OPEN ACCESS
Potravinarstvo Slovak Journal of Food Sciences
Crossref Similarity Check Powered by iThenticate

potravinárstvo®

Slovak Journal of Food Sciences

*Potravinarstvo Slovak Journal of Food Sciences*
**vol. 13, 2019, no. 1, p. 344-350**
**https://doi.org/10.5219/1062**
Received: 10 February 2019. Accepted: 11 March 2019.
Available online: 28 May 2019 at www.potravinarstvo.com

ISSN 1337-0960 (online)

# THE EFFECT OF COFFEE BEANS ROASTING ON ITS CHEMICAL COMPOSITION

*Pavel Diviš, Jaromír Pořízka, Jakub Křikala*

## ABSTRACT

Drinking coffee has become part of our everyday culture. Coffee cultivation is devoted to over 50 countries in the world, located between latitudes 25 degrees North and 30 degrees South. Almost all of the world's coffee production is provided by two varieties, called 'Arabica' and 'Robusta' whereas the share of Arabica is 70% of the world's coffee harvest. Green (raw) coffee can not be used to prepare coffee beverages, coffee beans must first be roasted. Roasting coffee and reaching a certain degree of coffee roasting determine its flavor and aroma characteristics. In the present study the fate of sucrose, chlorogenic acid, acetic acid, formic acid, lactic acid, caffeic acid, total phenolic compounds and 5-hydroxymethylfurfural was studied in coffee (Brazil Cerrado Dulce, 100% Arabica) roasted in two ways (Medium roast and Full city roast). It has been found that almost all sucrose has been degraded (96 – 98%) in both roasting ways. During Medium roast 65% of chlorogenic acid contained in green coffee was degraded while during Full city roast it was 85%. During both Medium and Full city roasting, the formation of acetic acid but especially formic and lactic acid was recorded. The highest concentration of organic acids was recorded at Full City roasting at medium roasting times (3.3 $mg.g^{-1}$ d.w. acetic acid, 1.79 $mg.g^{-1}$ d.w. formic acid, 0.65 $mg.g^{-1}$d.w. lactic acid). The amount of phenolic substances also increased during roasting up to 16.7 $mg.g^{-1}$ d.w. of gallic acid equivalent. Highest concentrations of 5-hydroxymethylfurfural were measured at medium roasting times at both Medium (0.357 $mg.g^{-1}$ d.w.) and French city (0.597 $mg.g^{-1}$ d.w.) roasting temperatures. At the end of roasting, the 5-hydroxymethylfurfural concentration in coffee were 0.237 $mg.g^{-1}$ d.w. (Medium roast) and 0.095 $mg.g^{-1}$ d.w. (Full city roast).

**Keywords:** coffee; roasting; hydroxymethylfurfural; sucrose; organic acids

## INTRODUCTION

Coffee is made up of modified seed of the fruit of various tropical to subtropical trees or coffee shrubs. Coffee has a large number of varieties, only a few of them have economic significance. Almost all of the world's coffee production is provided by two varieties, called 'Arabica' and 'Robusta' **(Butt and Tauseef Sultan, 2011)**. Arabica (*Coffea arabica*), is the most important botanical species, especially for the high quality of its fruits. It comes from about 70% of the world's green coffee production. Robusta (*Coffea canephora*), is the second most important variety of coffee, and its share of world production is steadily growing mainly due to its greater adaptability to habitats and disease resistance. Other reasons to increase demand of Robusta coffee in the market are the growing demand for instant coffee, which is preferentially made from Robusta coffee and last but not least, lower price of Robusta coffee compared to Arabica coffee **(Kemsley et al., 1995)**. World coffee production in 2017 was about 9.5 million tonnes, which makes coffee the second most important commodity of world trade **(FAOSTAT, 2018)**.

After processing the coffee beans by wet or dry drying technologies **(Arya and Jagan Mohan Rao, 2007; Guimar, Berbert and Silva, 1998),** coffee beans are roasted. During coffee roasting, coffee beans get brown colour and their characteristic flavour and aroma **(Yeretzian et al., 2002)**. In different countries, different roasting styles have been created according to population preferences. These roasting styles differ from each other at the roasting temperature used and the total coffee roasting time **(Moon, Yoo and Shibamoto, 2009; Dórea and DaCosta, 2005)**.

Due to the popularity of coffee in the world many researchers were involved in coffee research in the last quarter of a century. Most studies on coffee are health-related studies **(Ciaramelli, Palmioli and Airoldi, 2019; Poole et al., 2017; Ludwig et al., 2014; Butt and Tauseef Sultan, 2011; Dórea et al., 2005)**. Other studies are focused on the role of roasting conditions of the coffee in the level of selected compounds. Information on what is happening in roasted coffee beans is quite sufficient in the available literature, but there are only few studies that deal with the complex monitoring of changes in the chemical composition of coffee beans during roasting **(Wei et al., 2012)**.

In the present study the fate of sucrose, chlorogenic acid, acetic acid, formic acid, lactic acid, caffeic acid, total phenolic compounds and 5-hydroxymethylfurfural was studied in coffee roasted in two ways (Medium roast and Full city roast).

### Scientific hypothesis

Higher temperature and higher time of coffee beans roasting cause higher amounts of 5-hydroxymethylfurfural, organic acids and phenolic compounds while reducing the carbohydrate content in the coffee beans.

## MATERIAL AND METHODOLOGY

### Chemicals and reagents

All water used in this study was ultrapure water (Elga pure lab classic, Veolia water systems, UK). All chemicals used in this study were analytical grade chemicals purchased from Sigma-Aldrich (Germany) company except of Karl-Fisher titration reagent and water standard which have been purchased from Labicom (Czech Republic).

### Sample preparation

The 100% Arabica coffee (Brazil Cerrado Dulce, 4coffee, Czech Republic) was used in this study. Total amount of 25g of green coffee beans was roasted in a home coffee roaster (Gene café CBR101, 4coffee, Czech Republic). Coffee was roasted with two roasting degrees as Medium roast and Full city roast. Roasting on Medium roast degree was done at 210 °C and the total roasting time was 14 min. Roasting on Full city roast degree was done at 225 °C and the total roasting time was 19 min. Extraction of organic acids, sucrose, 5-hydroxymethylfurfural and total phenolic compounds was performed in 25 mL Erlenmeyer flasks. One gram of sample weighted on analytical balancer and 10 mL of solvent (80 °C water mixed with ethanol in 60:40 volume ratio) were used for extraction. Extraction was carried out on a magnetic stirrer for 30 minutes. After the extraction, the samples were centrifuged at 5000 rpm in centrifuge and the supernatant was filtered using nylon syringe filters (0.45 μm, Labicom, Czech Republic) and used for analysis. All samples were prepared in two replicates.

### Chemical analysis

Acetic, formic and lactic acid were determined using ion chromatography (Metroohm 850 professional IC, Metroohm, Switzerland) with conductivity detector. An Agilent Infinity 1260 liquid chromatograph (Agilent Technologies, USA) equipped with ELSD detector was used for determination of sucrose. Both methods are described in detail at work published by **Diviš et al. (2018)**. Total phenolic compounds were determined using Helios gamma spectrophotometer (Spectronic Unicam, Great Britain) through the Folin-Ciocalteus method **(Singleton et al. 1999)** and expressed as gallic acid equivalent. Concentration of 5-hydroxymethylfurfural was determined on Agilent Infinity 1260 liquid chromatograph with DAD detector using Kinetex EVO-C18 column and acetonitrile mixed with water in 15:85 volume ratio. Chlorogenic and caffeic acid were determined on Agilent Infinity 1260 liquid chromatograph with DAD detector using Kinetex EVO-C18 column and mixture of 2.5% formic acid and acetonitrile in 90:10 volume ratio as mobile phase. Water content in all samples was determined by Karl-Fisher titration **(Verhoef and Barendrecht, 1977)** using KF Titrino 701 titrator (Metroohm, Switzerland)**.** The pH value was measured using pH meter with combined electrodes (WTW, Germany). All parameters for a single sample were measured in three replicates. All measured concentrations were recalculated to dry weight of coffee.

### Statistic analysis

All experimental data were statistically processed using software XLstat (Addinsoft, USA). Obtained data were pre-treated by using Analysis of Variance (ANOVA) to find statistical significant differences between groups. Tukey's comparative test on the significance level 0.05 has been performed for individual parameters observed during coffee roasting. The pre-treated data were used as input parameters in Principal Component Analysis (PCA) to find correlation between the chemical composition changes during the roasting process.

## RESULTS AND DISCUSSION

Coffee beans contain, in addition to water and minerals, a large number of organic substances. The main component of coffee beans are carbohydrates. The coffee beans contain various hemicelluloses, starch, oligosaccharides and mainly sucrose. The amount of monosaccharides is relatively small. Other substances contained in coffee are proteins, non-protein nitrogenous substances, phenolic substances, non-volatile organic acids, volatile substances and oils **(Arya and Jagan Mohan Rao, 2007; Farah and Marino Donagelo, 2006; Redgwell and Fisher, 2006)**.

Concentration of sucrose in green coffee beans and in roasted coffee beans is presented in Table 1 and Table 2. The results show that sucrose degradation occurs during the roasting process. Sucrose degradation is explained by sucrose hydrolysis to glucose and fructose, which may be further fragmented to form aliphatic acids, or which may participate in Maillard reactions with proteins or amino acids **(Ginz et al. 2000)**. The sucrose concentration decreased in the middle of the roasting process by 47% in the case of Medium roast and by 59% in the case of Full city roast. At the end of the roasting process, almost all sucrose has already been degraded (96 – 98%).

Another substance that has been observed to reduce the concentration during the roasting process was chlorogenic acid. Concentration of chlorogenic acid in green coffee beans and in roasted coffee beans is presented in Table 3 and Table 4. Chlorogenic acid concentration decreased in the middle of the roasting process by 45% in the case of Medium roast and by 42% in the case of Full city roast. At the end of the roasting process, 67% of chlorogenic acid contained in green coffee was degraded during Medium roast and 85% during Full city roast. Chlorogenic acid is involved in colour, flavour and aroma formation of coffee **Farah and Marino Donagelo, 2006; Farah et al., 2005)**. Major degradation products of chlorogenic acid are melanoids and low molecular weight compounds.

Strong significant correlation was found between sucrose concentration and concentration of organic acid during coffee roasting ($r$ >0.9).

Concentration of organic acid in coffee during the roasting process is shown in Table 3 and Table 4. While the sucrose concentration in coffee decreases during roasting, the concentration of organic acids significantly increases. The most significant change was found in the lactic and formic acid content. The content of these acids in coffee beans rose almost 100 times after coffee roasting. Trend of changes in the concentration of organic acids was similar for Medium roasting and French roasting, however in the case of French roasting decrease in organic acid content was observed in the later stage of roasting. **Ginz et al. (2000)** lists the content of organic acids in Robusta coffee after roasting to be approximately 2 $mg.g^{-1}$ in the case of formic acid and acetic acid and 0.2 $mg.g^{-1}$ in the case of lactic acid. Formation of organic acids in coffee is described by Lobry-deBruyn-vanEckenstein rearrangement reaction in which fructose or glucose produced by sucrose hydrolysis is involved, and by formation of 1,2-endiole or 2,3-endiole as acid precursors **(Ginz et al., 2000)**. Formation of organic acids in coffee during roasting process did not significantly affect the pH of the coffee (Table 1 and Table 2.). This finding can be caused due to highly complex buffering effects and the wide distributions of salts and acids present in coffee. **Jeszka- Jeszka-Skowron et al. (2016)** measured pH value

**Table 1** Content of sucrose, 5-hydroxymethylfurfural, total phenolic compounds and pH value of coffee roasted to Medium roast degree.

| Time | pH ($mg.g^{-1}$ ±SD) | sucrose ($mg.g^{-1}$ ±SD) | HMF ($mg.g^{-1}$ ±SD) | TPC ($mg.g^{-1}$ ±SD) |
|---|---|---|---|---|
| **0** | 6.09 ±0.05$^{a}$ | 70.1 ±4.9$^{a}$ | <0.010 | 8.5 ±0.8$^{e}$ |
| **4** | 5.93 ±0.05$^{ab}$ | 58.5 ±2.1$^{b}$ | <0.010 | 8.9 ±0.8$^{e}$ |
| **5** | 5.89 ±0.05$^{ab}$ | 57.0 ±6.4$^{bc}$ | <0.010 | 9.6 ±0.9$^{de}$ |
| **6** | 5.78 ±0.05$^{ab}$ | 50.1 ±3.5$^{c}$ | 0.013 ±0.004$^{d}$ | 10.8 ±0.6$^{cd}$ |
| **7** | 5.89 ±0.05$^{ab}$ | 38.8 ±3.8$^{d}$ | 0.044±0.016$^{d}$ | 12.8 ±0.6$^{ab}$ |
| **8** | 5.68 ±0.05$^{ab}$ | 23.8 ±2.5$^{e}$ | 0.136 ±0.013$^{c}$ | 12.0 ±0.7$^{bc}$ |
| **9** | 5.73 ±0.05$^{ab}$ | 14.3 ±2.5$^{f}$ | 0.281 ±0.031$^{ab}$ | 12.7 ±0.3$^{ab}$ |
| **10** | 5.68 ±0.05$^{ab}$ | 12.2 ±1.9$^{f}$ | 0.232±0.014$^{b}$ | 13.0 ±0.2$^{ab}$ |
| **11** | 5.72 ±0.05$^{ab}$ | 6.3 ±1.8$^{gh}$ | 0.139 ±0.021$^{c}$ | 13.7 ±0.3$^{a}$ |
| **12** | 5.65 ±0.05$^{ab}$ | 4.4 ±0.5$^{gh}$ | 0.264 ±0.046$^{b}$ | 14.4 ±0.4$^{a}$ |
| **13** | 5.68 ±0.05$^{ab}$ | 4.1 ±0.7$^{gh}$ | 0.346 ±0.016$^{a}$ | 14.0 ±0.5$^{a}$ |
| **14** | 5.65 ±0.05$^{ab}$ | 3.0 ±0.4$^{h}$ | 0.224 ±0.018$^{b}$ | 13.4 ±0.4$^{ab}$ |

Note: Values in the same column with different letters are significantly different at $p$ <0.05.

**Table 2** Content of sucrose, 5-hydroxymethylfurfural, total phenolic compounds and pH value of coffee roasted to Full city roast degree.

| Time | pH ($mg.g^{-1}$ ±SD) | sucrose ($mg.g^{-1}$ ±SD) | HMF ($mg.g^{-1}$ ±SD) | TPC ($mg.g^{-1}$ ±SD) |
|---|---|---|---|---|
| **0** | 6.09 ±0.05$^{a}$ | 70.1 ±4.9$^{a}$ | <0.010 | 8.5 ±0.8$^{e}$ |
| **4** | 5.95 ±0.05$^{a}$ | 62.8 ±3.9$^{ab}$ | <0.010 | 8.9 ±0.3$^{e}$ |
| **5** | 5.95 ±0.05$^{a}$ | 59.3 ±3.4$^{b}$ | <0.010 | 11.5 ±0.7$^{d}$ |
| **6** | 5.76 ±0.05$^{ab}$ | 59.5 ±5.1$^{ab}$ | 0.017 ±0.003$^{h}$ | 13.7 ±0.9$^{c}$ |
| **7** | 5.73 ±0.05$^{ab}$ | 41.6 ±4.2$^{c}$ | 0.091 ±0.006$^{gh}$ | 13.9 ±0.5$^{c}$ |
| **8** | 5.69 ±0.05$^{ab}$ | 30.6 ±2.8$^{d}$ | 0.326 ±0.018$^{bcd}$ | 13.1 ±0.7$^{c}$ |
| **9** | 5.78 ±0.05$^{ab}$ | 16.3 ±2.5$^{e}$ | 0.341 ±0.025$^{bc}$ | 13.2 ±0.9$^{c}$ |
| **10** | 5.77 ±0.05$^{ab}$ | 12.1 ±2.2$^{f}$ | 0.259 ±0.021$^{de}$ | 13.8 ±0.8$^{c}$ |
| **11** | 5.75 ±0.05$^{ab}$ | 5.7 ±1.3$^{g}$ | 0.207 ±0.013$^{ef}$ | 14.9 ±0.9$^{bc}$ |
| **12** | 5.69 ±0.05$^{ab}$ | 3.4 ±0.4$^{gh}$ | 0.549 ±0.029$^{a}$ | 15.8 ±1.2$^{ab}$ |
| **13** | 5.62 ±0.05$^{ab}$ | 2.5 ±0.3$^{h}$ | 0.510 ±0.017$^{a}$ | 14.0 ±0.3$^{bc}$ |
| **14** | 5.59 ±0.05$^{ab}$ | 2.3 ±0.2$^{h}$ | 0.408 ±0.022$^{b}$ | 14.1 ±0.5$^{bc}$ |
| **15** | 5.55 ±0.05$^{b}$ | 2.0 ±0.2$^{hi}$ | 0.406 ±0.019$^{b}$ | 14.8 ±0.3$^{bc}$ |
| **16** | 5.62 ±0.05$^{ab}$ | 1.9 ±0.3$^{hi}$ | 0.303 ±0.023$^{cd}$ | 14.6 ±0.7$^{bc}$ |
| **17** | 5.72 ±0.05$^{ab}$ | 1.7 ±0.3$^{hi}$ | 0.236 ±0.015$^{de}$ | 16.7 ±0.8$^{a}$ |
| **18** | 5.66 ±0.05$^{ab}$ | 1.5 ±0.2$^{i}$ | 0.121 ±0.014$^{fg}$ | 15.6 ±0.6$^{ab}$ |
| **19** | 5.70 ±0.05$^{ab}$ | <1.0 | 0.108 ±0.017$^{g}$ | 14.4±0.9$^{bc}$ |

Note: Values in the same column with different letters are significantly different at $p$ <0.05.

**Table 3** Content of organic acids in coffee roasted to Medium roast degree.

| Time | Organic acids | | | | |
|---|---|---|---|---|---|
| | Acetic ($mg.g^{-1}$ ±SD) | Formic ($mg.g^{-1}$ ±SD) | Lactic ($mg.g^{-1}$ ±SD) | Chlorogenic ($mg.g^{-1}$ ±SD) | Caffeic ($mg.g^{-1}$ ±SD) |
| **0** | 0.345 ±0.036$^{gh}$ | <0.005 | <0.005 | 22.7 ±1.8$^{a}$ | 0.741 ±0.082$^{c}$ |
| **4** | 0.262 ±0.055$^{h}$ | 0.032 ±0.005$^{f}$ | 0.019 ±0.009$^{e}$ | 17.8 ±0.5$^{b}$ | 0.873 ±0.033$^{c}$ |
| **5** | 0.345 ±0.013$^{gh}$ | 0.055 ±0.016$^{f}$ | 0.037 ±0.006$^{e}$ | 15.7 ±0.9$^{bc}$ | 0.971 ±0.021$^{bc}$ |
| **6** | 0.378 ±0.033$^{g}$ | 0.069 ±0.004$^{f}$ | 0.036 ±0.004$^{e}$ | 14.5 ±0.6$^{cd}$ | 0.932 ±0.029$^{bc}$ |
| **7** | 0.726 ±0.067$^{f}$ | 0.133 ±0.027$^{ef}$ | 0.039 ±0.007$^{e}$ | 13.6 ±0.4$^{de}$ | 1.03 ±0.08$^{abc}$ |
| **8** | 1.07 ±0.08$^{e}$ | 0.291 ±0.028$^{de}$ | 0.114 ±0.011$^{d}$ | 13.7 ±0.3$^{de}$ | 1.05 ±0.11$^{abc}$ |
| **9** | 1.16 ±0.06$^{e}$ | 0.383 ±0.014$^{d}$ | 0.099 ±0.021$^{d}$ | 12.2 ±0.2$^{def}$ | 1.17 ±0.12$^{ab}$ |
| **10** | 1.21 ±0.03$^{de}$ | 0.432 ±0.029$^{cd}$ | 0.144 ±0.013$^{d}$ | 11.7 ±0.3$^{ef}$ | 1.03 ±0.07$^{abc}$ |
| **11** | 1.39 ±0.04$^{cd}$ | 0.571 ±0.025$^{bc}$ | 0.198 ±0.009$^{c}$ | 10.4 ±1.1$^{fg}$ | 1.02 ±0.14$^{abc}$ |
| **12** | 1.58 ±0.07$^{c}$ | 0.633 ±0.063$^{b}$ | 0.239 ±0.017$^{c}$ | 8.9 ±0.9$^{gh}$ | 1.18 ±0.05$^{ab}$ |
| **13** | 1.81 ±0.04$^{b}$ | 0.717 ±0.113$^{ab}$ | 0.317 ±0.018$^{b}$ | 7.9 ±0.8$^{gh}$ | 1.17 ±0.08$^{a}$ |
| **14** | 2.17 ±0.07$^{a}$ | 0.875 ±0.057$^{a}$ | 0.392 ±0.022$^{a}$ | 7.2 ±0.4$^{h}$ | 1.05 ±0.13$^{abc}$ |

Note: Values in the same column with different letters are significantly different at $p$ <0.05.

**Table 4** Content of organic acids in coffee roasted to Full city roast degree.

| Time | Organic acids | | | | |
|---|---|---|---|---|---|
| | Acetic ($mg.g^{-1}$±SD) | Formic ($mg.g^{-1}$±SD) | Lactic ($mg.g^{-1}$±SD) | Chlorogenic ($mg.g^{-1}$±SD) | Caffeic ($mg.g^{-1}$±SD) |
| **0** | 0.345 ±0.036$^{j}$ | <0.005 | <0.005 | 22.7 ±1.8$^{a}$ | 0.741 ±0.082$^{abc}$ |
| **4** | 0.214 ±0.015$^{k}$ | 0.011 ±0.005$^{i}$ | 0.013 ±0.004$^{i}$ | 17.1 ±0.3$^{b}$ | 0.852 ±0.130$^{abc}$ |
| **5** | 0.484 ±0.016$^{i}$ | 0.061 ±0.008$^{h}$ | 0.046 ±0.006$^{h}$ | 16.2 ±0.7$^{bc}$ | 0.97 ±0.112$^{abc}$ |
| **6** | 0.492 ±0.012$^{i}$ | 0.104 ±0.011$^{gh}$ | 0.053 ±0.006$^{h}$ | 15.3 ±0.6$^{bcd}$ | 0.932 ±0.091$^{abc}$ |
| **7** | 0.856 ±0.025$^{h}$ | 0.293 ±0.041$^{fg}$ | 0.051 ±0.004$^{h}$ | 14.1 ±0.5$^{cde}$ | 0.974 ±0.133$^{abc}$ |
| **8** | 1.26 ±0.08$^{g}$ | 0.421 ±0.013$^{ef}$ | 0.180 ±0.025$^{g}$ | 12.9 ±0.8$^{def}$ | 1.25 ±0.18$^{ab}$ |
| **9** | 1.46 ±0.09$^{fg}$ | 0.519 ±0.038$^{e}$ | 0.208 ±0.028$^{g}$ | 12.5 ±0.9$^{def}$ | 1.42 ±0.19$^{a}$ |
| **10** | 1.41 ±0.03$^{fg}$ | 0.559 ±0.029$^{de}$ | 0.217 ±0.025$^{fg}$ | 12.2 ±0.6$^{efg}$ | 1.03 ±0.09$^{abc}$ |
| **11** | 1.72 ±0.08$^{ef}$ | 0.732 ±0.047$^{cd}$ | 0.315 ±0.023$^{ef}$ | 11.1 ±0.5$^{fgh}$ | 0.95 ±0.07$^{abc}$ |
| **12** | 1.85 ±0.09$^{de}$ | 0.786 ±0.040$^{bc}$ | 0.343 ±0.013$^{de}$ | 9.9 ±0.6$^{ghi}$ | 1.45 ±0.15$^{a}$ |
| **13** | 2.17 ±0.17$^{cd}$ | 0.906 ±0.045$^{abc}$ | 0.394 ±0.029$^{cde}$ | 9.5 ±0.4$^{ghi}$ | 1.22 ±0.13$^{ab}$ |
| **14** | 3.22 ±0.11$^{a}$ | 1.13 ±0.21$^{a}$ | 0.628 ±0.043$^{a}$ | 9.0 ±0.7$^{hij}$ | 1.05 ±0.09$^{abc}$ |
| **15** | 2.61±0.12$^{b}$ | 1.07 ±0.09$^{a}$ | 0.442 ±0.041$^{bcd}$ | 8.6 ±0.5$^{ij}$ | 0.951 ±0.141$^{abc}$ |
| **16** | 2.51 ±0.14$^{b}$ | 0.917 ±0.048$^{abc}$ | 0.497 ±0.021$^{bc}$ | 7.5 ±0.4$^{jk}$ | 0.873 ±0.062$^{bc}$ |
| **17** | 2.43 ±0.05$^{bc}$ | 0.921 ±0.050$^{abc}$ | 0.410 ±0.016$^{bcde}$ | 6.8 ±0.8$^{jk}$ | 0.852 ±0.015$^{bc}$ |
| **18** | 2.61 ±0.06$^{b}$ | 0.984 ±0.033$^{ab}$ | 0.454 ±0.061$^{bc}$ | 5.8 ±0.5$^{k}$ | 0.755 ±0.073$^{bc}$ |
| **19** | 2.51 ±0.05$^{b}$ | 1.02 ±0.05$^{a}$ | 0.513 ±0.032$^{b}$ | 3.2 ±0.9$^{l}$ | 0.613 ±0.082$^{c}$ |

Note: Values in the same column with different letters are significantly different at $p$ <0.05.

of water treated Brazil Arabica green coffee to be 4.92. **Ginz et al. 2000** monitored pH changes in Robusta coffee during the roasting process and recorded pH change from 6.1 to 5.7 similar to this study (Table 1 and Table 2).

Another strong correlation was found between chlorogenic acid concentration and caffeic acid concentration in the case of Medium roast ($r$ = 0.8025). However, in the case of Full city roast, this correlation was not significant and week ($r$ = 0.2403). Chlorogenic acid is an ester of quinic acid and phenolic acid, mostly caffeic, ferulic or 3-hydroxycinnamic acid **(Farah and Marino Donagelo, 2006)**. During shorter roasting at lower temperatures chlorogenic acid can be hydrolysed and concentration of caffeic acid in coffee beans may temporarily increase. On the other side, with longer roasting times and higher temperatures, caffeic acid released from chlorogenic acid can be further degraded. From the results summarized in Table 4 it can be seen a significant increase of caffeic acid concentration in roasted coffee beans and subsequent reduction of caffeic acid concentration over longer periods of roasting. The formation of phenolic substances during roasting of coffee is also evident from the total concentration of phenolic compounds presented in Table 1 and Table 2. Measured concentrations of chlorogenic acid, caffeic acid or total phenolic compounds in this study are comparable with data published in literature. Chlorogenic acid concentration in green coffee beans is reported within the

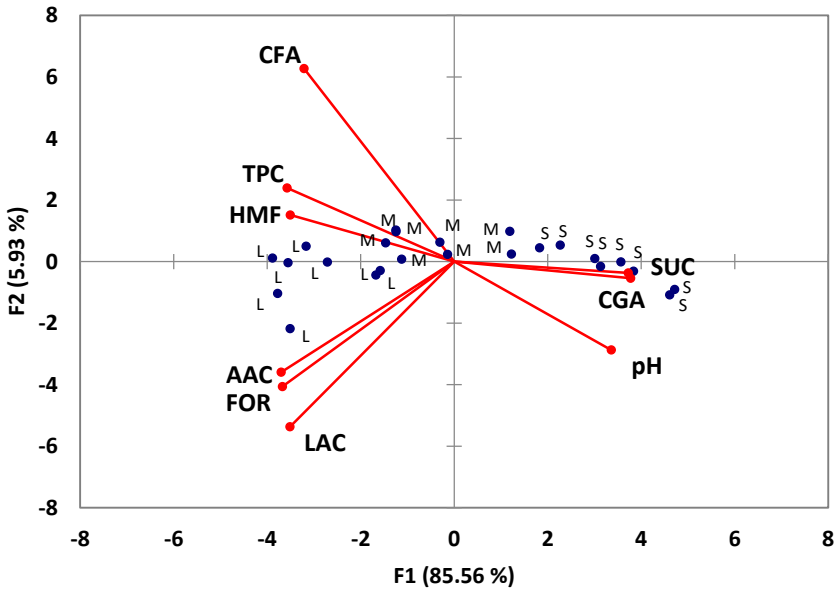


**Figure 1** PCA score of the monitored analytes in coffee beans roasted on Medium roast degree. Note: S = short time of roasting (0 – 6 min), M = medium time of roasting (7 – 10 min), L=long time of roasting (8 – 14min). CGA = chlorogenic acid, SUC = sucrose, LAC = lactic acid, FOR = formic acid, AAC = acetic acid, HMF = hydroxymethylfurfural,
TPC = total phenolic compounds, CFA = caffeic acid.

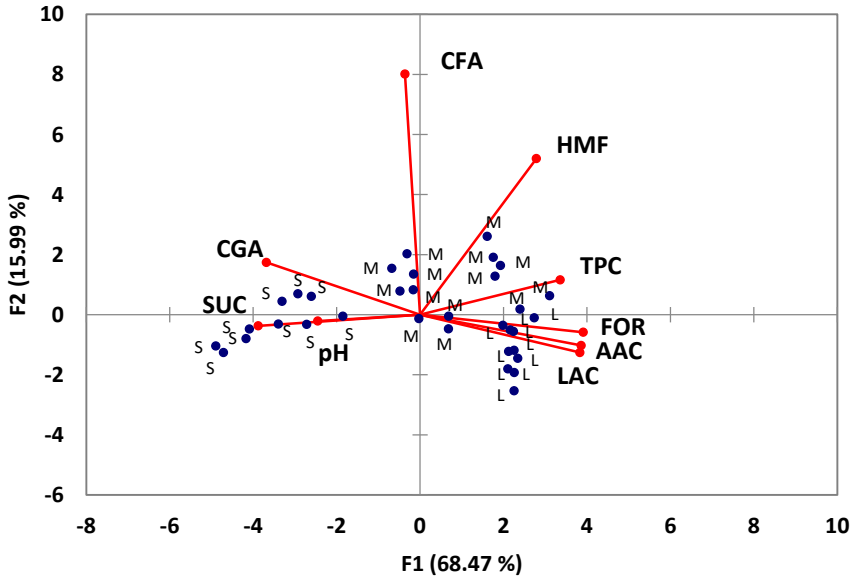


**Figure 2** PCA score of the monitored analytes in coffee beans roasted on Full city roast degree. Note: S = short time of roasting (0 – 7 min), M = medium time of roasting (8 – 14 min), L = long time of roasting (15 – 19 min). CGA = chlorogenic acid, SUC = sucrose, LAC = lactic acid, FOR = formic acid, AAC = acetic acid, HMF = hydroxymethylfurfural, TPC = total phenolic compounds, CFA = caffeic acid.

range of 34 – 57 mg.g$^{-1}$ while in roasted coffee beans in the range of 2 – 19 mg.g$^{-1}$ **(Ludwig et al., 2014; Narita and Inouye, 2015; Farah and Marino Donagelo, 2006; Moon, Yoo and Shibamoto, 2009)**.
Total phenolic compounds content in coffee is reported to be 14 – 30 mg.g$^{-1}$ (gallic acid equivalent) while caffeic acid content in coffee is reported to be 1.4 – 3 mg.g$^{-1}$ **(Bauer et al., 2018; Hall, Yuen and Grant, 2018)**.

Almost all foods that are heat-treated are monitored for content of 5-hydroxymethylfurfural. This compound is generated in food by the Maillard reaction **(Antal et al., 1990)**. Increased interest in 5-hydroxymethylfurfural stems from a partially verified suspicion that this compound is a health hazard compound that may be mutagenic, carcinogenic and cytotoxic **(Abraham et al., 2011)**. The content of 5-hydroxymethylfurfural in roasted coffee is reported to be 0.3 – 1.9 mg.g$^{-1}$ **(Murkovic and Pichler, 2006)**. In this study, maximum concentration of 5-hydroxymethylfurfural was measured to be 0.549 mg.g$^{-1}$ in coffee during Full city roast. During Medium roast

maximum content of 5-hydroxymethylfurfural was found to be 0.346 mg.g$^{-1}$. Relatively interesting is the course of 5-hydroxymethylfurfural concentration during roasting. During both Medium and Full city roast two sharp maxima in 5-hydroxymethylfurfural concentration were recorded, which could correspond to the first and second crack in coffee beans. After reaching the second maximum, concentration of 5-hydroxymethylfurfural in coffee decreases, because of its degradation to organic acids **(Murkovic and Bornik, 2007)**.

To investigate the overall composition changes during the roasting process, PCA was performed on the data for all coffee bean extracts at different time of roast. The roasting process was divided into three categories according to the total roasting time (short, medium and long time). The results are shown in Figure 1 and Figure 2. The PCA plots confirmed that sucrose and chlorogenic acid degraded during the roasting process and also that with longer roasting times the content of organic acids in coffee increases. Both Figures 1 and Figures 2 also show that content of 5-hydroxymethylfurfural is the highest in medium roasting times.

## CONCLUSION

This study proved that coffee roasting is a complex chemical process. The basic processes detectable during coffee roasting are the decomposition of sucrose and chlorogenic acid. Almost all sucrose is degraded during roasting independently of the roasting method. Degradation of chlorogenic acid is higher with longer roasting at higher temperatures. During the Full city roast (225 °C, 19 min) up to 85% of chlorogenic acid was degraded. Degradation products of sucrose and chlorogenic acid are low molecular organic acids and phenolic acids. Formic or lactic acid concentrations in coffee beans increased up to 100-fold during roasting. The increase in the concentration of phenolic compounds was not so steep, but it was observable. From the measured results, it cannot be clearly stated that with higher temperature and with higher roasting time concentration of 5-hydroxymethylfurfural is increasing. Highest concentrations of 5-hydroxymethylfurfural were measured at medium roasting times at both Medium and French city roasting temperatures. Conversely, at shorter roasting time and lower temperature higher concentrations of 5-hydroxymethylfurfural were found at the end of roasting.

## REFERENCES


Abraham, K., Gürtler, R., Berg, K., Heinemeyer, G., Lampen, A., Appel, K. E. 2011. Toxicology and risk assessment of 5-Hydroxymethylfurfural in food. *Mol. Nutr. Food Res.*, vol. 55, no. 5, p. 667-678. https://doi.org/10.1002/mnfr.201000564

Antal, M. J., Mok, W. S. L., Richards, G. N. 1990. Mechanism of formation of 5-(hydroxymethyl)-2-furaldehyde from d-fructose and sucrose, *Carbohydr. Res.*, vol. 199, no. 1, p.91-109. https://doi.org/10.1016/0008-6215(90)84096-D

Arya, M., Jagan Mohan Rao, L. 2007. An impression on coffee carbohydrates. *Crit. Rev. Food Sci. Nutr.*, vol. 47, no. 1, p. 51-67. https://doi.org/10.1080/10408390600550315

Bauer, D., Abreu, J., Jordao, N., Santos daRosa, J., Freitas-Silva, O., Teodoro, A. 2018. Effect of roasting levels and drying process of Coffea canephora on the quality of bioactive compounds and cytotoxicity. *Int. J. Mol. Sci.*, vol. 19, no. 11, p. 3407. https://doi.org/10.3390/ijms19113407

Butt, M. S., Tauseef Sultan, M. 2011. Coffee and its Consumption: Benefits and Risks, *Crit. Rev. Food Sci. Nutr.*, vol. 51, no. 4, p. 363-373. https://doi.org/10.1080/10408390903586412

Ciaramelli, C., Palmioli, A., Airoldi, C. 2019. Coffee variety, origin and extraction procedure: Implications for coffee beneficial effects on human health. *Food Chem.*, vol. 278, p. 47-55. https://doi.org/10.1016/j.foodchem.2018.11.063

Diviš, P., Smilek, J., Pořízka, J., Štursa, V. 2018. The quality of ketchups from the Czech Republic market in terms of their physico-chemical properties. *Potravinarstvo Slovak Journal of Food Sciences*, vol. 12, no. 1, p. 233-240. https://doi.org/10.5219/898

Dórea, J. G., daCosta, T. H. M. 2005. Is coffee a functional food? *The British Journal of Nutrition*, vol. 93, no. 6, p. 773-82. https://doi.org/10.1079/BJN20051370

FAOSTAT. 2018. Trade and markets. Available at: http://www.fao.org/statistics/en/

Farah, A., DePaulis, T., Trugo, L. C., Martin, P. R. 2005. Effect of roasting on the formation of chlorogenic acid lactones in coffee. *J. Agric. Food Chem.*, vol. 53, no. 5, p. 1505-1513. https://doi.org/10.1021/jf048701t

Farah, A., Marino Donangelo, C. 2006. Phenolic compounds in coffee. *Braz. J. Plant Physiol.*, vol. 18, no. 1, p. 23-36. https://doi.org/10.1590/S1677-04202006000100003

Ginz, M., Balzer, H. H., Bradbury, A. G. W., Maier, H. G. 2000. Formation of aliphatic acids by carbohydrate degradation during roasting of coffee. *Eur. Food. Res. Technol.*, vol. 211, no. 6, p. 404-410. https://doi.org/10.1007/s002170000215

Guimarã, A. C., Berbert, P. A., Silva J. S. 1998. Ambient-Air Drying of Pre-Treated Coffee (*Coffea Arabica* L.). *J. Agric. Eng. Res.*, vol. 69, no. 1, p. 53-62. https://doi.org/10.1006/jaer.1997.0222

Hall, S., Yuen, J. W., Grant G. D. 2018. Bioactive constituents in caffeinated and decaffeinated coffee and their effect on the risk of depression-A comparative constituent analysis. *Beverages*, vol. 4, no. 4, p. 79. https://doi.org/10.3390/beverages4040079

Jeszka-Skowron, M., Sentkowska, A., Pyrzynska, K., Paz dePena, M. 2016. Chlorogenic acids, caffeine content and antioxidant properties of green coffee extracts: influence of green coffee bean preparation. *Eur. Food Res. Technol.*, vol. 242, no. 8, p. 1403-1409. https://doi.org/10.1007/s00217-016-2641-y

Kemsley, E. K., Ruault, S., Wilson, R. H. 1995. Discrimination between Coffea arabica and Coffea canephora variant robusta beans using infrared spectroscopy. *Food Chem.*, vol. 54, no. 3, p. 321-326. https://doi.org/10.1016/0308-8146(95)00030-M

Ludwig, I. A., Clifford, M. N., Lean, M. E. J., Ashihara, H., Crozier, A. 2014. Coffee: Biochemistry and potential impact on health. *Food Funct.* vol. 5, no. 8, p. 1695-1717. https://doi.org/10.1039/c4fo00042k

Ludwig, I. A., Mena, P., Calani, L., Cid, C., DelRio, D., Lean, M. E. J., Crozier, A. 2014. Variations in caffeine and chlorogenic acid contents: what are we drinking? *Food Funct.*, vol. 5, no. 8, p. 1718-1726. https://doi.org/10.1039/c4fo00290c

Moon, J. K., Yoo, H. S., Shibamoto, T. 2009. Role of roasting conditions in the level of chlorogenic acid content in coffee beans: correlation with coffee acidity. *J. Agric. Food*

*Chem*., vol. 57, no. 12, p. 5365-5369. https://doi.org/10.1021/jf900012b

Murkovic, M., Bornik, M. A. 2007. Formation of 5-hydroxymethyl-2-furfural (HMF) and 5-hydroxymethyl-2-furoic acid during roasting of coffee. *Mol. Nutr. Food Res*., vol. 51, no. 4, p. 390-394. https://doi.org/10.1002/mnfr.200600251

Murkovic, M., Pichler, N. 2006. Analysis of 5-hydroxymethylfurfual in coffee, dried fruits and urine. *Mol. Nutr. Food Res*., vol. 50, no. 9, p. 842-846. https://doi.org/10.1002/mnfr.200500262

Narita, Y., Inouye, K. 2015. Chlorogenic acids from coffee. In Preedy, V. R. *Coffee in health and disease prevention*. Amsterdam, Netherlands : Elsevier, p. 189-199. ISBN 978-0-12-409517-5. https://doi.org/10.1016/B978-0-12-409517-5.00021-8

Poole, R., Kennedy, O. J., Roderick, P., Fallowfield, J. A., Hayes, P. C., Parkes, J. 2017. Coffee consumption and health: Umbrella review of meta-analyses of multiple health outcomes. *BMJ : British Medical Journal*, vol. 359, p. 1-18. https://doi.org/10.1136/bmj.j5024

Redgwell, R., Fisher, M. 2006. Coffee carbohydrates. *Braz. J. Plant Physiol.*, vol. 18, no. 1, p. 165-174. https://doi.org/10.1590/S1677-04202006000100012

Singleton, V. L., Orthofer, R., Lamuela-Raventós, R. M. 1999. Analysis of total phenols and other oxidation substrates and antioxidants by means of folin-ciocalteu reagent. *Methods in Enzymology*, vol. 299, p. 152-178. https://doi.org/10.1016/s0076-6879(99)99017-1

Verhoef, J. C., Barendrecht, E. 1977. Mechanism and reaction rate of the Karl Fischer titration reaction. Analytical implications. *Anal. Chim. Acta*, vol. 94, no. 2, p. 395-403. https://doi.org/10.1016/S0003-2670(01)84541-4

Wei, F., Furihata, K., Koda, M., Hu, F., Miyakawa, T., Tanokura, M. 2012. Roasting process of coffee beans as studied by nuclear magnetic resonance: Time course of changes in composition. *J. Agric. Food Chem*, vol. 60, no. 4, p. 1005-1012. https://doi.org/10.1021/jf205315r

Yeretzian, C., Jordan, A., Badoud, R., Lindinger, W. 2002. From the green bean to the cup of coffee: Investigating coffee roasting by on-line monitoring of volatiles. *Eur. Food Res. Technol.*, vol. 214, no. 2, p. 92-104. https://doi.org/10.1007/s00217-001-0424-7

**Acknowledgments:**

This work was financially supported by project FCH-S-18-5334 (The Ministry of Education, Youth and Sports of the Czech Republic).

**Contact address:**

*Pavel Diviš, Brno University of Technology, Faculty of Chemistry, Department of Food chemistry and Biotechnology, Purkyňova 118, 612 00 Brno, Czech Republic, Tel.: +420541149454,
E-mail: divis@fch.vut.cz
ORCID: https://orcid.org/0000-0001-6809-0506

Jaromír Pořízka, Brno University of Technology, Faculty of Chemistry, Department of Food chemistry and Biotechnology, Purkyňova 118, 612 00 Brno, Czech Republic, Tel.: +420 54114 9320,
E-mail: porizka@fch.vut.cz
ORCID: https://orcid.org/0000-0002-2742-8053

Jakub Křikala, Brno University of Technology, Faculty of Chemistry, Department of Food chemistry and Biotechnology, Purkyňova 118, 612 00 Brno, Czech Republic, Tel.: +420541149393,
E-mail: xckrikala@fch.vut.cz
ORCID: https://orcid.org/0000-0002-4776-9517

Corresponding author: *