samples the diluted TDS was 1.98 % with a standard deviation of 0.04 %.
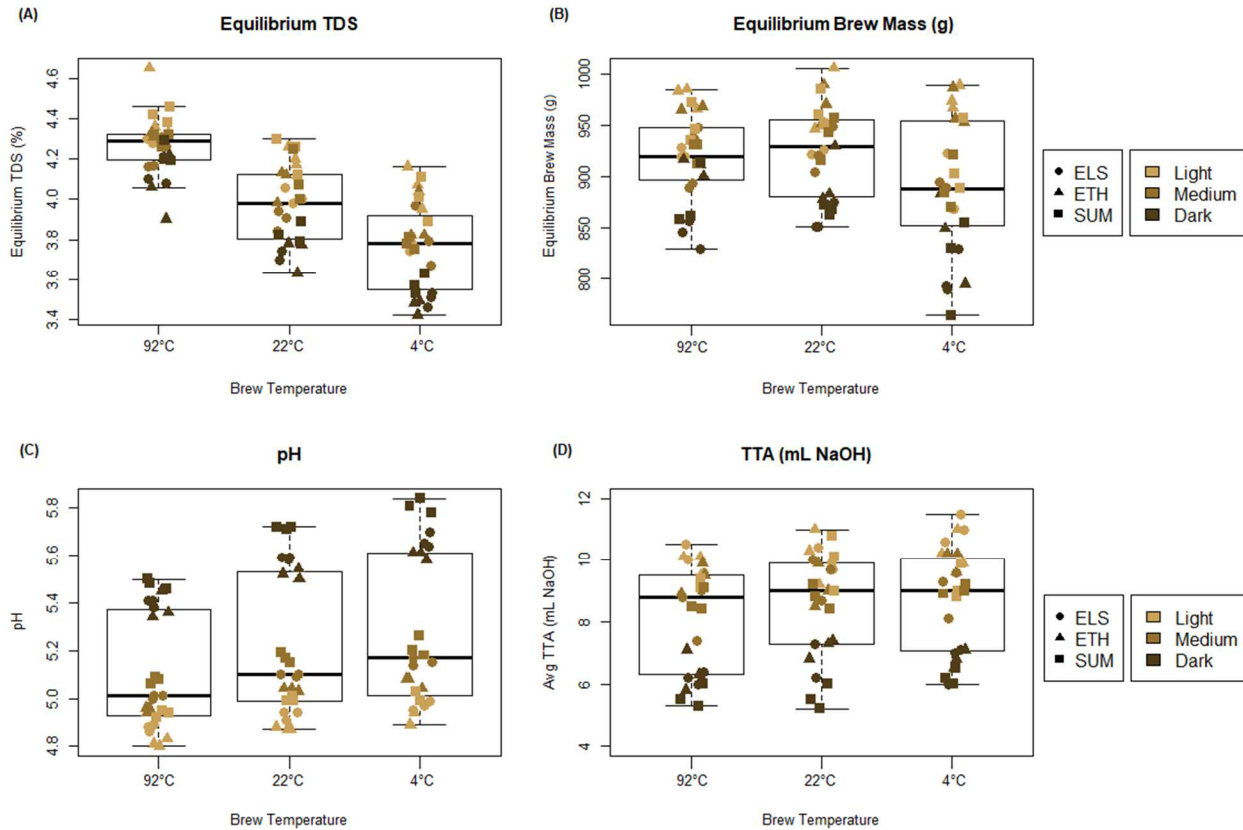
Figure 3.3: Brew characteristics of the 81 different brews, separated by brew temperature. The equilibrium TDS (A) and equilibrium brew mass (B), were measured prior to dilution. The pH (C) and titratable acidity (D) were measured after dilution.

After taking care to dilute the brews to the same TDS, it was readily apparent that the brews varied significantly in color. Figure 3.4 shows representative photos of the brews when poured into glass test tubes. These six samples (of the 27 total sample types) were chosen to represent the spectrum of color present in the coffee brews. Qualitatively, the lightest brew, Sumatra light roast brewed at 22°C, looked orange in appearance, especially compared to the brown-black of the El Salvador dark roast brewed at 92°C. In general, the cold brews (22°C and 4°C) were more reddish in appearance than the hot (92°C) brews, which were browner.

Additionally, the darker the roast, the darker the color of the brew, as shown in the comparison

between a light, medium, and dark roast brewed all brewed at 92°C (tubes 1-3, Figure 3.4).
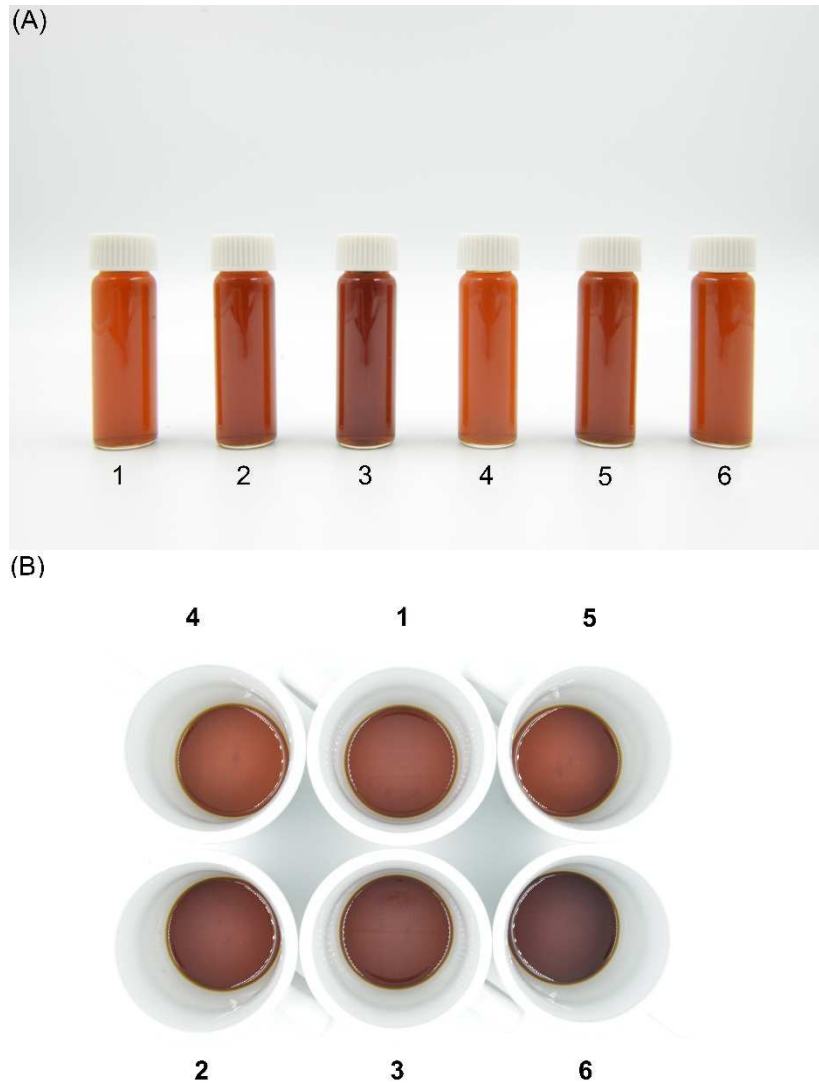

Figure 3.4: True color images, using a natural white balance, of six representative brews placed as (A) 5 mL in glass vials or (B) 20 mL in white ceramic mugs. Number codes indicate: 1: ETH Light 92˚C; 2: ELS Medium 92˚C; 3: ELS Dark 92˚C; 4: SUM Light 22˚C; 5: ETH Medium 4˚C; 6: SUM Dark 4˚C.

Notably, the brewed coffee exhibited a different color than the coffee grounds from which

it was derived, with the difference depending on roast and brew temperature (Table 3.3).

Across roasts and temperatures, the brews were redder (higher a* value) than the grounds themselves. Moreover, both roast level and brew temperature influenced the color of the brew, as shown in the hexadecimal swatches for each brew.

Table 3.3: L*a*b* values and representative color swatch by origin, roast, and temperature, presented as mean ± one standard deviation of three trial replicates. Colors in "Roast" and "Brew Temperature" columns are illustrative only; colors in the "Hexadecimal Swatch" column correspond to the equivalent L*a*b* values.

Origin	Roast	Brew Temperature	L*	a*	b*	Hexadecimal Swatch
ELS	Light	92°C	33.64 ± 2.17	26.08 ± 1.99	19.03 ± 4.08	
		22°C	36.42 ± 2.02	25.91 ± 2.05	22.05 ± 3.75	
		4°C	32.53 ± 3.00	21.29 ± 4.43	15.33 ± 5.43	
	Medium	92°C	29.44 ± 0.94	23.57 ± 1.50	12.44 ± 1.96	
		22°C	31.02 ± 1.71	21.85 ± 2.67	13.51 ± 3.03	
		4°C	30.51 ± 2.65	20.28 ± 4.76	13.02 ± 5.62	
	Dark	92°C	25.94 ± 1.49	17.77 ± 3.12	7.28 ± 2.48	
		22°C	26.32 ± 0.94	16.17 ± 1.75	7.26 ± 1.44	
		4°C	25.98 ± 1.47	13.50 ± 2.98	5.73 ± 1.96	
ETH	Light	92°C	33.45 ± 0.51	25.96 ± 0.59	18.59 ± 1.21	
		22°C	36.45 ± 1.30	26.46 ± 0.66	22.14 ± 1.93	
		4°C	37.41 ± 1.43	26.95 ± 1.70	24.76 ± 2.98	
	Medium	92°C	29.19 ± 1.25	22.60 ± 1.74	12.10 ± 1.92	
		22°C	32.38 ± 1.82	24.35 ± 2.47	15.86 ± 3.79	
		4°C	31.85 ± 2.18	22.89 ± 2.66	15.40 ± 4.00	
	Dark	92°C	25.35 ± 1.00	15.15 ± 2.90	5.45 ± 1.70	
		22°C	27.09 ± 0.53	16.28 ± 2.07	7.21 ± 1.95	
		4°C	25.70 ± 0.50	12.96 ± 2.78	5.33 ± 1.91	
SUM	Light	92°C	31.86 ± 0.75	23.84 ± 0.87	15.20 ± 1.19	
		22°C	37.52 ± 0.94	27.68 ± 0.89	24.10 ± 2.23	
		4°C	34.65 ± 4.11	24.65 ± 3.60	19.96 ± 7.29	
	Medium	92°C	29.44 ± 0.98	22.42 ± 1.23	11.96 ± 1.56	
		22°C	32.62 ± 1.73	24.28 ± 2.38	16.61 ± 3.01	
		4°C	31.45 ± 2.04	22.57 ± 3.06	14.91 ± 4.32	
	Dark	92°C	25.53 ± 0.35	16.35 ± 0.87	6.09 ± 0.63	
		22°C	28.67 ± 3.86	19.68 ± 7.28	11.02 ± 6.35	
		4°C	25.42 ± 1.02	12.96 ± 1.89	5.15 ± 1.50	

To further examine the differences in tristimulus values among brew temperatures, the L*a*b* values were graphed for each origin, roast level, and brew temperature. Increased roast level led to decreases in L*a*b* values across origins and brew temperatures. Differences

between brew temperature were most common in light roasts (Fig. 3.5A-C, 3.4G-I). Within the

light roasts, there was at least one brew temperature that had a significantly different L* value

(Fig. 3.5A-C). Across both roast levels and brew temperatures, the a* values had the fewest

significant differences (Fig. 3.5D-F). In dark roasts, differences between brew temperatures

decreased as the tristimulus values themselves decreased. Hot brews tended to have the

lowest tristimulus values. Interestingly, Sumatra room temperature brews had higher

tristimulus values than their hot or fridge counterparts for all three roasts.
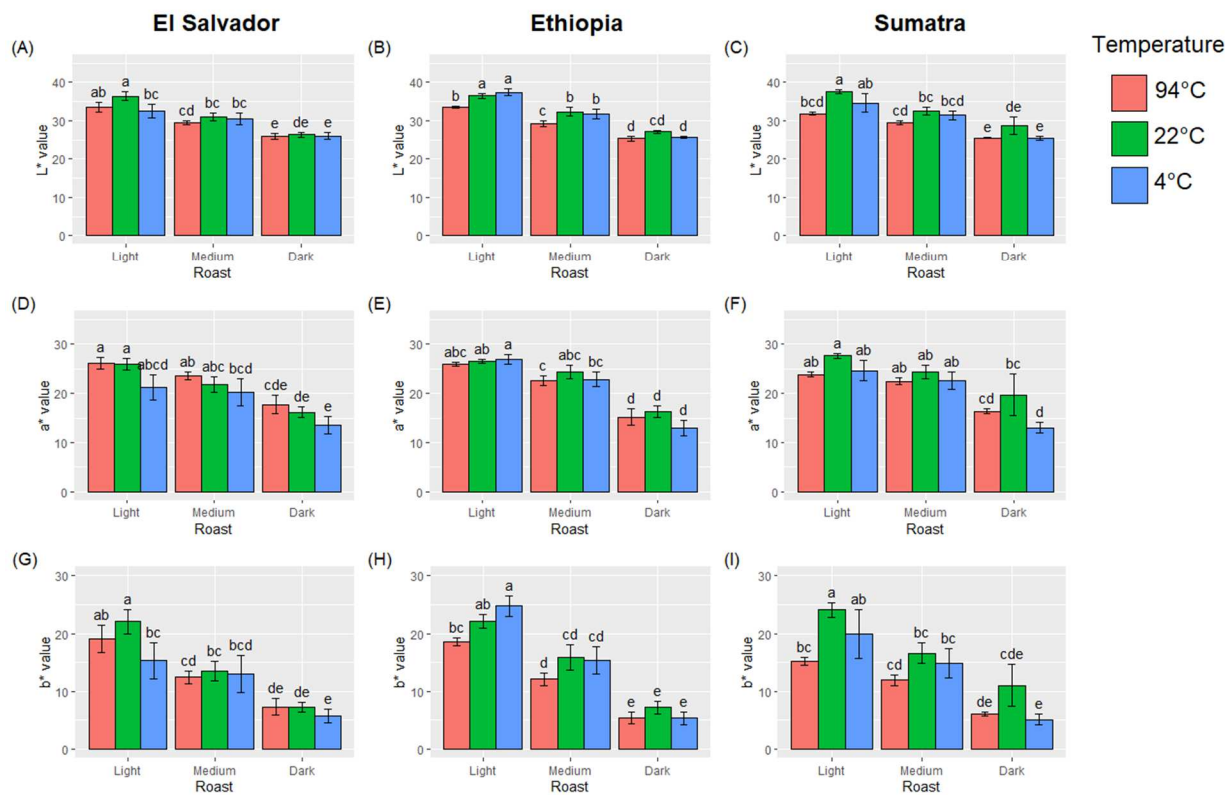
Figure 3.5: L*a*b* values for each origin, roast, and temperature. Different lowercase letters (a-e) denote statistically significant different groups. Brews with the same lowercase letter (a-e) are not significantly different.

Because the tristimulus values represent a three-dimensional color space, the values for

each of the brews can be graphed in three dimensions as well. In Fig. 3.6, each data point

within the box represents the L*a*b* values for that brew, and the color of the data point is the

is representative of roast level (light, medium, or dark) while the color of the text is

representative of brew temperature (4°C, 22°C, and 92°C)(Fig. 3.5). Each of the points can be

grouped two ways – by roast and by brew temperature. Brews of the same roast are clustered

together, with light roasts having the highest L*a*b* values and dark roasts having the lowest.

Brews with different brew temperatures are dispersed evenly throughout – brew temperature

does not have a clear trend across both origins and roast levels on the tristimulus values.

The color data points follow a line in three-dimensional space given by the three parametric

equations:

$$L^* = 30.66 + 12.33t; \ a^* = 21.28 + 14.13t; \ b^* = 13.61 + 19.29t \ \text{for} -0.477 \le t \le 0.523, \qquad (1)$$

where t represents distance along the line from the center point. Solving for variable t gives the

following equivalent set of parametric equations:

$$t = \frac{(L^*-30.66)}{12.33}; t = \frac{(a^*-21.28)}{14.13}; \ t = \frac{(b^*-13.61)}{19.29} \qquad\qquad (2)$$

Since variable t will be equivalent in all three equations, the three parametric equations can be

set equal to give a symmetric form:

$$\frac{(L^*-30.66)}{12.33} = \frac{(a^*-21.28)}{14.13} = \frac{(b^*-13.61)}{19.29} \qquad\qquad (3)$$

In other words, the L*a*b* values are linked in a positive linear relationship; as one of

the values decreased, so did the other two. Plotting the tristimulus values in three-dimensional

space also gives insight into the difference in color between brews, based on the distance

between the points. For example, Ethiopia light roast brewed at 4°C had the largest absolute difference in tristimulus values from Sumatra dark roast brewed at 4°C, placing the two brews furthest apart in three-dimensional space (Fig. 3.6). Additionally, Sumatra light roast brewed at 92°C was more like a Sumatra medium 4°C brew than a Sumatra light roast at 4°C (Fig. 3.6); in other words, brewing at a hot temperature resulted in a color more indicative of medium roast than light roast.
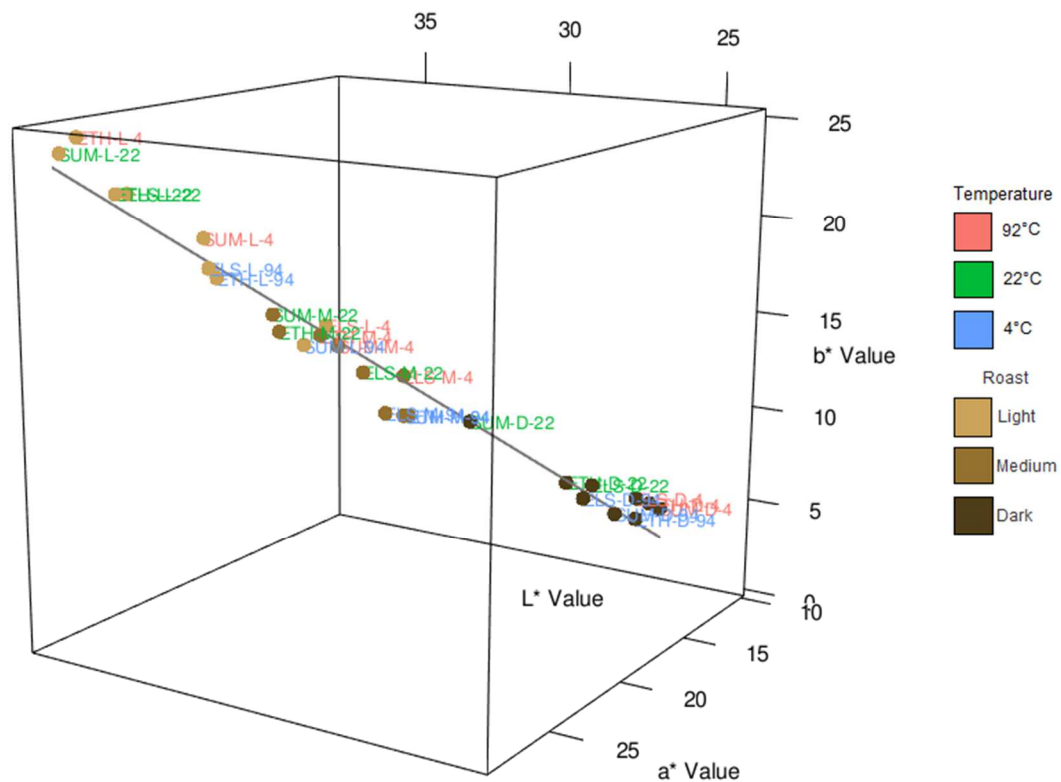

Figure 3.6: Three-dimensional plot of the L*a*b* values for each sample type grouped by roast and brew temperature. The black line denotes the linear best fit (cf. equations 1-3). See also supplementary movie 3.1.

Lastly, the absorbance spectra between 350 nm and 750 nm of each of the brews was examined (Fig. 3.7). With the exception of El Salvador light and medium roasts, the hot (92°C) brews had separate UV-Vis absorbance curves than the room (22°C) or fridge (4°C) brews. Because the 22°C and 4°C brews had absorbance spectra that are farther left on the visible spectrum, they appeared more reddish in color than the 92°C brews. The closeness (or even overlap) of the 22°C and 4°C brews suggest that they were more similar in appearance compared to the 92°C brews.
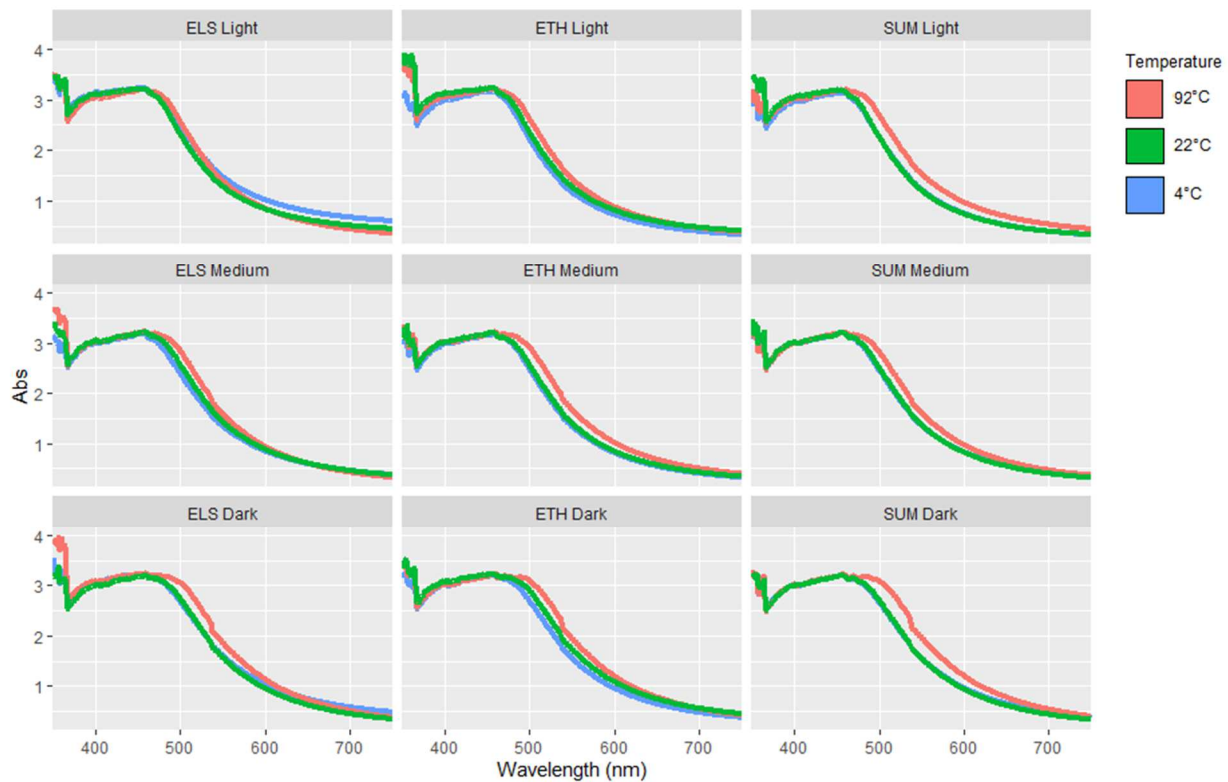
Figure 3.7: UV-Vis absorbance spectra from 350 nm-750 nm.

3.4 Discussion

The color of the coffee beverage is strongly influenced not only by roast level, but by brew temperature as well, especially within light and medium roast levels. Based on previous work

linking increased roasting with darker bean colors (Da Porto 1991; Nicoli 1997), it is perhaps

unsurprising that roast level would be a major factor in the final color of the coffee brew.

However, it is more surprising that brew temperature would also affect the color of the coffee

brew. Understanding how these two factors ultimately impact the final beverage can lead to

opportunities to brand and market the color of the coffee by manipulating roast level and brew

temperature.

The photos of the grounds and brews provide important insight into how color is extracted

into the brew. Even though the grounds for each roast level look almost identical (Fig. 3.2), the

color of the coffee brew itself does not follow the same pattern. The grounds provide a

foundational layer of color that is then altered during the extraction process, based on origin

and brew temperature. Similarly, the color of the grounds is drastically different than the color

of the coffee brew, regardless of origin and temperature. In other words, brewing coffee

grounds of a certain color does not yield a direct translation of the color from grounds to cup.

Moreover, the photo of the coffee brew in the mugs (Fig. 3.3B) highlights the visual disparity

that consumers may face when sampling different beverages. The color of the coffee brew can

serve as an indicator for brew strength (Pangborn 1982), but also for flavor compounds that are

generated during roasting (Lawless and Heymann 2010); such large differences in color can

affect the perceived sensory characteristics.

However, color differences are usually measured in a subjective manner (dos Santos Scholz

et al. 2018; Kalschne et al. 2019; Pangborn 1982) because it is a rather subjective sensory

modality. Measuring the appearance and color of objects is traditionally performed by

instruments due to the wide variation in human vision and the tricky nature of color itself

(Lawless and Heymann 2010). The color can be affected by composition of the object itself, the spectral illumination on the object, and the sensitivity of the viewer's eyes (Lawless and Heymann 2010). Performing colorimetric analysis with instruments depends solely on the composition of the object, removing any variations in illumination or sensitivity of the viewer's eyes, producing reliable and objective measurements of the object's color. Qualitative judgements about the difference in color may give insight into the perception of the coffee product, but instrumental analysis is needed to concretely find differences between products.

Quantitatively, these differences in color are translated into the L*a*b* values for both the coffee beans, grounds, and the coffee brew. The tristimulus values for the coffee grounds (Table 3.2) follow the same pattern as previously discovered; increased roast level leads to lower L*a*b* values (Bicho 2011; Da Porto 1991; Illy 1995; Nicoli et al. 1997). Dark roasts, which approach the color black as roasting continues, will have the lowest tristimulus values as there is an increasing absence of color (Lawless and Heymann 2010). This is intuitive for the L* measure, which is determined by lightness, but it also applies to a* (greenness-redness) and b* (blueness-yellowness). As the color of the bean approaches black, a* and b* will approach a value of 0. Moreover, it becomes harder to detect differences in color the closer to black the values become, which is why dark roasts tended to have fewer significant differences. Lastly, higher Agtron Gourmet readings and L*a*b* values in the grounds when compared to the beans can be explained by the process of grinding that homogenizes the mixture and exposes the less roasted interior of the bean (Illy 1995).

Visualizing the tristimulus values in three-dimensional space led to a very interesting, strongly linear relationship between the L*a*b* values across the roast levels. Equation 1,

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which links each value together, implies that the color of a coffee beverage can be predicted a priori for given coffee grounds based on the roast level and anticipated brew temperature.

The color of the coffee beverage can have profound effects on perceived sensory characteristics. Reddish colored beverages can taste less bitter and sweeter than those with lower intensities of red coloring (Johnson and Clydesdale 1982; Maga 1974), although it is unclear whether the color differences observed here will have as large an effect. Nonetheless, a plausible hypothesis is that the differences in color between different brewing temperatures may affect the perceived flavor of the beverage, since the 4°C and 22°C brews tended to be redder in color (Figs 3.3, 3.6). Sensory analysis of coffee is sometimes performed with panelists in sensory booths illuminated with red light to minimize the impact of sample color perception (Frost et al. 2020, Batali et al. 2020), but most often coffee is cupped under regular illumination. Further research is necessary to elucidate how brew color affects flavor perception of coffee.

It is unclear how the chemical compositions for different roast levels and brew temperatures affects the final observed color. It is well established that the brown color in roasted coffee is a result of melanoidins produced during the roasting process as well as the caramelization of sucrose (Bradbury 2001; Illy 1995; Macrae 1985). Melanoidins are polymeric products of the Maillard reaction and can be separated into three classes based on their molecular weight: low, intermediate and high (Bekedam et al. 2008). The amount of each class of melanoidin differs by roast level; the darker the roast, the higher the percentage of high molecular weight melanoidins (Bekedam et al. 2008). Increased levels of high molecular weight melanoidins could account for the darker colors of the dark roast coffee brews. Brown pigmentation also comes from the caramelization of sucrose, which occurs whenever the

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roasting temperature reaches above 130˚C (Trugo 1985). The resulting product is a water-soluble heterocyclic compound, which can then polymerize to form the Maillard-like brown pigments (Tressl et al. 1998; Bradbury 2001). The inclusion of two different classes of colored compounds (melanoidins and caramels) hints at the possibility of differential extraction across different brew temperatures. The size and solubility of these compounds would affect their overall extraction into the brew, accounting for the changes in color. The slight differences in equilibrium TDS we observe (Fig. 3.2A) suggest that differences in the size and solubility of colored compounds has an effect on color; higher equilibrium TDS levels should yield a darker color. Here we performed only simple chemical measurements of pH and TTA (Fig. 3.2C,D). Further research into the chemical composition into coffees brewed at the same temperature would elucidate why roast level and brew temperature influence the color of the coffee liquid.

The importance of color as an indicator of coffee quality and its role in sensory perception highlights possible marketing and branding opportunities. Harnessing the power of roast level and brew temperature to control the color of the final coffee liquid creates a novel approach to making unique coffee products.

3.5 Conclusions

Our systematic analysis of the color of different coffee brews yielded insights regarding an underappreciated aspect of coffee extraction. Perhaps unsurprisingly, coffee beans roasted to different colors yielded brews of different colors. More surprisingly, use of "cold" brewing temperatures (4°C or 22°C) led to a beverage that was much more reddish in color than the

typical brown-black color of hot (92°C) brewed coffee. Our finding that the color of the grounds

is not directly translated into the brew, and that the brew color varies significantly based on

brew temperature and origin, does complicate the choice of coffee and brewing parameters to

achieve brewed coffee of a desired color. However, the results also offer additional opportunity

for branding and marketing of cold brew, as 'reddish' in color. Additionally, differential

extraction of chemical species could be behind those color differences, thus warranting the

need for further research into the molecules and the physical and chemical processes that

affect coffee color.

3.6 Acknowledgments

3.7 References

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3.8 Supplementary Figures and Tables

Table S3.1: Roast profile details for each sample type, including bean density, time of first crack, duration of roast, development time, development time ratio, start and end temperature, and percent weight loss.

| Origin	Roast	Density (g/mL)	First crack (s)	Duration (s)	Dev. Time (s)	Dev. time ratio	Start temp. (˚C)	End temp. (˚C)	Weight loss
El Salvador	Green	0.69							
	Light	0.37	595.60	663.80	68.20	10.28	186	204	13%
	Medium	0.35	597.00	717.20	120.20	16.74	189	210	14%
	Dark	0.31	631.00	905.20	270.20	30.30	185	221	17%
Ethiopia	Green	0.67							
	Light	0.39	587.80	693.40	99.00	14.16	188	208	14%
	Medium	0.36	599.00	714.60	115.60	16.18	190	210	15%
	Dark	0.32	637.60	913.20	277.60	30.32	190	219	17%
Sumatra	Green	0.69							
	Light	0.38	637.80	711.40	73.60	10.38	187	205	12%
	Medium	0.38	618.60	747.80	129.20	17.28	188	211	13%
	Dark	0.34	657.00	958.00	301.00	31.42	180	221	16%
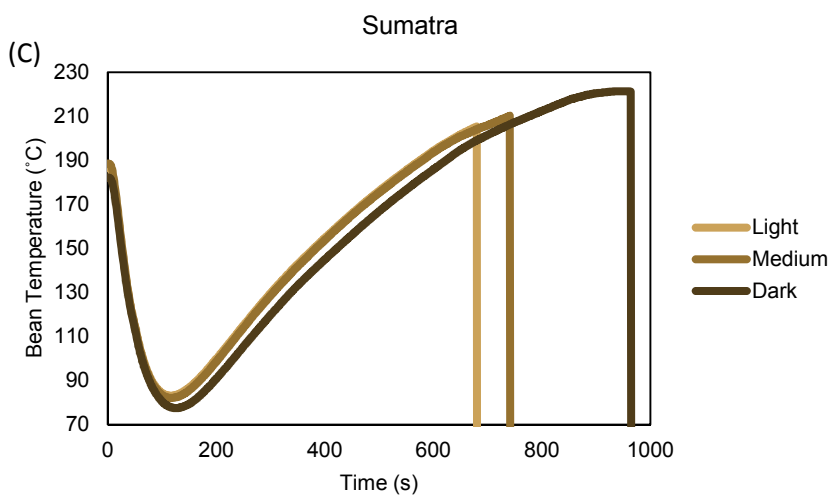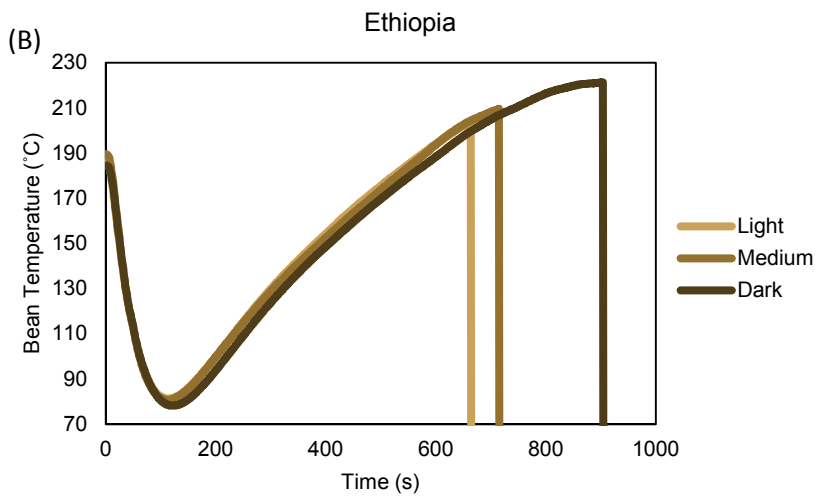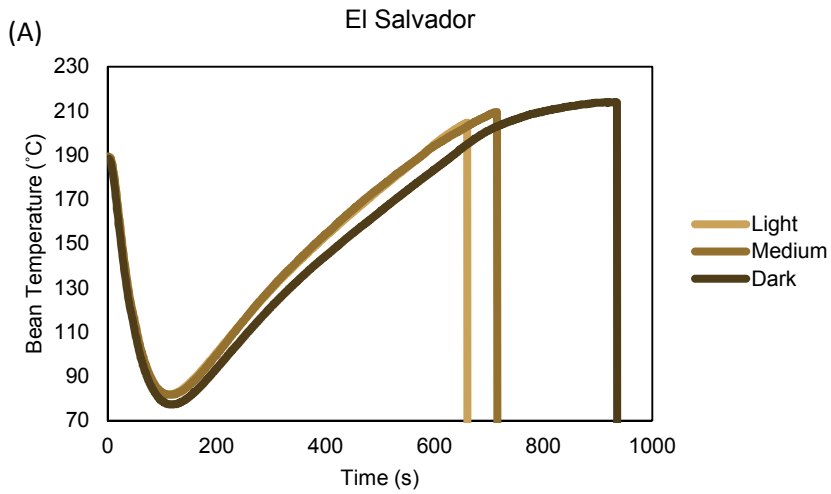
Figure S3.1: Roast curves for each of the 9 roast types, shown as increase in bean temperature (˚C) over time. A) El Salvador origin roasts. B) Ethiopia origin roasts. C) Sumatra origin roasts.
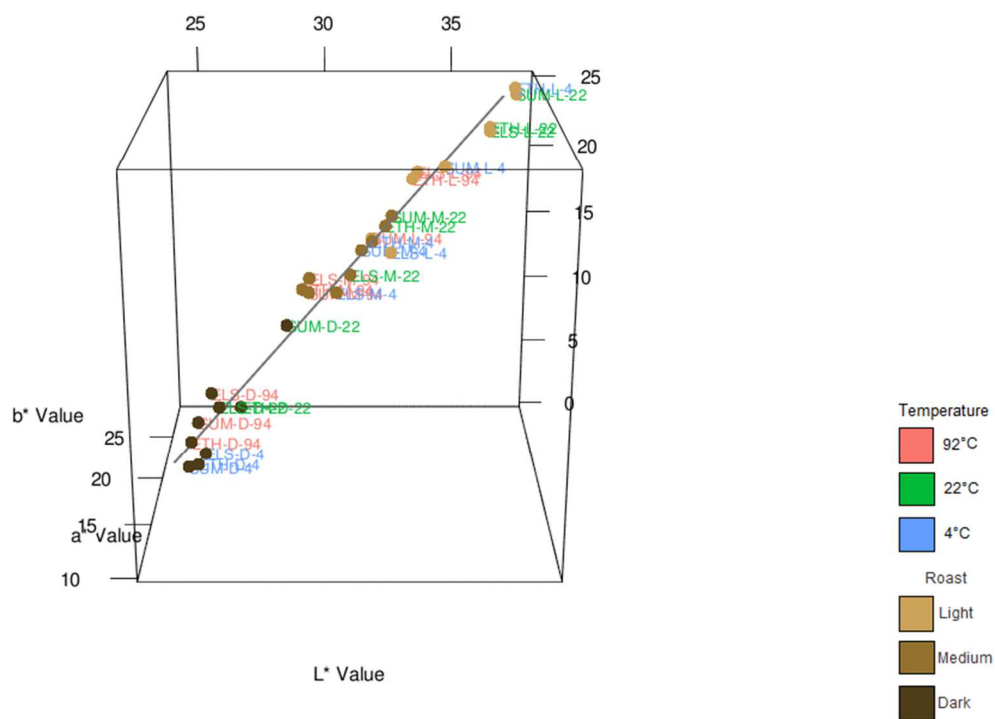
Movie S3.1: Rotation of three-dimensional plot of the L*a*b* values for each sample type grouped by roast and brew temperature. The black line denotes the linear best fit (cf. equations 1-3)