Effect of roasting degree of coffee beans on sensory evaluation: Research from the perspective of major chemical ingredients

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**ABSTRACT**

As the most consumed beverage in the world, the material basis of the sensory quality for roasted coffee beans has always received much attention. The objective of the present study was to clarify the physical morphology changes, main chemical ingredients and cupping scores of arabica coffee beans of different roasting degrees, by scanning electron microscopy (SEM), nuclear magnetic resonance (NMR) and sensory analysis, respectively. Statistical analysis of the data by multivariate analysis demonstrated that trigonelline, sugars, malate, quinic acids, \(\gamma\)-butyro-lactone and acetate have the potential to be new roasting markers. Additionally, in all the sensory indicators, body and acidity were found to be susceptible to roasting degree. Basing on cluster heatmap and sensory molecular network, the complex relationships between sensory indicators and ingredients were discussed. The results of partial least squares regression (PLSR) showed that the content of the main coffee ingredients can be used to predict the body score.

1. Introduction

As the second most frequently consumed drink after water, coffee, which has been grown in more than 70 countries, is closely related to the lives of billions of people around the world and has become the second largest traded commodity worldwide after petroleum (Butt & Sultan, 2011). The quality of coffee beverages is influenced by multiple factors such as altitude, soil, climate, processing procedures, roasting degree, and brewing methods; among all the factors, roasting plays a key role in coffee beverage quality (Dutra, Oliveira, Franca, Ferraz, & Afonso, 2001).

Once green beans are roasted, intricate physical and chemical changes occur. Physical changes are mainly reflected in the dramatic changes in the shape, water content, density, color, and internal structure of beans (Schenker, Handschin, Frey, Perren, & Escher, 2000). For the observation of the microscopic appearance of coffee beans, SEM is the most effective method. Although Schenker et al. (2000) have tried to observe the structure of roasted coffee beans using SEM, the morphology of coffee beans at different roasting levels has not been clearly explained. The chemical changes are marked with Maillard reaction and caramelization reaction to produce pleasant or unpleasant substances, which can directly decide the quality of the beverage (Baggenstoss, Poisson, Kaegi, Perren, & Escher, 2008; Steen, Waehrens, Petersen, Munchow, & Bredie, 2017, Liu et al., 2019). Previous studies have shown that some of the main components, especially sugars and chlorogenic acids (CGAs) (Farah, De Paulis, Moreira, Trugo, & Martin, 2006; Sittipod, Schwartz, & Paravissi, 2019), will be reduced by participating in the reactions, however, the main chemical composition changes at different roasting stages have not been well elucidated.

Beverage quality can be usually determined by sensory analysis in which a panel of trained, specialized “cuppers” evaluates coffee quality using either a table with scoring values (scoring method) or a sensory lexicon (descriptive method) (Worku, Duchateau, & Boeckx, 2016). The most widely adopted evaluation standard is the “Coffee Cupping Protocol of Specialty Coffee Association of America”, which includes ten sensory indicators: aroma, flavor, aftertaste, acidity, body, overall, clean up, uniformity, sweetness and balance.

Given that sensory analysis is affected by a variety of subjective factors which may lead to injustice (Romano et al., 2014; Worku et al., 2016), a theoretical alternative method is to find the material basis of the abovementioned sensory indicators, and based on these substances, to objectively evaluate the quality of coffee. In the past 30 years,

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considerable works have been devoted to the discovery of aromatic volatiles produced during roasting, and have led to the identification of over 1000 volatile organic compounds (VOC) (Colzi et al., 2017; Barie, Bucking, Stahl, & Rapp, 2015; Lindinger et al., 2008). In addition to the research on aroma, there are also reports on the material basis of acidity, body and bitterness (Santos, Lopo, Rangel, & Lopes, 2016; Blumberg, Frank, & Hofmann, 2010; Frank, Zehtbauer, & Hofmann, 2006; Rizzi, Boekley, & Ekanayake, 2004). Due to the intricacies of the roasted products, there is still a long way to match the indicators of sensory evaluation with the trace ingredients produced in roasting; actually, even the relationship between the main ingredients and sensory indicators has not been fully understood, which makes it hard to realize the coffee quality evaluation model based on chemical compositions. To best of our knowledge, there is no precedent for directly using the content of chemical components to predict the sensory score.

In the past few decades, in addition to direct use of instrumentiation combined with expert assessment to find flavor components, represented by gas chromatography–olfactometry–mass spectrometry (GC-O-MS) (Zou, Liu, Song, & Liu, 2018), instrumental detection combined with multivariate analysis has also been tried for the excavation of flavor substance and quality control of roasted coffee beans (Sittipod et al., 2019). For example, proton transfer reaction–mass spectrometry was employed in the discrimination of coffee beans of different roasting degree (Romano et al., 2014), and near infrared spectroscopy was exploited as an analytical tool for on-line monitoring of acidity during coffee roasting (Worku et al., 2016). As complicated the aromatic contents of coffee are, nearly all of the volatiles are derived from nonvolatile ingredients of green beans, which breakdown and react during roasting, forming a complex mixture (Hashim & Chaveron, 1995). Therefore, in the current study, the main chemical ingredients were chosen as research subjects to clarify their influences of roasting on sensory indicators. On the other hand, influences of roasting on sensory indicators were studied. Further, an in-depth study of the relationship between major chemical ingredients and sensory evaluation was carried out and a sensory molecular network based on major chemical ingredients was constructed. Finally, an exploratory study was conducted to build a sensory scores prediction model based on the characteristic signal of the main coffee ingredients.

2. Material and methods

2.1. Materials and instruments

D2O (99.9%) for NMR detection was purchased from Saen Chemical Technology (Shanghai) Co., Ltd. Samples were ground by a Jiuyang JYL-B060 grinder. Centrifugation was performed on an 80–2 benchtop centrifuge (Shanghai Medical Devices Co., Ltd.). The Bruker DRX-600 MHz NMR instrument (Bruker, Zurich, Switzerland) was used to detect 1H NMR spectra. SEM images were acquired with a Sigma300 (CARL ZEISS) field emission scanning electron microscope. The malic acid (99.0%), citric acid (99.0%), and quinic acid (98.0%) for 1H NMR spectra confirmation were purchased from J&K Chemical Co., Ltd. Trigonelline (98.0%) was purchased from Acme Biochemical Co. Ltd. Shanghai. Sucrose (98.0%), glucose (98.0%) and xylose (98.0%) were purchased from Aladdin Reagent (Shanghai) Co., Ltd. Caffeine (99.0%) was prepared and tested for purity by HPLC.

2.2. Coffee bean samples

All sample coffee beans for cupping and 1H NMR detection, including 24 light roasted bean (LRB) samples, 24 moderate roasted bean (MRB) samples and 24 dark roasted bean (DRB) samples, were produced in Pu’er City, Yunnan Province, China and all belong to Arabica (Catimor) species. The roasting degree was mirrored by the color value of the beans: LRB, 80–95; MRB, 60–75; DRB, 40–55.

2.3. Morphological characterization of coffee beans with different roasting degrees

For SEM characterization, three green beans, MBbs, and DRBs with uniform shape were selected, respectively. The beans were cut in the direction of the axis to expose the inner section, and the inner section was cut into 1–2 mm thick slices. For each bean, 2–3 sections were taken for SEM observation. The surface was uniformly plated with silver and then placed under a SEM (CARL ZEISS) to collect images. SEM magnification was ranged from 40 to 600 times.

2.4. Detection of major chemical constituents by 1H NMR

2.4.1. Extraction solvent screening

Before formal 1H NMR analysis, the extraction solvent was first screened. The solvents of four different polarities, n-hexane (b. p 68.7 °C), ethyl acetate (b. p 77.2 °C), ethanol (b. p 78.4 °C), and water (b. p 100.0 °C), were used to extract coffee of three roasting degrees (from the same green bean sample), respectively. In total, 500 g beans of three roasting degrees were crushed and passed through an 80 mesh sieve. For each individual experiment, 50 g (M0) of coffee powder and 200 mL (V0) of extraction solvent were added to a 500 mL Erlenmeyer flask, and extracted in a 60 °C water bath for 1 h with the aid of ultrasound. After that, 10 mL (V1) of the extraction solution was removed and concentrated under vacuum. The weight of the concentrate (M1) was accurately weighed and the extraction rate (Y) was calculated by the following formula:

\[ Y = \frac{V_1M_1}{V_0M_0} \times 100\% \]

2.4.2. 1H NMR signal acquisition

Six samples were randomly selected from three roasting degree bean samples, respectively. A total of 18 samples were obtained for 1H NMR analysis. For each sample, the beans were pulverized and sieved through an 80 mesh sieve to obtain uniform powder. Accurately weighed samples of 40.0 mg were placed in a 100 mL centrifuge tube, and 800 μL D2O was added. The samples were treated ultrasonically in a water bath at 80 °C for 1 h and centrifuged at 4000 rpm for 15 min. Then, 450 μL of the supernatant solution was stored in a nuclear magnetic tube at a constant temperature of 4 °C. The collection of 1H NMR data was performed on the same day as sample extraction on a Bruker DRX-600 MHz NMR instrument. 1H NMR sampling parameters were as follows: sampling data point 65536; peak width: 12,019 HZ; acquisition time: 2.7 s; relaxation time 10 s; number of scans 4. Presaturation method was used for water peak suppression.

1H NMR data was displayed in MestReNova and the main chemical ingredients were identified against literature and standards (Wei, Furihata, Hu, Miyakawa, & Tanokura, 2011). The characteristic chemical shifts of the main compounds were integrated to obtain their absolute peak areas, and the result are shown in Table S2.

2.5. Sensory evaluation

The sensory analysis was conducted by 4 Q-Grader panelists trained on the SCAA cupping protocol (Association, 2015). A total of 10 indicators including aroma, flavor, aftertaste, acidity, body, balance, overall, clean cup, uniformity and sweetness were scored during the sensory evaluation. The sensory indicators were evaluated on a scale from 6 to 10 with 0.25 increments and the sum of all ten sensory indicators’ scores was the final score of an individual sample.
2.6. Data processing

Multivariate analysis was performed using SIMCA 14.1 (Umetrics, Sweden). For the main chemical ingredients data set (n = 18), centralized was performed for the $^1$H NMR absolute peak area, then, principal component analysis (PCA) was performed. The chemical ingredients data set was centered and normalized for partial least squares discriminant analysis ((PLS-DA)). For the cupping score data set (n = 72), the data were centered and normalized, after which, PLS-DA was performed to explore the effect of roasting degree on sensory evaluation. The data set for the body score prediction was also centralized before PLS modeling. Analysis of variance (ANOVA) was conducted for the significance examination of all the models.

The Pearson correlation matrix between 7 cupping indicators and compounds was calculated by SPSS 16.0. The cluster heatmap was drawn based on the numpy, matplotlib and seaborn packages in python 3.5, and the sensory molecular network was drawn in Cytoscape 3.6.1.

3. Results and discussion

3.1. The production and change of coffee flavor substances

3.1.1. Changes in microstructure and main chemical ingredients during roasting

The change in microstructure caused by roasting has major influence on the final quality of coffee beverage. During roasting, the green beans are heated at 200–240 °C for 10–15 min. External temperature, roasting time, coffee bean size, shape, water content and other factors will affect the change of coffee microstructure and the occurrence of chemical reactions, thus affecting the generation and release of flavor substances.

Due to unusually thick cell walls and the tight alignment between cells, the green coffee beans are very hard (Fig. 1A, 1D), so they can be regarded as aggregates of microreactor units, which provide considerable support during roasting pressure buildup (Baggenstoss et al., 2008). The continued increase in temperature is accompanied by degradation of flavor precursor compounds such as sugars, amines, and CGAs to produce a large amount of flavor compounds. It is generally believed that when the temperature rises to approximately 154 °C, the Maillard reaction between sugars and amines begins, and the Maillard reaction products, coffee melanoidins, make the color of the beans darker.

The resulting volatile flavor compounds and CO$_2$ accumulate in the cavity inside the coffee bean, causing pressure inside the beans to rise. Roasted coffee beans can withstand theoretical pressures up to 16 bar (Baggenstoss et al., 2008). When the vapor pressure and the CO$_2$ pressure inside the beans build up, the “1st crack” occurs. The “blow holes” produced at this time become the outlets of the flavor compounds inside the beans. As shown in Fig. 1B, 1E, after the “1st crack” (MRB), a loose pore-like structure was observed under SEM, the micropores gradually became dense from the periphery to the middle, and an obvious crack appeared in the middle. Oil droplets can be observed around and at the bottom of the pore structure.

The combustion causes the CO$_2$ to continue to accumulate. After reaching a certain pressure, the “2nd crack” occurs and the interior begins to coke or carbonize. Previous study found that although there were high pressure conditions during the roasting process, no signs of cell wall rupture were observed in the SEM image (Baggenstoss et al., 2008; Schenker et al., 2000), which may be due to the change of the cell wall from the glass state to a more elastic state at high temperatures. From our observation, after the “2nd crack”, the pore size did not change significantly, but the crack in the middle became obviously longer, the oily substance on the surface increased, and the cell structure in the center of the bean began to be destroyed (Fig. 1C, F).
3.1.2. Exploring changes in the main chemical ingredients based on $^1$H NMR

To further clarify the changes in the main chemical ingredients in beans during roasting, $^1$H NMR was adopted in the analysis of roasted beans. First, the extraction solvent screening experiment was carried out. n-hexane, ethyl acetate, ethanol and water were used to extract coffee bean of three roasting degrees, respectively, and their extraction rate and $^1$H NMR profiles are shown in Figs. S4 and S5, respectively. Interestingly, the extraction rate of n-hexane, ethyl acetate and ethanol increased with the roasting degree, which may be due to the reaction of carbohydrates during roasting to form small or moderately polar melanoids. Although these macromolecular compounds do not show obvious $^1$H NMR signals, their content can increase with roasting degree, resulting in an increase in the organic solvent extraction rate. The extraction rate of water was much higher than that of the other three solvents, and no significant difference was detected in the water extraction rates of the three roasting degrees. $^1$H NMR spectra of the extracts of the four solvents showed that the water extract contained the most abundant types of compounds. Sugar, caffeine, CGAs, and trigonelline are all very water soluble (Upadhyay, Ramalakshmi, & Rao, 2012; Jezska-Skowron, Zgola-Greszkowiak, & Greszkowiak, 2015), but are very low soluble in n-hexane, ethyl acetate. Although caffeine and CGAs have good solubility in hot ethanol, sugars, as the most important flavor precursor compounds in coffee, are almost insoluble in ethanol. Among the four solvents, water has the highest boiling point, which means that when water is used as extraction solvent, not only can the main chemical components in the coffee be extracted to the utmost extent, but also the error caused by the evaporation of the solvent can be reduced. In addition, hot water is also the extraction solvent in coffee brewing. Therefore, although a small portion of the fat-soluble component may be neglected, in consideration of various advantageous, water was used as extraction solvent, not only can the main chemical components in the coffee be extracted to the utmost extent, but also the error caused by the evaporation of the solvent can be reduced. In addition, hot water is also the extraction solvent in coffee brewing. Therefore, although a small portion of the fat-soluble component may be neglected, in consideration of various advantageous, water was used as extraction solvent, not only can the main chemical components in the coffee be extracted to the utmost extent, but also the error caused by the evaporation of the solvent can be reduced. In addition, hot water is also the extraction solvent in coffee brewing. 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Therefore, Although detecting the external color of the beans is still the main means of determining roasting degree (Ruosu et al., 2012), considering the influence of geography, climate, variety and other factors on the flavor precursor compounds, it is hard to become an unified standard; thus, more factors must be concluded to conduct more accurate and unified assessment. Due to their characteristic changes

3.1.3. Roasting degree marker mining based on multivariate analysis

To accurately describe the influence of roasting on the content of the main coffee ingredients, the characteristic chemical shift intervals of the compounds were integrated to obtain the absolute peak area information of the compounds (Table S2), and further PCA and PLS-DA analysis was conducted.

PCA and PC2 of the PCA analysis model explained 80.0% and 16.4% of variance, respectively. In the score plot, three groups of samples were divided into three clusters from bottom left to top right in increasing order of roasting (Fig. S8), and no outlier existed in all samples. The PLS-DA model fit four principal components (p < 0.01). The goodness of fit of the model was $R^2 = 0.938$, $R^2 = 0.944$, and the predictive power was $Q^2 = 0.866$. The score plot of the PLS-DA model showed that the samples of three groups were well distinguished from left to right in descending order of roasting (Fig. 3A). The corresponding loading plot showed that compounds marked with blue, including CGAs, trigonelline, sucrose, other sugars, choline, and caffeine, had the highest content in LRB, while N-methylpyridinium, quinic acids, γ-butyrolactone, malate, 2-furfuryl methanol and acetate, which are marked with brown, had the highest content in DRB.

The clarification of the changes in the main chemical ingredients of roasted beans is also meaningful to the selection of roasting degree markers. Although detecting the external color of the beans is still the main means of determining roasting degree, it is hard to become an unified standard; thus, more factors must be concluded to conduct more accurate and unified assessment. Due to their characteristic changes
During roasting, CGAs, free amino acids, alkylpyrazines, 2-furfuryl alcohol and 5-methylfurfural/2-acetylfuran ratio have been proposed as roasting markers (Dutra et al., 2001; Hashim & Chaveron, 1995; Dorfner, Ferge, Yeretzian, Kettrup, & Zimmermann, 2004; Ruosi et al., 2012). The variable importance in projection (VIP) value of the PLS-DA model, first published by Wold and Johansson (1993), is a parameter of screening biomarkers in metabolomics, and the variable with VIP value greater than 1 can be considered as a differential variable between groups (Farres, Platikanov, Tsakovski, & Tauler, 2015). Among the VIP values corresponding to the first component of the current PLS-DA discriminant model, nine (class) compounds, including N-methyl-pyridinium, quinic acids, CGAs, γ-butyro-lactone, other sugars, trigonelline, 2-furyl-methanol, sucrose, and acetate had VIP values greater than 1 (Fig. S9), indicating that these compounds play important roles in the differentiation of roasting degree.

In addition to the roasting markers already reported in previous articles, from the results of PLS-DA analysis, other ingredients, such as trigonelline, sugars, malate, quinic acids, γ-butyro-lactone and acetate also have the potential to be markers of roasting degree. As discussed in section 3.1.2, the contents of sugars (sucrose and other sugars) and quinic acids in beans of different roasting degree were varied significantly, making them ideal markers for distinguishing roasting degree. Although obvious changes occurred mainly in DRB, the content of trigonelline, γ-butyro-lactone and acetate have the potential to become auxiliary indicators for evaluating the degree of roasting. It is worth noting that although the content of γ-butyro-lactone in roast coffee is relatively low, the significant changes make it a great contribution to the discriminant model.

3.2. Sensory evaluation

To minimize human error in sensory evaluation, all 72 samples of three roasting degree were included. To intuitively see overall change, the aroma, flavor, aftertaste, acidity, body, balance, and overall were plotted with heatmap (Fig. S10). On the whole, in addition to body score, which increases as the degree of roasting, the MRB samples had higher cupping scores in terms of aroma, flavor, aftertaste, acidity, balance, and overall than LRB and DRB.

To quantify the extent to which the roasting degree affects the score of the evaluation, multivariate data analysis was further conducted. Based on aroma, flavor, aftertaste, acidity, body, balance, and overall score of 72 samples, a 72*7 data matrix was constructed, and the matrix was further analyzed by PLS-DA analysis. The goodness of fit of the model was $R^2_X = 0.9$, $R^2_Y = 0.825$ the predictive power was $Q^2 = 0.785$, and the p value for ANOVA was lower than 0.01. As seen from the score plot, three different categories of coffee can be well classified (Fig. 4A). In this experiment, VIP value was used to determine the contribution of the input sensory indicators to the discriminant model. It can also directly reflect the influence of the roasting degree on sensory indicators. The model fitted a total of four principal components, and VIP values of variables in each component are shown in Fig. 4B. In the first component, VIP values of body, acidity, balance, and flavor were greater than 1. Among other three main components, only VIP values of body and acidity were greater than 1, and total VIP value indicated that the influence of roasting degree on sensory indicators can be ranked as: body > acidity > balance > flavor > balance > overall > aroma.

3.3. Relationship between main chemical ingredients and sensory indicators

In this section, the data set including the main chemical ingredients, cupping score and color value for the 18 samples was used to calculate the Pearson correlation coefficient of the variables (Tables S4 and S5). The cluster heatmap shown in Fig. 5A was drawn based on the
calculation result. Usually, the correlation strength of the variables is judged by the following range of values: correlation coefficient 0.8–1.0, extremely strong correlation; 0.6–0.8, strong correlation; 0.4–0.6, moderate correlation; 0.2–0.4, weak correlation; 0.0–0.2, weakly correlated or uncorrelated. To intuitively clarify the complex relationship between compounds, sensory indicators, total cupping score and color value, and variables with moderate to extremely strong correlation were screened to construct a sensory molecular network, in which correlation was represented by lines of different colors and thicknesses (Fig. 5B).

As the maximum amount of ingredients present in coffee water extract, the content of sugars (sucrose and other sugars) was extremely strongly negatively correlated with body and was strongly negatively correlated with balance, aftertaste, flavor, and overall. A reasonable explanation is that the insufficient Maillard reaction of sucrose resulting in the inadequate formation of favorable flavor compounds, indirectly leads to a lower cupping score. Indeed, a large body of literature reported that sugars can produce various flavor compounds that are favorable for cupping by the Maillard reaction during roasting (Liu et al., 2019; Velasquez, Pena, Bohorquez, Gutierrez, & Sacks, 2019). In addition, from the results of cluster analysis, it can be seen that the effect of choline on sensory quality was very similar to that of sugars. Trigonelline, CGAs and caffeine were under the adjacent branches of the cluster analysis, indicating they have similar correlation between content and sensory evaluation. In previous reports, the degradation products of trigonelline and CGAs along with caffeine were considered to be related to the bitterness of coffee drinks (Locas & Yaylayan, 2004). CGAs can be thermally transformed into the bitter-tasting CGA lactones 5-O-caffeoyl-muco-γ-quinide, 3-O-caffeoyl-γ-quinide, 4-O-caffeoyl-muco-γ-quinide, 5-O-caffeoyl-epi-δ-quinide, 4-O-caffeoyl-γ-quinide, 3,4-O-dicaffeoyl-γ-quinide, 4,5-O-dicaffeoyl-muco-γ-quinide, and 3,5-O-dicaffeoyl-epi-δ-quinide (Frank et al., 2006; Rizzi et al., 2004).
Additionally, CGAs or its analogues were found to be important flavor regulating substances (Sittipod et al., 2019). Similar to sugars, the content of these three ingredients was extremely strongly negatively correlated with body. In addition, CGAs showed moderately negative correlation with balance.

The remaining nine (classes) compounds, including formate, citrate, malate, 2-furyl-methanol, lipids, γ-butyro-lactone, quinic acids, acetate and N-methyl-pyridinium, are distributed in the same cluster. Combined with the score plot and loading plot of the PLS-DA analysis in Fig. 3, the content of these compounds was found to be relatively high in MRB or DRB. The correlation heat map showed that they were all positively correlated with the body score. Among them, 2-furyl-methanol, γ-butyro-lactone, quinic acids, acetate and N-methyl-pyridinium showed strong correlation. In addition, these nine compounds showed overall low positive correlation with balance, flavor, aftertaste, aroma and overall.

Although acetic acid content was significantly increased in DRB, the acidity of coffee did not increase. In fact, it is prone to produce bitter substances and mask the acid taste of coffee in DRB. For instance, several heterocyclics were suggested as potential bitter-tasting agents: benzene (Kreppenhofer, Frank, & Hofmann, 2011); 5-hydroxymethylseveral heterocyclics were suggested as potential bitter-tasting agents: benzene (Kreppenhofer, Frank, & Hofmann, 2011); 5-hydroxymethyl-

![Fig. 4. The score plot (A) and corresponding loading plot (B) of the first two dimensions of PLS-DA analysis based on the sensory evaluation data of samples. (n = 64).](image)

3.4. Establishment of a sensory prediction model

Although it has always been the mainstream evaluation method for coffee quality, sensory evaluation is thought to be fairly subjective and generally less replicable and consistent than physically based measurements. Genetic factors, health, age, education, past experiences, food habits, smoking habit, and cultural and religious patterns can all be factors that interfere with the objective score of the cupping panels (Romano et al., 2014; Worku et al., 2016). Therefore, researchers have long been exploring alternative methods for evaluating coffee quality (Worku et al., 2016; Romano et al., 2014).

In this research, 11 compounds with extremely strong or strong correlations with body (apart from lipids, citrate, malate and formate) were tested to be used as input variables to establish a body score prediction model. Data showed that there were high correlations between input variables (Table S5, marked by yellow), suggesting that the variables had a strong collinearity and it was not appropriate to establish the prediction model using the least squares regression (LSR) method. PLSR method combines the advantages of PCA and LSR, which can extract the latent variables (integrated variables) and satisfy the maximum extent linear correlation. This method can not only solve the problem of multicollinearity but also exhibit good modeling effects when the number of observed samples is small, so it was chosen as the modeling method.

The model fits a total of three principal components and the fit of the model was R²X = 0.993, R²Y = 0.834; the predictive power of the model was Q² = 0.755 (p < 0.01). The scatter plot of t₁/t₂ showed no outlier present in observed samples (Fig. S11). A linear relationship is shown in the scatter plot of t₁ and u₁ (Fig. 6A). Additionally, the predictive ability of the model was further checked by comparing between prediction and observed body value, and the result showed that the gaps between the predicted and observed score in all samples were within 0.2 (Fig. 6B). All the evidence suggests that it is feasible to predict the body score of coffee beverage by testing the content of the main ingredients.
4. Conclusion

The changes in microstructure and main chemical ingredients during the roasting of coffee beans were clarified by SEM and $^1$H NMR, respectively. $^1$H NMR combined with multivariate analysis was confirmed to be an effective strategy to monitor roasting degree. Trigonelline, sugars, malate, quinic acids, $\gamma$-butyro-lactone and acetate showed potential to be used to monitor the roasting degree of coffee beans.

The complexity of the chemical composition in roasted beans determines that it is impossible for researchers to describe a sensory feature using one or a kind of compounds. To more accurately clarify the material basis of sensory indicators, in the current research, the method of sensory molecular networks was proposed to reveal the intricate relationship between major compounds and sensory indicators.

Multivariate analysis and correlation analysis proved that the content of coffee’s main ingredients did have significant effects on acidity and body, especially the effect on body. The PLS model based on the main chemical components was used in an exploratory manner for prediction of body score and demonstrated good prediction performance. Other cupping indicators considered in this research, including balance, flavor, balance, overall and aroma, were less affected by the content of the main component. To replace these indicators, undetected volatile components or trace non-volatile components must be considered.

Fig. 5. A) The cluster heatmap for the correlation between coffee sensory indicators and major chemical ingredients. B) The flavor molecular network showing the correlation between total cupping score, sensory indicators, color value and major chemical ingredients. The thickness of the line corresponds to the strength of the correlation. Weak correlation and medium correlation (positive and negative) are indicated by gray lines; strong and extremely strong positive correlation are indicated by blue lines; strong and extremely strong negative correlation are indicated by pink lines. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
CRediT authorship contribution statement

Guilin Hu: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data curation, Writing - original draft, Writing - review & editing, Visualization. Xingrong Peng: Project administration. Ya Gao: Methodology. Yanjie Huang: Software. Xian Li: Conceptualization. Haiguo Su: Formal analysis. Minghua Qiu: Investigation, Resources, Supervision, Project administration, Funding acquisition.

Declaration of Competing Interest

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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Appendix A. Supplementary data

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References


