Comparison of Chemical Compounds and Their Influence on The Taste of Coffee Depending on Green Beans Storage Conditions

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Abstract

Currently, there is no technology for storing green coffee (GC), which results in obtaining high-quality roasted coffee (RC). The aim of this study was evaluating the effects of storage temperature (-10, 5, 10, 18, 20°C, uncontrolled), post-harvest treatment method (natural (N), washed (W)) and type of packaging material (GrainPro (G), jute (J) bags) on content of chlorogenic acids, caffeine and trigonelline as also on sensory profile of GC from “specialty” sector after 12 months of measured storage. HPLC results showed that GrainPro bags preserve considered compounds better than jute. Exception was 10oC chamber, where in the samples from jute have been reported higher contents of all analyzed compounds. Also natural way of grain processing retains more assayed compounds. The best results were obtained in 10°C for jute both, natural and washed, where the highest level of all considered compounds were noted. The tendency was supported by the sensory analysis.

Introduction

The coffee is one of the most widely consumed products in the world. In 2018/2019 season, global coffee production reached 170.22 million (60-kilo) bags and this quantity was 4.6% higher than in the previous season 2017/2018. The production of Arabica was about 100 while Robusta 70 million bags [1]. Since improving the cup quality and changing coffee image by the propagation of information about its health benefits, the coffee consumption has increased significantly. People are more and more conscious about what they consume and want to know where the coffee is coming from, what is its origin, how it was roasted [2]. The roasteries have noticed this trend and they are bringing out their special coffee products.

Generally not all beans can be used as a high quality coffee. According to the Specialty Coffee Association of America (SCAA), coffee with total score 80 points or more in a sensory analysis is classified as “specialty” [3]. The judges are assessing important flavour attributes for coffee: aroma, flavour, aftertaste, acidity, body, balance, uniformity, clean cup, sweetness and defects according to the Cupping Specialty Coffee Protocol. Specialty Coffee market is quite a young compared to the entire coffee market in the world. It is distinguished by the approach to the raw material, which is both the coffee plantation, and green and roasted bean. At every stage of production, from cultivation to the cup of brewed coffee everything takes place under controlled conditions. The coffee tree grows only in rural areas, it is harvested only by hand, so that only ripe cherries are picked. Then the cherries are processed carefully and under controlled conditions by various methods e.g. natural (dry, when entire cherry is first cleaned and then dried) and washed (wet, when the fruits covering the beans are removed prior to drying). Afterwards the beans are dried to the appropriate level of humidity, and then transported to their destination, i.e. a coffee roastery where the coffees are roasted in an craft way to bring out the full aroma and flavour. The recipients of such beans are specialty cafes that have perfected the entire process of coffee cup preparing. The specialty coffee is distinguished by its full aroma, unique flavour but also by its chemical composition. [4, 5]. Sanmiguel, Torrez & Pérez-Villarreal indicated that over the last decade, consumer interest in the behavior and sensory attributes of coffee has increased significantly [6]. Also Barahona, Sanmiguel & Yang show the relationship between the sensory attributes of coffee beverages and the price of coffee [7].

Few years ago, consumers perceived coffee mainly as a stimulant, today they are informed about beneficial components and suggested health benefits. Regular coffee drinkers are less likely to suffer from a range of chronic and degenerative diseases (e.g. cancer, cardiovascular disorders, diabetes and Parkinson's), than people who do not drink coffee [8, 9, 10]. The positive health effects of coffee consumption are attributed to the presence of caffeine, trigonelline and chlorogenic acids [11]. Caffeine is the most widely consumed psychoactive substance worldwide that has many biological effects: stimulant and allowing for maintained cognitive function [12]. Trigonelline is the second most predominant alkaloid in raw coffee beans. The roasting of coffee beans converts trigonelline to nicotinic acid, a water-soluble B vitamin also known as niacin. Trigonelline appears to have several biological activities: as an antimicrobial agent and regenerates of dendrites and axons in cortical neurons [13]. Moreover, trigonelline may indirectly effects on hypoglycemic and hypolipidemic [14]. Various studies indicate that coffee has the high concentrations of polyphenols [15, 16, 17]. The most studied polyphenols in coffee are chlorogenic acids. The 3-O-caffeoylquinic acid is thought to be the most abundant among of its isomers in coffee [18, 19]. Chlorogenic acids are considered to have a positive effect on the prevention of diabetes and in the treatment of its symptoms [20].

Harvesting processes, roast degree and conditions of GC beans storage are responsible for the production or degradation of several compounds, which give sensory characteristics to the coffee beverage [19]. Keeping coffee fresh is critical to preserving taste.

During inappropriate GC beans storage, there is decrease in the quality and level of chemical compounds, which is expressed by flattening of cup quality. During 12 months storage, Król, Gantner, Tatarak, & Hallmann [17] noticed degradation of polyphenolic compounds. Coradi, Borem, Saath, & Marques [21] noticed that washed coffee presents better quality when compared to the product in its natural form. While, high temperatures and high water content have been reported as the main factors causing sensory changes in coffee during storage [22, 23, 5].

GC beans spend a lot of time in storage before they reach the consumer. The literature indicates [24, 25, 26] that the storage conditions of raw beans are an important parameter influencing the quality of coffee beverages, but there is a lack of studies about optimal conditions of GC storage and their influence on the sensory characteristic and chemical composition in coffee. Ensuring that the storage areas have optimal conditions helps preserve the rich taste, safety and quality of GC beans. Due to the long time and high transport cost of coffees from the specialty sector, preservation of the chemical compounds presented in GC beans, seems to be crucial for specialty coffee roasters and for consumers who get used to the taste of coffee. That is why more coffees are contracted for 12 and even up to 24 months, because coffee from the same plantation may taste different in the next harvest. Finding the best storage conditions may not only slow down the degradation process of the bean, but also it could be the driving force behind the construction of a central, fully controlled warehouse for more than one coffee roaster. The central storage will also allow for consolidated purchases of raw material, which can be beneficial for both, farmer and the roaster. Therefore, in this study we have evaluated the influence of GC beans storage conditions on the chemical composition and cup quality. The GC beans were stored from 12 months in measured chambers at various temperatures (-10, 5, 10, 18, 20°C and uncontrolled, UC) and different packaging (polypropylene-GrainPro and natural fiber-jute) to determine their quality attributes, including taste loss during storage and level of caffeine, trigonelline and chlorogenic acids. It also seemed important to show the differences in the chemical composition of GC and RC brews as currently in many countries, including Poland, the GC brews become very popular as anti-obesity drinks [27]. The need to find the best temperature and type of packaging during GC beans storage which can allow to maintain high properties of green and hence roasted grain, is therefore legitimate.

Methods

Coffee samples

GC beans were delivered from Finca El Oregano (1700 masl)-natural processed coffee and Finca La Maravilla (1850 masl)-washed processed coffee, plantations located in Huehuetenango, Guatemala. Both type of coffees were drying until an 11% (wb) moisture and sealed in GrainPro and jute bags. After 5 months from harvesting coffees arrived in Poland by sea.

Reagents

Analytical standards of chlorogenic acid (3-CQA, CAS:327-97-9), neochlorogenic acid (5-CQA, CAS: 906-33-2), caffeine (CAS: 58-08-2), trigonelline (CAS: 535-83-1) were purchased from Sigma-Aldrich, Fluka, Chromadex. All standards used were of analytical grade ($\geq 99\%$ purity). The mobile phase was prepared by diluting formic acid (Fisher Scientific, LC-MS purity, CAS: 64-18-6) with ultrapure water (Direct-Q system, resistivity below 18 M Ω cm) to a concentration of 0,1% (w/w) and pH was adjusted to 2.4. The solution was filtered under vacuum system through a 0,45 μ m filter. The second part of the mobile phase was methanol (POCH, HPLC grade, CAS: 67-56-1). Stock solutions of 1000 mg/l were prepared by diluting each analyzed compound in HPLC grade methanol. These solutions were diluted in methanol to reach the intermediate concentrations. All solutions were stored in the fridge in 4°C.

Coffee storage

After arrival to Poland, GC beans were divided into the 100 g samples and packed separately in small G and J bags. In this form they were stored in measured chambers at various temperatures (-10, 5, 10, 18, 20°C and uncontrolled) during 12 months. The humidity level was set to be kept at 50% relative humidity (RH) except - 10°C chamber it was 39% RH.

Roasting

After 12 months storage, GC beans samples were removed from all measured chambers for stabilization. Half of them were used for further chemical analysis while the corresponding other half was roasted after day of stabilization. Sample roaster ROEST S100 designed for optimal workflow and efficiency in a coffee lab maintained the following conditions: roasting start temperature: 165°C,

final temperature: 205°C, roasting time: 6–7 min with fixed airflow and heater setting, development time: 53 seconds. Then, RC beans were subjected to sensory and chemical analysis.

Extraction

The samples of GC and RC were ground (Blender type GB25, Hamilton Beach Commercial, USA). Then, 0.5 g of milled beans were extracted by 15 ml of distilled water (90°C) on a shaker (Multi-Tube Vortexer, Benchmark, USA) for 10 min (500 rpm). Further, the sample solution was filtered using 0.45 µm nylon with glass pre-filter (GF/NY, PureLand) before analysis. Extraction of each sample was performed in triplicates.

HPLC analysis

The chromatographic analysis was performed on Dionex UltiMate 3000 chromatograph equipped with and automatic pump, injector, autosampler, column compartment, UV-VIS detector with photodiode array technology (PDA). Instrument control, data acquisition and processing were managed by Chromeleon 6.8 software. Compounds were separated with isocratic reverse-phase system. A 100 x 4.6 mm chromatographic column Kinetex XB C18 with iso-butyl side chains and with TMS endcapping stationary phase (3,5 µm, Phenomenex) and the guard column with similar composition were employed. 30°C was monitored in column compartment during all chromatographic runs. The mobile phase consisted of formic acid solution in water (0.1%, w/w) as a solvent A and methanol as a solvent B. The elution conditions were: 85% A and 15% B (0–12 min). During all analysis time, the flow rate of the mobile phase remained at the level of 1.0 ml/min and injection volume was 1 µl. The wavelengths scanned were 325 nm for 3-CQA, 4-CQA, 5-CQA and 272 nm for caffeine and trigonelline.

Sensory analysis

The sensory evaluation of coffee samples was performed using scaling method described by the SCAA (2015). Five certified judges in two independent cupping evaluated seven sensorial attributes (aroma, flavour, aftertaste, acidity, body, balance and overall impression). The GC samples were roasted 48 hours before the cupping, ground immediately prior to cupping, no more than 15 minutes before water infusion. The hot water (97°C) was poured directly into the measured grounds to the rim of the cup. The steeping time took 4 minutes before evaluation process started.

Statistical analysis

All HPLC results in the study were expressed as mean from three independent replicates measured in duplicate ($n = 6$) $\pm$ standard deviation. While for sensory analysis, results from 5 cuppers in 2 independent cupping using triangulation were used and also expressed as mean ($n = 10$) $\pm$ standard deviation. Classification techniques, such as: cluster analysis (CA, tree diagram using Ward's method with Euclidean distance) and principal component analysis (PCA) were used to interpret the obtained results. The calculations were performed using the software STATISTICA ver. 10. Correlation matrix was used to find significant correlation between considered variables. Differences were considered significant when $p < 0.05$.

Results And Discussion

HPLC analysis- Characterization of chlorogenic acids, caffeine and trigonelline

This part aims to separate, identify and quantify important for coffee extracts substances, especially two groups. The first are polyphenolic acids, namely, chlorogenic acids such as 3-CQA, 4-CQA, 5-CQA and alkaloids of which caffeine and trigonelline are the key components. The level of identified compounds is shown in Table 1. Content of these ingredients differ in GC and RC beans and depends on the number of factors, such as e.g. post-harvest techniques, storage temperature and type of bags [28, 29] separation, identification and quantification of mentioned compounds were carried out using high-performance liquid chromatography with diode array detection (HPLC-DAD). For confirmation, UV-VIS absorption spectrum for each compound in coffee samples was compared with corresponding standard spectrum (Fig. 1). Identification of individual compounds was made by comparing individual retention times of each compound peak obtained during the chromatographic analyze of the coffee samples with retention time of the corresponding standards. The content of the compounds was calculated based on five points calibration curve. Each point was injected in duplicate. Identification and quantification of studied compounds were performed using the

validated methodology confirmed its selective, linear, precise, and accurate character. Validation parameters and chromatographic data are shown in Table 2.

CQA profiles were significantly different among all experiment variants of temperature, type of packaging and grain processing. For GC samples after 12 months storage, 4-CQA (RDS 16%) and 5-CQA (RDS 15%) presented the highest diversity while in RC samples all compounds maintained at a similar level of diversity (RDS about 10%). 3-CQA was the predominant analyzed compound in GC samples corresponding to approximately 55–60%. Trigonelline and caffeine were 17 and 15% respectively while 4-CQA and 5-CQA constituted only 7 and 5% of analyzed ingredients. In RC samples, 3-CQA level lowered and corresponded to about 30% among the analyzed compounds and also was predominant. Trigonelline and caffeine remained the same level of 21%, while 4-CQA and 5-CQA constituted 13 and 10% respectively. Figure 2 shows the difference in analyzed compounds in GC and RC samples after 12 months storage. The highest level of caffeine and trigonelline for GC and RC, was found in JN samples stored in 10oC (about 1150 and 1300 mg/100g respectively), and the lowest in GW and JW in -10oC (about 840 and 960 mg/100g respectively). There were no significant differences between these compounds in all experiments of GC and RC extracts ($p < 0.05$). Despite the fact that in the JN bags in uncontrolled conditions and GN 18oC, content of the caffeine and trigonelline in roasted coffee was equally high (about 1200 and 1300 mg/100g respectively), a much lower content of these compounds in GC samples was noted (about 950 and 1100 mg/100g respectively) and thus, there was more variation between GC and RC samples.

Roasting of GC caused loss of the water inside coffee beans and then volatile compounds and carbon dioxide are formed. In general extracting of caffeine and trigonelline from RC is easier than from GC thus, higher level of these compounds were found in RC samples what is in accordance with [30, 31, 32].

CQAs content slowly decreased in GCs among different variants of temperature, type of packaging and grain processing. After 12 months storage, the smallest differences in the content of CQAs were noted in the chambers 10°C for J both, N (1% of difference from initial concentration-DFIC) and W (2% DFIC). While the greatest decrease was recorded in the chamber 5°C for both J bags, N (49% DFIC) and W (59% DFIC) as well. A similar relationship was observed for caffeine and trigonelline content.

For RC prepared from GC after 12 months storage, the smallest content variation for CQAs was observed in chamber 10°C for JW (1% DFIC), 18°C for both natural, GrainPro (4% DFIC) and jute (5% DFIC). This time the biggest difference from initial concentration was noted in the chamber – 10°C for JW (42% DFIC) and in 20°C for JN (48% DFIC). One more time, the same was recorded for the quantity of caffeine and trigonelline.

At the end of 12 months of storage, the sum of CQAs, caffeine and trigonelline contents of GC in washed samples were noted to be lower than in the GC samples prepared in natural process, while for RC prepared from GC after mentioned time of storage the situation was quite the opposite for CQAs (except stored in 18°C) and for caffeine (except stored in -10°C, 18°C and uncontrolled conditions). These trends in trigonelline content in RC brews were the same as in GC samples.

The results show, that for both, N and W coffee samples, G bag can preserve CQAs, caffeine and trigonelline in GC beans better than J bag during storage time. The exception is chamber 10°C where in the samples from J bag higher contents of all analyzed compounds have been reported. It was also noted that quantity of trigonelline and caffeine were also higher in jute bag than in G bag when samples were stored in the uncontrolled conditions. The same behavior of compounds was noticed in the RC samples.

Sensory analysis

One of the most important factors influencing consumer approval of a product are sensory features. The cupping form provides recording important flavour attributes for coffee: aroma, flavour, aftertaste, acidity, body, balance, uniformity, clean cup, sweetness and overall which are rated on a 16-point scale representing levels of quality in quarter point increments between numeric values from 6 to 9, when 6.00-6.75 is good, 7.00-7.75 is very good, 8.00-8.75 is excellent and 9.00-9.75 is outstanding. The final score is calculated by summing the individual scores given for each attributes and additionally for clean cup, uniformity and sweetness. This score allows the coffee to qualify as specialty quality when is above 80 points [3].

After delivering coffee to Poland, the first sensory evaluation, so-called calibration, took place the day before the coffee samples were put into temperature chambers. Then all the attributes for the natural coffee brews: El Oregano (86.0 points of total score) and washed coffee brews: Finca La Maravilla (86.8 points of total score) were determined. The results confirmed the specialty quality of

both coffees and were in accordance with Coradi, Borem, Saath, & Marques [21] who noticed that washed coffee presents better quality when compared to the product in its natural form.

The first sensory evaluation of the coffees stored in the chambers was done after 3 months after placing both types of coffees at the indicated temperatures. After 12 months in chambers, the highest total score was achieved for RC samples from -10°C GN (81.1 points), 10°C for both GN and JN bags (79.5 points), as also for 18°C and UC for GN (79.2 and 78.8 points respectively) (Table 3). While the lowest scores were recorded for the samples stored in UC in both jute bags: natural (76.5 points) and washed (76.8 points) as also for chamber 18°C for GW (76.7 points) and 20°C for JN (76.9 points) and GW (76.7 points). The highest diversity among the evaluated attributes occurred for acidity, where the difference between the best and worst results for all samples after 12 months storage was 0.94 points, followed closely by balance and overall, 0.87 points for both. The smallest differences were found within aroma- 0.56 points. However for all attributes fluctuations were at a similar level ranged from 2.3 to 3.0%. After 12 months of coffee samples storage, a decrease ranged from 12.8% to 17.3% in the attributes of sensory analysis was noted in relation to calibration values. The largest difference between the attributes after 12 months compared to the fresh coffee occurred in aroma and was 17.3% of decline in relation to initial values (DRIV), followed closely by acidity (16.0 % DRIV) and also in body and overall (15.8 and 15.9% DRIV respectively). The smallest decrease in sensory values was noted for the aftertaste (12.8% DRIV) among all assessed attributes. Despite the highest total score for the RCs stored 12 months in chamber -10°C GN, large fluctuations were recorded for the remaining types of packaging in this chamber (RSD=3.7%). Based on the results of the sensory analysis, it was found that the most flavour stable results were in chamber 10°C (RSD=2.1%) and the highest values of assessed attributes were found in JN bag. Therefore, only the 10°C chambers and JN bags were considered in the further description. The lowest results were noticed for 20°C and UC.

The results of the sensory evaluation regarding the taste characteristics are graphically presented by means of radar charts (Fig. 3). They illustrate the changes that took place in RC from beginning of sensory evaluation in chambers (Fig. 3A) to 12 months (Fig. 3C) of storage in 10°C chamber taking into account the type of bag and way of coffee bean processing. It is easy to notice a decrease in the taste values of RC in all analyzed variants. The shape of the radar charts for all bags within chamber 10°C at the beginning of sensory evaluation in chambers were similar to the shape of the charts after the 12 month storage time. In both cases, all attributes remain on a similar level, ranged 7.3-7.8 points on beginning of sensory evaluation in chambers and 6.7-7.2 points after 12 months of storage. At the beginning of sensory evaluation in chambers, the highest attributes were felt for JW coffees and the body was characterized by the highest value, while after 12 months in JN the most taste values were felt.

Compared to other chamber temperatures, changes after 12 months in relation to calibration values to individual attributes were the smallest in 10°C (below 14.2% DRIV) except for JW (17.2-18.1% DRIV). We can also notice that the differences of sensory analysis for JN maintain the highest values for all attributes (9.3-11.6% DRIV) except the slightly lower values for aroma (14.2% DRIV) and body (12.4% DRIV). The second pair of radar chart illustrates the changes within the jute natural bags on the beginning of sensory evaluation in chambers (Fig. 3B) and after 12 months storage (Fig. 3D), showing all tested temperatures. Comparing the shapes of the radar charts in all JN bags, we can observe that they differ significantly from each other. At the beginning of sensory evaluation in chambers, all attributes remained at a similar level (7.0-7.7 points) and the flavour was the most noticeable in chambers -10, 5 and 10°C, aroma in 18°C, acidity in 20°C and UC. The highest total score of quality classification was achieved for 10°C chamber (82.4 points) while the lowest for 18°C (79.9 points). While after 12 months of storage, acidity and overall play the main role in the assessment of taste and attributes ranged from 6.6 to 7.2 points. The highest total score of quality classification was achieved for 10°C chamber (79.5 points) while the lowest for UC (76.5 points). Here, the greatest decrease in relation to initial is noticeable for chambers: 20°C (13.7-17.8% DRIV), UC (13.7-18.5% DRIV) and -10°C (13.7-16.7% DRIV). While the results for RC samples stored in the JN bag at 10°C showed the smallest decrease among all assessed attributes (9.3-14.2% DRIV).

Statistical analysis

Correlations

Correlation matrix was used to find significant correlations between considered variables (Table 4). This compilation allowed to observe that the increase in storage temperature causes a loss of flavour and aroma of coffee brews at the same time causing a growth of the 4-CQA content. In addition, jute bag affected the body attribute. Washed post-harvest process showed the relationship

with the content of CQAs while natural process with the other parameters, furthermore trigonelline more strongly. All CQAs strongly positively correlate with each other, weaker with caffeine and 4-CQA further contributes to the aroma. The caffeine content corresponded strongly to the trigonelline and also affected on aftertaste, acidity and overall, while trigonelline correlates with all attributes except body.

Differentiation of green and roasted coffee brews after 12 months of storage, taking into account chemical discriminants

To illustrate the relationship between the concentration of the compounds in the GCs and RCs and different storage conditions, the chemometric analysis such as: PCA, CA was applied. On the basis of the presented tree diagram (Fig. 4A.), it can be concluded that taking into account the Sneath criterion, among the analyzed samples of GCs and RCs, two groups showing mutual similarity can be clearly distinguished. The first group includes RC (purple and blue marking), while the second GC brews (green marking). Inside the RC group the distinction between washed (purple) and natural (blue) coffees is also observed. The cluster analysis technique proved to be helpful in the identification of coffee samples in terms of both the type of grain (CG, RC) and the method of its post-harvest treatment (N.W).

Next, a principal component analysis (PCA) was performed to explain the differences between the GC and RC coffees in terms of storage conditions. These results are shown in the system of the two first principal components: PC1 and PC2. The analysis of factor loadings matrix of variables in the factor space shows that the first component consists of highly correlated (>0.96) variables such as positively correlated CQAs and negatively caffeine and trigonelline (Table 5A). Two main factors with eigenvalues higher than one explain over 98.5% of the data variance while the first distinguished factor (PC1) explains nearly 96.5% of the data variance, and its eigenvalue of 4.8 indicates that it contains information originally explained by nearly 5 variables used to describe the research object (Fig. 4B).

The factorial arrangement of coffee sample objects allowed for the identification of 3 groups: a. blue: RCs in GN and JN bags, b. purple: RCs in GW and JW bags, c. black GCs in JN and GN bags and also and green: GCs in JW and GW bags. The location of the group of GC extracts from all types of bags (ellipse c) indicates a greater importance of the discriminants related to the presence of CQAs, in relation to the both RC extract groups a and b. While the position of the group of RC extracts from JN and GN bags (ellipse a) shows a greater importance of caffeine and trigonelline - related factors compare to the rest groups. In the case of both RC and GC samples, the determined components have values at a similar level of differentiation along the first principal component. PCA analysis showed that in the chemical perception of GC and RC all the tested compounds have different significance. The high content of CQAs in coffee beverages is more important in the case of GC brews of all bag types and allow to visualize them as a group along positive PC1 values. In turn, high levels of caffeine and trigonelline group RC brews along negative values.

Differentiation of roasted coffee brews after 12 months of storage, taking into account chemical and sensory discriminants.

The analysis of factor loadings matrix of variables in the factor space shows that the first component consists of highly negative correlated (>0.94) all sensory attributes as also a little weaker trigonelline while 4-CQA was positively correlated. The second principal component was caffeine (in plus) and 3-CQA (in minus) (Table 5B). Figure 5 represents the CA and PCA of chemical and sensorial characteristics of RC grains after 12 months of storage in different conditions. The presented dendrogram (Fig. 5A) graphically shows the partition of the analyzed RC in terms of its post-harvest treatment method into two groups: coming from natural and washed process (Sneath criterion).

A similar tendency was repeated in the PCA (Fig. 5B) taking into consideration data obtained for CQAs, caffeine, trigonelline and sensory characteristics. PCA analysis allowed to visually divide the analyzed coffee samples into two sectors: natural- with negative PC1 and positive PC2 values as also washed- with positive PC1 and negative PC2 values. The factorial arrangement of coffee sample objects allowed for the identification of 4 groups: a. light green: RC derived from natural process and stored in G and J in 5 and 10°C chamber, b. dark green: RC derived from natural process and stored in G and J in -10, 18, 20°C and UC chamber, c. dark blue: RC derived from washed process and stored in G and J in -10, 18, 20°C and UC chamber, d. light blue: RC derived from washed process and stored in G and J in 5 and 10°C chamber. Two main factors with eigenvalues higher than one explain over 94.7% of the data variance.

The first distinguished factor (PC1) explains nearly 71.9% of the data variance, and its eigenvalue of 8.6 indicates that it contains information originally explained by nearly 9 variables used to describe the research object. The second distinguished factor (PC2) explains nearly 22.8% and translates the information of the other three variables. The location of the RC extracts group from JN and GN in 5 and 10°C (ellipse a) indicates a greater importance of the discriminants related to the high presence of trigonelline and all sensory attributes which translates into a high total score value. In contrast to light blue group (ellipse d) where presence of 4-CQA is more important while the caffeine and 3-CQA content within both groups fluctuate at similar levels. In the case of both washed and natural RCs from b and c ellipse, the determined components have values at a similar level of differentiation along the first principal component. While in b group infusions with high caffeine importance and lower 3-CQA can be distinguished in opposite to c group.

In this work it has been shown that there is a huge effect of packaging materials, temperature and time of storage on CQAs, caffeine and trigonelline as well. The results show, that for both, natural and washed coffee samples, GrainPro bag can preserve CQAs, caffeine and trigonelline in GC beans better than jute bag during storage time. The exception is chamber 10°C where in the samples from jute bag higher contents of all analyzed compounds have been reported. In sensory analysis, the highest grade in terms of general quality was the coffee stored in the -10°C chamber in GN bag. However, large fluctuations for the remaining types of packaging in this chamber and lower profitability of keeping such a low temperature in warehouses influenced the selection 10°C chamber and JN bags where quality was comparably high. In this case, the decrease in taste values in relation to fresh coffee (calibration value) was only 7.6% and the most noticeable taste was acidity as also overall and the total result in the quality classification was 79.5 points. While the lowest results were noticed for 20°C and UC. A score >79 can be defined to be almost a specialty level. Certainly, these are Premium quality coffees, which constitute a relatively low percentage of the total coffee production in the world.

The PCA analysis showed that in the perception of the chemical and sensory properties of RCs, all tested compounds have different meanings, however, it allows them to be grouped. In order to optimize GC storage conditions, it would be advisable to continue the research in the future by narrowing the temperature range to 7, 10 and 13°C, as well as checking the vacuum packaging.

Declarations

Author contributions statement

M.Z., N.S., K.B., R.K. conceived the experiments, M.Z., N.S., K.B., A.J., D.A., R.M. conducted the experiments, M.Z., N.S., K.B., R.K., Ł.B. analysed the results. All authors reviewed the manuscript.

Additional information

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Tables

Table 1. The level of identified chemical compounds (mg/100 g) in green and roasted coffee. The values represent average $\pm$ standard deviation, n=6.

Temp. [°C]	Type of packaging*	[mg/100g], n=6									
		Green coffee (GC)					Roasted coffee (RC)				
		3-CQA*	5-CQA*	4-CQA*	Caffeine	Trigone- lline	3-CQA*	5-CQA*	4-CQA*	Caffe- ine	Trigone- lline
-10	GN	3955±85	356 ±11	508 ±15	1148 ±76	1273 ±72	1567 ±25	553 ±16	562 ±11	1010 ±17	1232 ±29
	JN	3744±157	327 ±16	474 ±26	1019 ±50	1169 ±48	1294 ±88	448 ±56	487 ±38	890 ±67	1092 ±72
	GW	3231±67	254 ±7	381 ±10	836 ±26	963 ±18	1388 ±58	458 ±22	543 ±26	836 ±38	973 ±34
	JW	3305±28	259 ±3	388 ±7	835 ±11	961 ±8	1335 ±19	429 ±9	518 ±8	871 ±12	979 ±10
5	GN	3148±38	283 ±6	400 ±7	953 ±14	1135 ±20	1343 ±7	426 ±5	515 ±8	980 ±11	1170 ±8
	JN	3170±29	281 ±4	396 ±7	988 ±16	1156 ±21	1314 ±12	410 ±6	505 ±8	985 ±12	1170 ±9
	GW	2681±81	206 ±4	302 ±7	868 ±14	984 ±9	1790 ±110	594 ±37	734 ±52	1123 ±75	1215 ±86
	JW	2427±133	189 ±10	278 ±16	830 ±30	980 ±25	1669 ±71	543 ±34	673 ±29	1033 ±40	1133 ±36
10	GN	2770±36	250 ±2	350 ±7	949 ±13	1159 ±15	1405 ±47	440 ±22	540 ±22	1093 ±35	1243 ±60
	JN	4279±315	396 ±31	567 ±34	1162 ±86	1289 ±85	1574 ±29	500 ±16	624 ±13	1157 ±19	1325 ±25
	GW	4116±125	334 ±10	507 ±17	920 ±25	979 ±27	1614 ±28	526 ±13	644 ±13	1025 ±18	1121 ±14
	JW	3860±78	312 ±9	472 ±12	871 ±27	949 ±11	1649 ±7	540 ±9	665 ±5	1037 ±12	1121 ±7
18	GN	3595±46	323 ±5	469 ±9	944 ±19	1103 ±9	1544 ±26	489 ±11	607 ±11	1178 ±19	1361 ±20
	JN	3524±38	327 ±4	465 ±11	966 ±3	1116 ±7	1612 ±11	516 ±8	638 ±6	1149 ±10	1342 ±9
	GW	3589±63	295 ±8	437 ±13	848 ±15	969 ±7	1427 ±8	459 ±6	556 ±3	920 ±7	1029 ±3
	JW	3597±84	294 ±7	438 ±12	876 ±8	981 ±2	1481 ±18	464 ±5	591 ±13	919 ±13	1033 ±2
20	GN	3425±65	312 ±5	439 ±8	982 ±29	1172 ±12	1437 ±17	447 ±8	584 ±28	990 ±18	1181 ±17
	JN	3290±46	310 ±3	430 ±4	943 ±25	1141 ±7	1324 ±71	407 ±25	540 ±39	948 ±55	1121 ±48
	GW	3093±50	254 ±5	368 ±8	879 ±16	1016 ±12	1607 ±22	516 ±8	650 ±12	900 ±14	1041 ±8
	JW	3970±150	331 ±10	508 ±19	856 ±31	911 ±23	1610 ±36	516 ±13	654 ±19	943 ±25	1080 ±20
Uncontrolled conditions	GN	3686±100	312 ±6	498 ±50	814 ±19	903 ±8	1561 ±25	491 ±8	654 ±42	1086 ±20	1314 ±26
	JN	3566±51	331 ±2	472 ±5	956 ±33	1119 ±16	1468 ±67	456 ±23	625 ±41	1179 ±61	1333 ±68

GW	3568±46	296 ±5	445 ±11	824 ±9	935 ±5	1613 ±20	517 ±6	651 ±8	972 ±12	1117 ±2
JW	3601±56	296 ±18	456 ±50	864 ±21	1008 ±6	1547 ±22	486 ±8	617 ±10	993 ±13	1114 ±11

*3-CQA- 3-O-caffeoylquinic acid, 4-CQA- 4-O-caffeoylquinic acid, 5-CQA- 5-O-caffeoylquinic acid, GN- Grain-Pro natural, JN- Juta natural, GW- Grain-Pro washed, JW- Juta washed

Table 2. Validation parameters and chromatographic data of the HPLC-DAD method.

Compound	Equation of analytical curve	λ^*	LOD*	LOQ*	Linear range	R*	RSD* %	Accuracy [%]	tR* [min]
		[nm]	[mg/100g]	[mg/100g]	[mg/100g]				
5-CQA*	y=0.9342x-0.0292	325	10	34	1-6	0.999	2.3	103.4	3.6
3-CQA*	y=0.8928x-2.6578	325	64	213	15-60	0.998	2.9	104.7	7.9
4-CQA*									9.9
Trigonelline	y=0.3824x-1.8094	272	109	363	5-30	0.992	2.8	97.6	1.0
Caffeine	y=1.1672x-0.2488	272	12	39	3-30	0.997	1.9	88.2	8.7

* λ - wavelength, **LOD**- Limit of detection, **LOQ**- Limit of quantification, **R**- Correlation coefficient, **RSD**- Relative standard deviation, **t_R**- retention time, **3-CQA**- 3-O-caffeoylquinic acid, **4-CQA**- 4-O-caffeoylquinic acid, **5-CQA**- 5-O-caffeoylquinic acid.

Table 3. The level of identified sensor attributes (points) in roasted coffee. The values represent average ± standard deviation, n=10.*GN- Grain-Pro natural, JN- Juta natural, GW- GrainPro washed, JW- Juta washed

Temperature	Type of packaging*	[points], n=10							
[°C]									
Roasted coffee (RC)									
		Aroma	Flavour	Aftertaste	Acidity	Body	Balance	Overall	Total score
-10	GN	7.19 ±0.18	7.31 ±0.09	7.13 ±0.09	7.47 ±0.04	7.31 ±0.00	7.34 ±0.04	7.31 ±0.09	81.06 ±0.09
	JN	6.81 ±0.09	6.84 ±0.31	6.69 ±0.27	6.78 ±0.31	6.81 ±0.35	6.72 ±0.31	6.72 ±0.22	77.38 ±1.86
	GW	6.94 ±0.00	6.94 ±0.09	6.72 ±0.13	6.69 ±0.00	6.78 ±0.04	6.75 ±0.00	6.75 ±0.09	77.56 ±0.35
	JW	6.91 ±0.31	6.75 ±0.27	6.72 ±0.04	6.81 ±0.09	6.72 ±0.04	6.78 ±0.13	6.78 ±0.13	77.47 ±0.93
5	GN	6.94 ±0.09	6.81 ±0.09	6.69 ±0.27	6.97 ±0.13	6.94 ±0.00	6.84 ±0.13	6.84 ±0.04	78.03 ±0.31
	JN	7.03 ±0.13	6.91 ±0.04	6.66 ±0.04	6.88 ±0.00	6.94 ±0.09	6.91 ±0.04	6.88 ±0.00	78.19 ±0.09
	GW	6.63 ±0.18	6.88 ±0.00	6.88 ±0.18	6.84 ±0.04	6.75 ±0.09	6.81 ±0.09	6.78 ±0.04	77.56 ±0.09
	JW	6.78 ±0.22	6.91 ±0.13	6.78 ±0.04	6.75 ±0.18	6.59 ±0.04	6.75 ±0.09	6.81 ±0.18	77.38 ±0.88
10	GN	7.13 ±0.09	7.13 ±0.18	7.03 ±0.13	7.13 ±0.00	7.00 ±0.00	7.06 ±0.09	7.06 ±0.09	79.53 ±0.57
	JN	6.97 ±0.22	7.06 ±0.44	7.03 ±0.22	7.19 ±0.44	7.06 ±0.53	7.03 ±0.40	7.13 ±0.53	79.47 ±2.78
	GW	6.84 ±0.13	6.88 ±0.27	6.88 ±0.18	6.94 ±0.09	6.88 ±0.09	6.88 ±0.09	6.94 ±0.09	78.22 ±0.40
	JW	6.91 ±0.31	6.75 ±0.27	6.72 ±0.04	6.81 ±0.09	6.72 ±0.04	6.78 ±0.13	6.78 ±0.13	77.47 ±0.93
18	GN	7.16 ±0.04	7.06 ±0.35	6.91 ±0.13	7.03 ±0.22	7.00 ±0.00	6.94 ±0.18	7.09 ±0.22	79.19 ±1.06
	JN	7.00 ±0.35	6.91 ±0.31	6.94 ±0.27	7.03 ±0.04	6.59 ±0.13	6.81 ±0.27	6.91 ±0.31	78.19 ±1.68
	GW	6.78 ±0.22	6.72 ±0.22	6.59 ±0.22	6.59 ±0.31	6.72 ±0.22	6.66 ±0.22	6.59 ±0.22	76.66 ±1.64
	JW	6.72 ±0.04	6.84 ±0.22	6.81 ±0.09	6.97 ±0.40	6.75 ±0.35	6.81 ±0.18	6.88 ±0.27	77.78 ±1.55
20	GN	6.75 ±0.09	6.84 ±0.13	6.81 ±0.09	6.88 ±0.00	6.81 ±0.27	6.81 ±0.18	6.84 ±0.22	77.75 ±0.62
	JN	6.78 ±0.04	6.63 ±0.18	6.69 ±0.18	6.81 ±0.09	6.72 ±0.04	6.69 ±0.09	6.63 ±0.18	76.94 ±0.53
	GW	6.63 ±0.00	6.56 ±0.18	6.69 ±0.09	6.75 ±0.00	6.75 ±0.35	6.66 ±0.13	6.69 ±0.09	76.72 ±0.84
	JW	6.66 ±0.04	6.69 ±0.09	6.56 ±0.09	6.66 ±0.13	6.81 ±0.09	6.72 ±0.04	6.69 ±0.00	77.23 ±1.03
Uncontrolled	GN	6.97 ±0.13	7.03 ±0.31	6.88 ±0.18	7.00 ±0.35	7.03 ±0.22	6.97 ±0.31	6.97 ±0.13	78.84 ±1.64

Conditions	JN	6.63 ±0.18	6.59 ±0.13	6.69 ±0.18	6.72 ±0.13	6.59 ±0.22	6.63 ±0.18	6.66 ±0.22	76.50 ±1.24
	GW	6.63 ±0.00	6.81 ±0.09	6.84 ±0.13	6.91 ±0.31	6.78 ±0.22	6.78 ±0.13	6.78 ±0.13	77.53 ±0.84
	JW	6.69 ±0.00	6.56 ±0.18	6.50 ±0.27	6.53 ±0.04	6.50 ±0.00	6.47 ±0.04	6.44 ±0.09	76.81 ±0.98

Table 4. Correlation between individual parameters. Bold results – correlation coefficient greater than the absolute value of 0.4 and p value<0,05.*3-CQA- 3-O-caffeoylquinic acid, 4-CQA- 4-O-caffeoylquinic acid, 5-CQA- 5-O-caffeoylquinic acid, G-GrainPro, J-jute, N-natural, W-washed

	Temperature [°C] (-10,5,10,18,20,UC)	Bag (G/J)	Grain preparation (N/W)	3-CQA*	5-CQA*	4-CQA*	Caffeine	Trigonelline
3-CQA*	0.294	-0.134	-0.413	1.000	0.948	0.952	0.461	0.266
	p=0.163	p=0.532	p=0.045		p=0.000	p=0.000	p=0.023	p=0.209
5-CQA*	0.029	-0.177	-0.404	0.948	1.000	0.832	0.346	0.186
	p=0.895	p=0.409	p=0.050	p=0.000		p=0.000	p=0.098	p=0.384
4-CQA*	0.471	-0.069	-0.411	0.952	0.832	1.000	0.479	0.269
	p=0.020	p=0.749	p=0.046	p=0.000	p=0.000		p=0.018	p=0.203
Caffeine	0.352	-0.004	0.458	0.461	0.346	0.479	1.000	0.932
	p=0.092	p=0.985	p=0.024	p=0.023	p=0.098	p=0.018		p=0.000
Trigonelline	0.300	-0.057	0.712	0.266	0.186	0.269	0.932	1.000
	p=0.155	p=0.792	p=0.000	p=0.209	p=0.384	p=0.203	p=0.000	
Aroma	-0.423	-0.1680	0.550	-0.246	-0.150	-0.414	0.265	0.405
	p=0.039	p=0.433	p=0.005	p=0.247	p=0.486	p=0.044	p=0.211	p=0.050
Flavour	-0.423	-0.354	0.426	0.083	0.208	-0.107	0.342	0.455
	p=0.040	p=0.090	p=0.038	p=0.700	p=0.329	p=0.620	p=0.102	p=0.026
Aftertaste	-0.190	-0.345	-0.396	0.296	0.356	0.152	0.523	0.571
	p=0.373	p=0.099	p=0.055	p=0.161	p=0.088	p=0.479	p=0.009	p=0.004
Acidity	-0.2358	-0.261	0.548	0.094	0.177	-0.077	0.415	0.549
	p=0.267	p=0.218	p=0.006	p=0.664	p=0.408	p=0.719	p=0.043	p=0.005
Body	-0.3175	-0.455	0.484	-0.088	0.033	-0.246	0.155	0.338
	p=0.131	p=0.026	p=0.016	p=0.683	p=0.879	p=0.246	p=0.469	p=0.106
Balance	-0.369	-0.345	0.468	0.068	0.184	-0.118	0.323	0.448
	p=0.076	p=0.099	p=0.021	p=0.753	p=0.390	p=0.585	p=0.124	p=0.028
Overall	-0.300	-0.307	0.475	0.137	0.219	-0.035	0.432	0.535
	p=0.154	p=0.144	p=0.019	p=0.522	p=0.303	p=0.872	p=0.035	p=0.007

Table 5. Correlation between analyzed compounds and two first principal components PC1 and PC2. A. In green coffee (GC) and roasted coffee (RC), all analyzed compounds. B. In roasted coffee (RC), all analyzed compounds and sensory attributes. Bold results - loads greater than the absolute value of 0.7.

A. Green coffee and roasted coffee			B. Roasted coffee	
Compound	PC1	PC2	PC1	PC2
3-CQA	0,984	0,015	0,684	-0,724
5-CQA	0,975	0,181	0,678	-0,576
4-CQA	0,965	-0,248	0,738	-0,444
Caffeine	-0,991	-0,066	-0,606	0,744
Trigonelline	-0,996	0,017	-0,728	0,637
Aroma	-	-	-0,948	-0,310
Flavour	-	-	-0,946	-0,322
Aftertaste	-	-	-0,944	-0,325
Acidity	-	-	-0,948	-0,312
Body	-	-	-0,940	-0,334
Ballance	-	-	-0,944	-0,328
Overall	-	-	-0,946	-0,321

Figures

Figure 1

Typical high performance liquid chromatogram of exemplary green coffee extract, indicating the presence of five main ingredients: 1. 5-CQA, 2. 3-CQA, 3. 4-CQA, 4. trigonelline, 5. caffeine. Data collected at two wavelengths: A. 325 nm, B. 272 nm.

Figure 2

Comparison of compounds found in the green and roasted coffee via HPLC-DAD after 12 months storage, A. 3-CQA, B. 4-CQA, C. 5-CQA, D. trigonelline, E. caffeine. Content in [mg/100g] as mean from three independent replicates measured in duplicate (n=6).

Figure 3

Sensory profile of coffee samples A. 10oC chamber on the beginning of sensory evaluation in chambers, B. jute natural bags on the beginning of sensory evaluation in chambers, C. 10oC chamber after 12 months storage, D. jute natural bags after 12 months storage. Mean values (n=10) GN-Grain Pro natural, JN-jute natural, GW-Grain Pro washed, JW-jute washed, storage temperature in oC: -10, 5, 10, 18, 20, UC-Uncontrolled Conditions.

Figure 4

GCs and RCs stored 12 months-chemical discriminants. A. Tree diagram. RC-roasted coffee, GC-green coffee, JN-jute natural, GN-Grain-Pro natural, JW-jute washed, GW-Grain-Pro washed, -10, 5, 10, 18, 20oC, UC-uncontrolled conditions. B. Biplot of the projection of variables into the factor plane. Blue dots (a group) represent roasted coffees derived from natural process and stored in Grain Pro and jute. Purple dots (b group) represent roasted coffees derived from washed process and stored in Grain Pro and jute. Green dots (c group) represent green coffees derived from washed process and stored in Grain Pro and jute. Black dots (c group) represent green coffees derived from natural process and stored in Grain Pro and jute. Black names in blue frames represent analyzed compounds such as: 3-CQA- 3-O-caffeoylquinic acid, 4-CQA-4-O-caffeoylquinic acid, 5-CQA- 5-O-caffeoylquinic acid, caffeine, trigonelline.

Figure 5

RCs stored 12 months-chemical and sensory discriminants. A. Tree diagram RC-roasted coffee, GC-green coffee, JN-jute natural, GN-Grain-Pro natural, JW-jute washed, GW-Grain-Pro washed, -10, 5, 10, 18, 20oC, UC-uncontrolled conditions. B. Biplot of the projection of variables into the factor plane. Light green dots (a group) represent roasted coffees derived from natural process and stored in Grain Pro and jute in 5 and 10oC chamber. Dark green dots (b group) represent roasted coffees derived from natural process and stored in Grain Pro and jute in -10, 18, 20oC and UC chamber. Dark blue dots (c group) represent roasted coffee derived from washed process and stored in Grain Pro and jute in -10, 18, 20oC and UC chamber. Light blue dots (d group) represent roasted coffees derived from washed process and stored in Grain Pro and jute in 5 and 10oC chamber. Black names in blue frames represent analyzed compounds: 3-CQA- 3-O-caffeoylquinic acid, 4-CQA-4-O-caffeoylquinic acid, 5-CQA- 5-O-caffeoylquinic acid, caffeine, trigonelline. Red names in blue frames represent all sensory attributes.