



# Effect of harvesting altitude, fermentation time and roasting degree on the aroma released by coffee powder monitored by proton transfer reaction mass spectrometry

Martina Bodner<sup>1</sup> · Ksenia Morozova<sup>1</sup> · Prapaijit Kruathongsri<sup>2</sup> · Prodpran Thakeow<sup>2</sup> · Matteo Scampicchio<sup>1</sup>

Received: 5 February 2019 / Revised: 27 March 2019 / Accepted: 31 March 2019 / Published online: 11 April 2019  
© Springer-Verlag GmbH Germany, part of Springer Nature 2019

## Abstract

This study investigates the effect of harvesting altitude, fermentation time and roasting degree on the volatile profile released by coffee (*Coffea arabica*, variety Catimor) powder. The analysis of the volatile organic compounds was performed by proton transfer reaction mass spectrometer (PTR-MS). The experimental design consisted of three factors: altitude at two levels (900 m and 1500 m, milder and harsher climate, respectively), four different fermentation times (0, 24, 48 and 72 h) and roasting at three levels (light, medium and dark). Analysis of the released volatile organic compounds (VOCs) revealed that the intensity of  $m/z$  45 and 59 dramatically decreases at a higher harvesting altitude. Longer fermentation times induce a decrease of  $m/z$  61 and 75, probably related to the activity of the isocitrate lyase. Finally, a prolonged roasting degree induces a rise of the  $m/z$  61, 75, 81 and 97. The total count per second measured by PTR-MS was used as an index of “overall coffee aroma intensity” to build a linear regression model. The model was used to predict the total VOCs intensity on the basis of the altitude, fermentation time and roasting level. The validation of the model (adjusted  $R^2=0.91$  and normalized relative standard deviation in prediction of 7%) reveals that, although the degree of roasting clearly affects the resulting aroma intensity, altitude and fermentation time also play a role in the formation of the volatile profile. Moreover, a significant interaction was observed between the altitude where the bean were grown and the roasting level. These results support the hypothesis that the type of process of the seeds has a strong impact on the resulting coffee’s quality. Furthermore, PTR-MS coupled with linear regression models is a powerful tool for the quality control of coffee process.

**Keywords** PTR-MS · Coffee powder · Aroma · VOCs · Linear regression model

## Introduction

Roasted coffee has an aroma characterized by more than 1000 volatile organic compounds (VOCs) [1, 2]. However, it has been also demonstrated that only a small fraction of these volatiles can be perceived by the human olfactory system [2]. Such chemical species include: (1) pyrazines and furans, (2) aldehydes and ketones, (3) phenols, (4) sulfur compounds, (5) monoterpenes and (6) acids [3–5]. Each

odorant class contributes to the final coffee aroma with an extent that is greatly dependent on the variety of green coffee, but also on the conditions set during the manufacturing process.

Because of the growing competition in the market of coffee powders and capsules, industries must tune precisely their manufacturing process to achieve specific sensorial attributes and satisfy the consumer demand. Thus, there is an increasing interest to apply analytical devices to measure the presence of volatiles responsible for the coffee aroma and mathematical models able to correlate their content with the manufacturing conditions used [3, 4].

At this purpose, several attempts have been addressed recently to develop powerful gas analyzers enabling the detection of the volatile organic compounds of coffee aroma. One of the most advanced techniques for volatile analysis is proton transfer reaction mass spectrometry (PTR-MS). This device measures the headspace above the analyzed sample

✉ Matteo Scampicchio  
matteo.scampicchio@unibz.it

<sup>1</sup> Faculty of Science and Technology, Free University of Bolzano, Piazza Università 1, 39100 Bolzano, Italy

<sup>2</sup> Department of Product Development Technology, Faculty of Agro-Industry, Chiang Mai University, Chiang Mai 50100, Thailand

directly without any sample preparation. Several studies have demonstrated the advantages offered by PTR-MS to analyze coffee samples, in particular low fragmentation, high time resolution, and broad linear detection range [5].

However, very little is known about the potential use of PTR-MS to develop methods to predict the coffee powder aroma as a function of the manufacturing process. Few authors applied PTR-MS to investigate the effect of roasting on the release of VOCs from coffee beans. Yeretizian et al. monitored the VOCs formation in green coffee beans and during coffee roasting [6]. Gloess et al. applied PTR-MS in the analysis of flavor formation in coffee from different origins during light, medium and dark roasting [7]. Mateus et al. developed a mathematical model of the release kinetics of roasted coffee powder [8]. Indeed, the manufacturing process, together with the green coffee variety, is mainly responsible for the resulting aroma of roasted coffee powder. First, green coffee quality, with its specific composition on precursors, reflects the altitude of the orchard where coffee beans are grown [1]. Altitude together with latitude and slope exposure is responsible for the so-called “Terrain effect”. These geographical factors contribute to the development of volatile and non-volatile compounds responsible for the coffee aroma [9]. In example, previous studies on coffee beans grown at high altitudes have shown that the harsh climate conditions affect the transpiration and photosynthesis activity of the plant, which, ultimately, lead to a more delicate coffee aroma, with increased fruity, acidic and floral notes [9, 10]. A second important factor in the development of the aroma of coffee powder is the fermentation period. After the harvest, coffee beans are fermented by wet or dry processing [11–13]. In wet processing, different strains of bacteria and/or yeast are inoculated in the coffee beans. These microorganisms produce metabolic compounds, which can affect the final aroma of coffee [14]. It has been demonstrated that the fermentation time corresponds to a decrement of free low molecular weight sugars, free amino acids and an increase of phenolic compounds [11], likely induced by the activity of isocitrate lyase [15]. Overall, the total amount of VOCs is decreasing at longer fermentation times. Another important factor that influences coffee flavor is the type of roasting. Roasting greatly affects flavor intensity by reducing sugars and amino acids into furans, pyridines, pyrazines and pyrroles [2, 11, 16–18]. Depending on the extent of roasting, coffee is commercially categorized as light, medium or dark. The roasting process generates VOCs as products of Maillard, Strecker, hydrolysis and pyrolysis reactions [1, 3]. Although light roasting can emphasize some positive potential of filter and espresso coffee, in some cases it leads to a non-uniform bean color with a sour, grassy, and underdeveloped flavor. Lighter roasting may prevent full aroma development and result in lower VOCs concentration, which makes some sensory attributes

(sweetness and acidity in particular) more prominent [19]. The medium roasting process leads to a more balanced taste and aroma, often with notes of citrus flavor. Finally, a dark roast process is likely to produce coffee where the contribution of highly volatile compound, i.e., acids and furans, to the overall aroma is minor. On the contrary, the contribution of less volatile compounds, for example, pyrazine and pyridine become more important [1, 20].

To put in the hands of coffee industry a predictive tool for the identification of those processing variables that influence the resulting coffee powder aroma, it is essential to have an analytical device that can measure the headspace concentration of the characteristic volatile compounds of coffee powder aroma, online and with high reproducibility. For this purpose, this work aims to apply PTR-MS-type gas analyzer to develop a predictive model that correlates the volatile intensity of coffee powder (i.e., strong vs. delicate aroma) with the main processing conditions, including the altitude of the orchard, the fermentation time and the roasting level. In this work, we demonstrate that it is possible to use PTR-MS to develop a predictive tool to design coffee characteristics from specific processing conditions.

## Materials and methods

### Sample preparation

Coffee beans (*Coffea arabica*, variety Catimor) were harvested at 900 and 1500 m above sea level in the Doi Chang area, Chiang Rai Province, Thailand by WaweeCoffee Co., Ltd. The coffee cherries were harvested in the same period at both altitudes. The ripe cherries from different altitudes were selectively picked by coffee pickers who have experience in coffee harvesting for more than 20 years. The ripening stage of the hand-picked cherries was assessed by visual evaluation of the cherry skin color. 1 kg of mucilaginous parchment beans, harvested at each altitude, was placed in 10 × 10 cm boxes. 5 L fresh distilled water was added to fill the boxes completely. The beans were fermented in a growth chamber at 28 °C, in dark, for 24, 48 and 72 h. 300 g of green coffee beans harvested at 900 and 1500 m were not fermented. After each time of fermentation, the resulting parchment coffee was dried in a laboratory drying oven at temperatures of 35–40 °C until the desired water content of 12% (wet basis) was achieved. Fermented and not fermented coffee beans (100 g) were roasted at 200 °C by Wawee Coffee Co., Ltd using a PRE1Z small-scale roaster (Probat Inc., Vernon Hills, USA.) Three different roasting profiles were achieved: light, medium and dark. Light-roasted coffee beans were roasted for 6 min, show 1–5% of weight loss and a light brown color; medium-roasted coffee beans were treated for 8 min, show 5–8% of weight loss and a medium brown color;

dark-roasted coffee beans were roasted for 10 min, show 8–10% of weight loss and a dark brown color (Fig. 1).

Three different factors were analyzed: harvesting altitude (900 and 1500 m), fermentation time (0, 24, 48 and 72 h) and roasting degree (light, medium and dark), leading to the production of 24 different types of coffee beans. Samples were code named according to all three features (Table 1). 50 g of coffee beans of each type were then milled for 1 min at the frequency of  $30 \text{ s}^{-1}$  by Retsch MM 400 Mixer Mill (Retsch GmbH, Haan, Germany).

### Proton transfer reaction mass spectrometry (PTR-MS)

The headspace of coffee powder was measured by PTR-QMS 500 (Ionicon Analytik GmbH, Innsbruck, Austria). 35 mg of coffee powder was equilibrated in 40 mL glass vials at  $30 \text{ }^\circ\text{C}$  for 15 min under ambient air. Five replicates for each sample were analyzed. Four more similar replicates were averaged to perform statistical analysis. Four empty vials were analyzed and considered as blanks. The measurement order was randomized to avoid any possible memory effect. The instrumental conditions were the following: drift voltage 600 V, drift temperature  $75 \text{ }^\circ\text{C}$ , inlet temperature  $75 \text{ }^\circ\text{C}$  and drift pressure 2.10 mbar, affording an  $E/N$  value of 149 Townsend ( $1 \text{ Td} = 10^{-17} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ). The signal

intensities were corrected and normalized as previously described [21], with the following equation:

$$\text{ncps}(\text{RH}^+) = \frac{\text{cps}(\text{RH}^+) \cdot 10^7 \cdot \text{transmission rate}}{500 \cdot \text{cps}(\text{H}_3^{18}\text{O}^+) + \text{cps}(\text{H}_2\text{O} \cdot \text{H}_3\text{O}^+)}, \quad (1)$$

where  $\text{ncps}(\text{RH}^+)$  is the normalized count rate for each ion intensity,  $\text{cps}(\text{RH}^+)$  is the count per second of each ionized molecule,  $\text{cps}(\text{H}_3^{18}\text{O}^+)$  is related to the primary ion ( $m/z$  21) and  $\text{cps}(\text{H}_2\text{O} \cdot \text{H}_3\text{O}^+)$  to water cluster ( $m/z$  37).

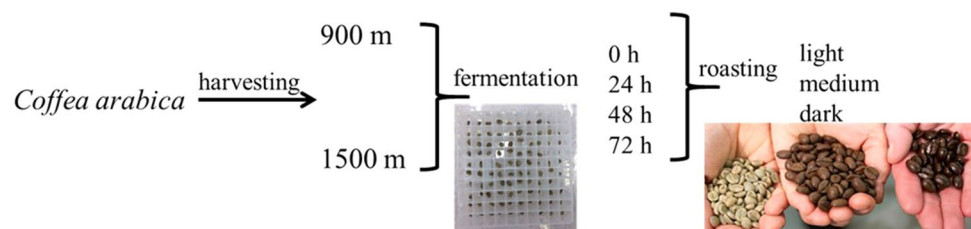
The total VOCs was calculated by summing the intensity of each of the 181 ion fragments, except  $m/z$  21 and 37, measured by the PTR-QMS.

Some ion fragments were tentatively identified accordingly to previous works on PTR-MS on coffee [2, 5, 22–25].

### Statistical analysis

All analyses were conducted using R-3.5.2 version from 20.12.2018 (R Development Core Team, 2010) (R Core Team 2013). The linear regression model was built with the caret package [Max Kuhn (2018). caret: Classification and Regression Training. R package version 6.0-81. <https://CRAN.R-project.org/package=caret>]. Briefly, the data set was randomly split into a training set (80% of the samples) and test set (20% of the samples and their replicates). Samples of the training set were used for the development of the

**Fig. 1** Schematic drawing of the experimental setup



**Table 1** Description of the 24 types of coffee used in this study  $170 \times 75 \text{ mm}$  ( $150 \times 150 \text{ DPI}$ )

ID	Altitude (m)	Fermentation (h)	Roasting	ID	Altitude (m)	Fermentation (h)	Roasting
L900	900	0	Light	L1500	1500	0	Light
L924	900	24	Light	L1524	1500	24	Light
L948	900	48	Light	L1548	1500	48	Light
L972	900	72	Light	L1572	1500	72	Light
M900	900	0	Medium	M1500	1500	0	Medium
M924	900	24	Medium	M1524	1500	24	Medium
M948	900	48	Medium	M1548	1500	48	Medium
M972	900	72	Medium	M1572	1500	72	Medium
D900	900	0	Dark	D1500	1500	0	Dark
D924	900	24	Dark	D1524	1500	24	Dark
D948	900	48	Dark	D1548	1500	48	Dark
D972	900	72	Dark	D1572	1500	72	Dark

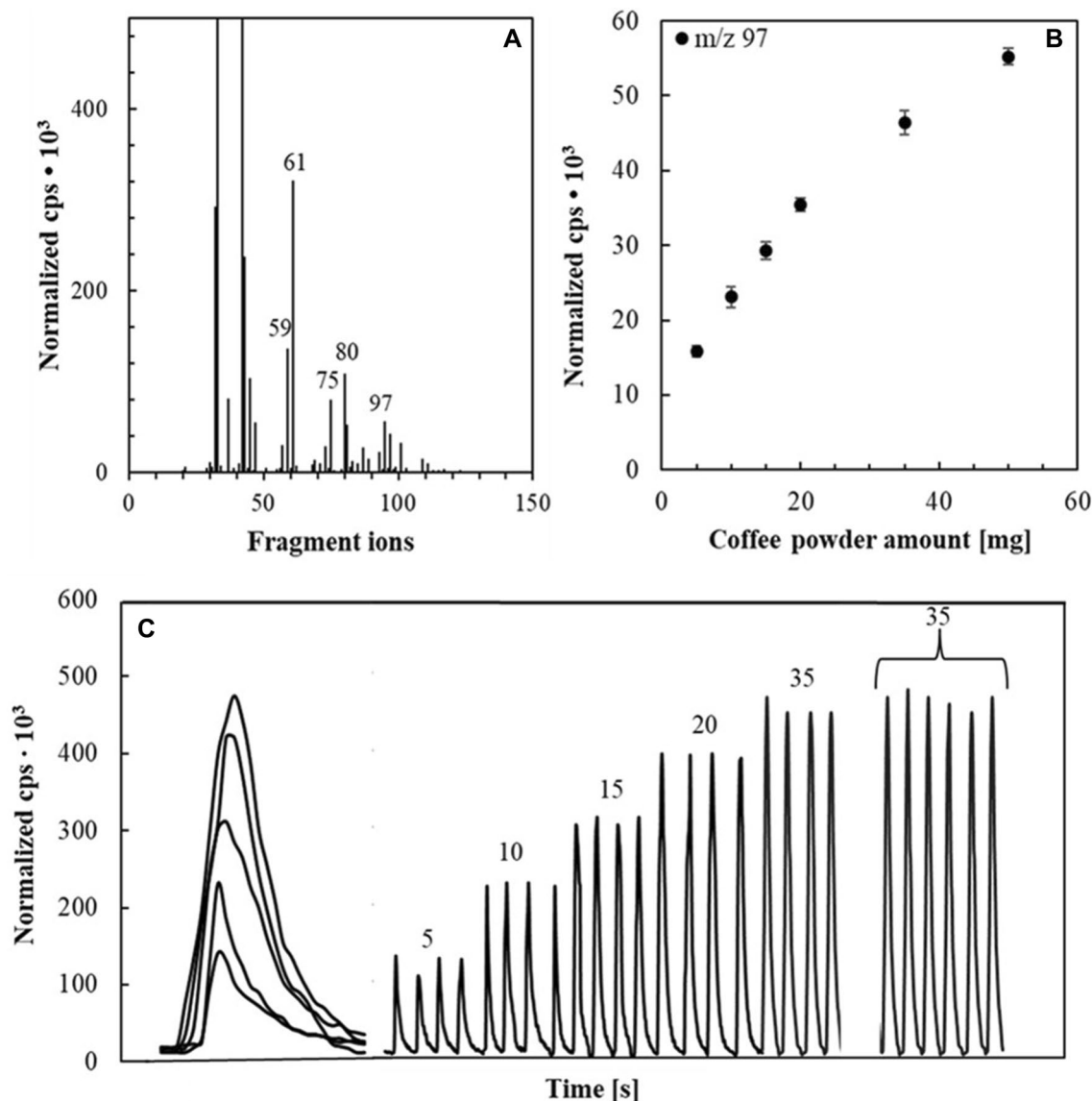
model. The model was then externally validated using the test set.

## Results

### PTR-MS spectrum

Figure 2a shows a typical PTR-MS spectrum of a coffee sample by highlighting some of the most abundant ions, such as  $m/z$  59, 61, 75 and 80. A similar signal pattern was reported in other works [22–25]. Figure 2b shows that the signal intensity of  $m/z$  97 (tentatively identified as furfural)

increases as a function of the amount of coffee samples loaded in the glass ampoule (fixed volume of 40 mL). Such increment is linear in the range from 5 to 35 mg. For sample loadings higher than 35 mg, the signal seems saturated, reaching a plateau level. At the highest amount of the sample (50 mg of coffee powder), a depletion of the primary ion ( $m/z$  21, ( $H_3^{18}O^+$ )) was observed. This confirmed the saturation of the drift chamber. Thus, the optimal amount for the detection of VOCs in coffee powder samples was selected as 35 mg. Figure 2c shows also the transient signal of the specific fragment ion  $m/z$  97. This fragment was tentatively identified to be furfural, a compound of great interest for coffee samples. The signal recorded for such a mass fragment



**Fig. 2** a Typical PTR-MS signal. b Signal intensity ( $n=4$ ) of  $m/z$  97 vs. increasing amounts of coffee powder. c Transient signal of  $m/z$  97 in relationship to different amounts of coffee powder (on the left). In

the middle, the signal of the four replicates of increasing concentrations of coffee powder is shown and on the right, six replicates of signal intensity measured for 35 mg of coffee powder

is linearly dependent ( $R^2=0.97$ ) on the amount of coffee sample. Sensitivity, determined as the slope of the calibration curve, is 1003 normalized cps and LOD below 60 normalized cps.

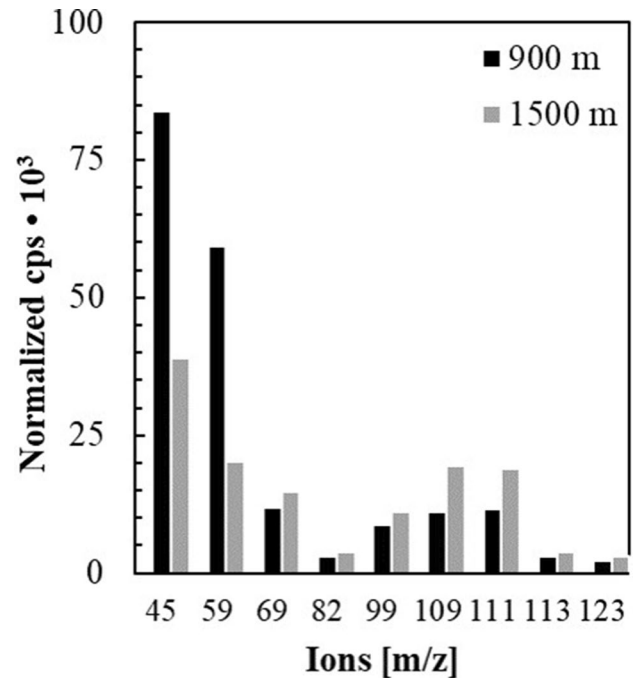
**ANOVA on the total VOCs**

Table 2 reports the mean values of total VOCs (expressed as normalized cps  $\times 10^6$ ) as a function of (1) the altitude of the coffee plant, (2) wet fermentation time and, (3) degrees of roasting. The minimum VOC intensity ( $2.61 \times 10^6$  ncps) was observed in coffee powders grown at high altitudes (1500 m), exposed to longer fermentation time (72 h) and to light roasting processes (6 min). Conversely, the highest VOC intensity was recorded for samples grown at low altitudes (900 m), exposed to shorter fermentation times (24 h) and longer roasting processes (10 min).

Table 2 also shows the result of the three-way analysis of variance. The main factors are all statistically significant ( $p < 0.001$ ). Altitude explained 53% of the total variance, followed by roasting (37%) and fermentation time (10%). The results also highlight a significant interaction between altitude and roasting. This confirms that the altitude plays an important role in developing specific precursors in green coffee, which sets the stage for later flavor development during roasting. 100 g of beans harvested at low 900 m weighed  $16.54 \text{ g} \pm 0.17 \text{ g}$ , while 100 g of high-altitude beans weighed  $17.35 \text{ g} \pm 0.19 \text{ g}$ . The different size of the beans harvested at the two altitudes may explain the interaction of altitude and roasting.

**Effect of altitude**

Figure 3 compares the most intense mass fragments observed among the non-fermented and lightly roasted samples (L900 vs. L1500) harvested at two different altitudes.



**Fig. 3** Volatile profile of non-fermented samples harvested at 900 and 1500 m and exposed to light roasting

**Table 2** Mean ( $n=4$ )  $\pm$  standard deviation of total VOCs ( $\times 10^6$  ncps) and the results of the three-way analysis of variance

Fermentation time	Altitude					
	900 m			1500 m		
	Degree of roasting					
	Light (6 min)	Medium (8 min)	Dark (10 min)	Light (6 min)	Medium (8 min)	Dark (10 min)
Short (24 h)	3.44 $\pm$ 0.88	4.11 $\pm$ 0.21	4.73 $\pm$ 0.46	2.88 $\pm$ 0.28	3.19 $\pm$ 0.57	3.48 $\pm$ 0.90
Medium (48 h)	3.17 $\pm$ 0.88	3.8 $\pm$ 1.0	4.37 $\pm$ 0.60	2.75 $\pm$ 0.28	2.94 $\pm$ 0.38	3.21 $\pm$ 0.36
Long (72 h)	3.07 $\pm$ 0.35	3.5 $\pm$ 1.3	3.97 $\pm$ 0.48	2.61 $\pm$ 0.04	2.83 $\pm$ 0.34	3.00 $\pm$ 0.95
Source of variability	Sum of squares $\times 10^6$		df	Mean square $\times 10^3$	F value	p value
Model	24.060		17	1.415	33.00	<0.0001
A—altitude	11.889		1	11.889	277.24	<0.0001
B—fermentation	2.733		2	1.367	31.87	<0.0001
C—roasting	7.822		2	3.911	91.20	<0.0001
AB	0.125		2	0.063	1.46	0.242
AC	1.273		2	0.637	14.84	<0.0001
BC	0.182		4	0.046	1.06	0.384
ABC	0.036		4	0.009	0.21	0.933
Experimental error	2.316		54	0.043		



The ions that showed a significant difference between the coffee samples harvested at 900 m and 1500 m were the mass ions 45 (tentatively identified as acetaldehyde) and 59 (tentatively identified as acetone). Other relevant ions include (tentatively identified as): 69 (furan), 82 (methylpyrrole), 99 (2-furanmethanol), 109 (dimethylpyrazine), 111 (acetylfuran), 113 (5-methylfurfuryl alcohol) and 123 (2-ethyl-5-methylpyrazine). Overall, the sum of these VOCs accounts for 75% of the total intensity.

These results support the hypothesis that high elevation can affect the final quality of the coffee beverage [15, 26]. Altitude has an impact not only on the total headspace intensity, but also in the contribution of VOCs. The two ion fragments that change the most are  $m/z$  45 and 59. This could also influence the aroma. At lower altitude, coffee will be more delicate, with more fruity, green ( $m/z$  45) and buttery ( $m/z$  59) notes [27]. This conclusion may be explained with the fact that the metabolism of coffee beans may change according to stress events, such as dry or cold climatic conditions [9, 15]. Accordingly, the growing conditions at high altitude may reflect a harsher environment and explain differences in total VOCs profile.

### Effect of fermentation

The fermentation time leads to a great change in the total VOCs. This is expected, because fermentation affects the development of aroma precursors. Table 2 shows that longer fermentation times correspond to lower total VOCs. This is in agreement with studies [1]. The amount of free low molecular weight sugars and free amino acids is decreasing during fermentation, while increasing the phenolic compounds [11]. These processes are induced by the activity of isocitrate lyase (ICL) [15]. ICL is a key enzyme responsible for the production of many aroma precursors. According to the literature, the activity of ICL is maximum in the first 24–48 h, and then it fades down [15], which explains the lower amount of VOCs in coffee beans exposed to longer fermentation times.

The evolution of total VOCs is characterized by the great changes of a few mass fragments. These include  $m/z$  61, 75, 45, 59, 81 and 97, tentatively identified as acetic acid, propionic acid, acetaldehyde, acetone, butene-2-one and furfural, respectively. Together, these ions accounted for 70% of the total VOCs signal. All these ions highly correlated with each other. As an example, Fig. 4 shows that the changes observed for the two mass ions with the highest intensity, respectively, the  $m/z$  61 and 75, followed an exponential decay ( $R^2 > 0.95$ ). A similar behavior was observed for the other ions. Overall, these results confirm that prolonged fermentation time decreases the evolution of total VOCs, as expected from a lower activity of ICL and lower production of aroma precursors.

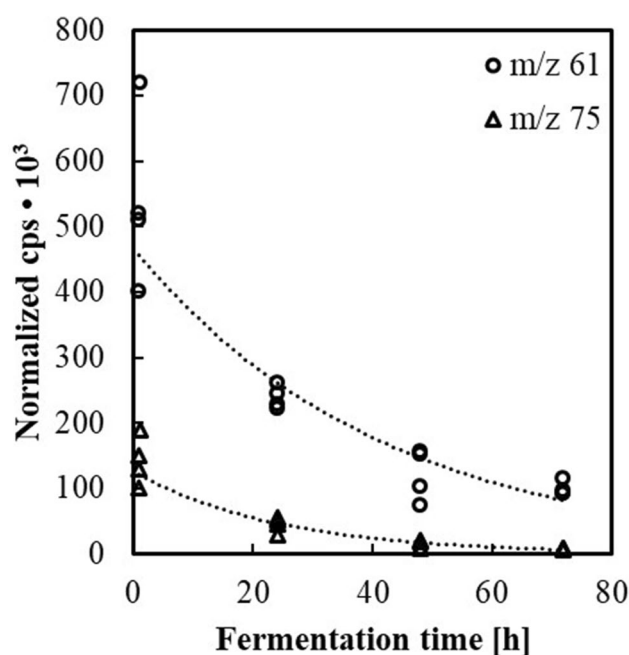


Fig. 4  $m/z$  61 and 75 intensity of coffee harvested at 900 m and light roasted at different fermentation time

### Effect of roasting

The roasting factor is known to generate in coffee a number of VOCs as products of Maillard, Strecker, hydrolysis and pyrolysis reactions [1, 3, 28]. Although we demonstrated that altitude and fermentation time could be important in developing specific VOC precursors, the final aroma taste is likely given during the roasting. Figure 5 shows that the greatest amount of VOCs is formed during medium (8 min) to long (10 min) stages of roasting level.

At any time, the highest signal intensity was always achieved with the  $m/z$  61. However, other important fragments were detected, such as the  $m/z$  75, 81 and 97. All are linearly correlated with the roasting level. Furthermore, the mass fragment  $m/z$  97 was tentatively identified as furfural, a typical compound found in coffee. Together, these ions accounted for 70% of the total VOC signal.

Cherries grown at 900 m had an average size of  $6.73 \text{ mm} \pm 0.46 \text{ mm}$  in width and  $8.76 \text{ mm} \pm 0.49 \text{ mm}$  in length; the ones harvested at 1500 m measured in average  $7.23 \text{ mm} \pm 0.75 \text{ mm}$  in width and  $8.06 \text{ mm} \pm 0.69 \text{ mm}$  in length. Regarding the weight, 100 g of low-altitude beans weighed  $16.54 \text{ g} \pm 0.17 \text{ g}$ , while high-altitude beans weighed  $17.35 \text{ g} \pm 0.19 \text{ g}$ . Smaller beans may undergo the chemical reactions happening during the roasting process faster than the bigger ones, thus leading to a higher release of VOCs.

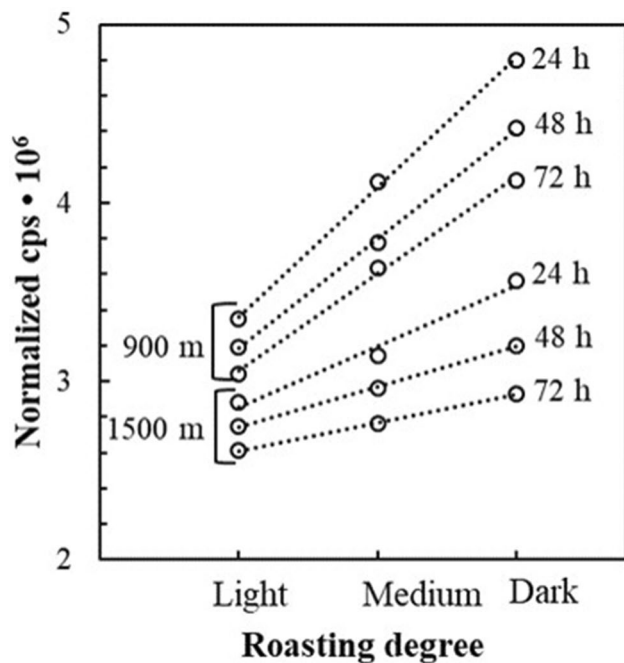


Fig. 5 Total VOCs as a function of the roasting level

### Prediction of total VOCs intensity

The total VOCs signal of coffee powder was used as an index for the overall aroma intensity. With this signal, a regression model was built to predict the total VOCs intensity of coffee samples as a function of the three environmental factors considered so far, i.e., harvesting altitude, fermentation time and roasting level. The samples were divided into a training set (80% of the samples) and test set (20% of the samples), respectively. With the training set, the resulting linear regression model was:

$$Y(10^6) = -0.41 \text{ altitude} - 0.27 \text{ fermentation} + 1.03 \text{ roasting} \\ + 0.11 \text{ altitude fermentation} - 0.31 \text{ altitude roasting} \\ - 0.07 \text{ fermentation roasting} + 3.3.$$

The adjusted  $R^2$  was 0.89 and the normalized relative standard deviation was 6%. Validation of the model was performed on the test set (20% of the samples) by a five-fold cross-validation repeated ten times. The resulting adjusted  $R^2$  was 0.89 and the normalized relative standard deviation was 7%. The regression analysis confirmed that the most important variable was the roasting level, followed by its interaction with altitude. From this model, the highest total VOC value (which corresponds likely with the most intense aroma) can be achieved with coffee bean roasted for long times and grown at low altitude,

and fermentation for short times. Conversely, the highest total VOC value (which corresponds likely with the most delicate aroma) can be achieved with coffee bean that is quickly roasted, fermented for longer times and grown at high altitudes.

### Conclusion

The results of this study show the potential of PTR-MS as a rapid tool in the monitoring of the volatile profile of coffee powder with respect to harvesting and processing treatments. Regarding altitude, 900 m asl seems to be ideal, with respect to total VOC intensity, compared with 1500 m asl. Although the degree of roasting greatly affects the development of intense aroma levels, the results suggest that altitude and fermentation time also play a role in the formation of the volatile profile. Low altitude is characterized by a wetter and warmer climate compared to high altitude and these leads to the development of VOCs related to fruity, green and buttery notes, resulting in a more delicate aroma. Beans fermented for a prolonged period contain less acidic notes, less low molecular weight sugars and more phenolic compounds. These findings are in agreement with Bytof [29], who suggested that the chemical reactions happening in the seeds during their processing have a strong impact in the composition of flavor and therefore in the quality of coffee. The linear model that was developed in this study has huge potential to be applied in predicting the total VOCs intensity based on the altitude, fermentation time and roasting level. The suitability of PTR-MS together with the linear regression model could be a powerful tool in quality control for coffee industry. Further studies are desirable in the future to correlate these results with sensory analysis.

**Acknowledgements** Prapaijit Kruathongsri was supported by The Thailand Research Fund (TRF), in the project Research and Researcher for Industry (RRI) “Development of Arabica coffee bean containing gamma-aminobutyric acid (GABA) and its application for ready-to-drink coffee beverage”. The partner industry is WaweeCoffee Co., Ltd., Chiang Mai, Thailand. We are grateful to the Province of Bolzano for financial support (Landesregierung mittels Beschluss Nr. 1472, 07.10.2013).

### Compliance with ethics standards

**Conflict of interest** No conflict of interest has been declared.

**Compliance with ethics requirements** This article does not contain any studies with human or animal subjects.

## References

- Toledo PRAB, Pezza L, Pezza HR, Toci AT (2016) Relationship between the different aspects related to coffee quality and their volatile compounds. *Compr Rev Food Sci Food Saf* 15(4):705–719
- Yeretzian C, Alfons J, Werner L (2003) Analysing the headspace of coffee by proton-transfer-reaction mass-spectrometry. *Int J Mass Spec* 223–224:115–139
- Sunarharum WB, Williams DJ, Smyth HE (2014) Complexity of coffee flavor: a compositional and sensory perspective. *Food Res Int* 62:315–325
- Toci AT, Farah A (2014) Volatile fingerprint of Brazilian defective coffee seeds: corroboration of potential marker compounds and identification of new low quality indicators. *Food Chem* 153:298–314
- Lindinger C, Labbe D, Pollien P, Rytz A, Juillerat MA, Yeretzian C, Blank I (2008) When machine tastes coffee: instrumental approach to predict the sensory profile of espresso coffee. *Anal Chem* 80(5):1574–1581
- 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. *Euro Food Res Technol* 214:92–104
- Gloess AN, Vietri A, Wieland F, Smrke S, Schönbacher B, Sánchez López JA, Petrozzi S, Bongers S, Kozirowski T, Yeretzian C (2014) Evidence of different flavour formation dynamics by roasting coffee from different origins: on-line analysis with PTR-TOF-MS. *Int J Mass Spec* 365–366:324–337
- Mateus M-L, Lindinger C, Gomy J-C, Liardon R (2007) Release kinetics of volatile organic compounds from roasted and ground coffee: online measurements by PTR-MS and mathematical modeling. *J Agric Food Chem* 55:10117–10128
- Hameed A, Hussain SA, Suleria HAR (2018) “Coffee Bean-Related” agroecological factors affecting the coffee. Co-evolution of secondary metabolites. Reference series in phytochemistry. Springer, Berlin
- Pongsak A (2002) Coffee production status and potential of organic arabica coffee in Thailand. *AU J Technol* 5:117–123
- Lee LW, Cheong MW, Curran P, Yu B, Liu SQ (2015) Coffee fermentation and flavor—an intricate and delicate relationship. *Food Chem* 185:182–191
- Kipkorir R, Muhoho S, Muliro P, Mugendi B, Frohme M, Broedel O (2015) Effects of coffee processing technologies on aroma profiles and sensory quality of Ruiru 11 and SL 28 Kenyan coffee varieties. *Asian J Agr Food Sci* 3:178–188
- Joët T, Laffargue A, Descroix F, Doubeau S, Bertrand B, Al De Kochko, Dussert S (2010) Influence of environmental factors, wet processing and their interactions on the biochemical composition of green Arabica coffee beans. *Food Chem* 118:693–701
- Hameed A, Hussain SA, Ijaz MU, Ullah S, Pasha I, Suleria HA (2018) Farm to consumer: factors affecting the organoleptic characteristics of coffee. II: postharvest processing factors. *Compr Rev Food Sci Food Saf* 17:1184–1237
- Selmar D, Bytof G, Knopp SE, Breitenstein B (2006) Germination of coffee seeds and its significance for coffee quality. *Plant Biol* 8:260–264
- Ruosi MR, Cordero C, Cagliero C, Rubiolo P, Bicchi C, Sgorbini B, Liberto E (2012) A further tool to monitor the coffee roasting process: aroma composition and chemical indices. *J Agric Food Chem* 60:11283–11291
- Cheong MW, Tong KH, Ong JJM, Liu SQ, Curran P, Yu B (2013) Volatile composition and antioxidant capacity of Arabica coffee. *Food Res Int* 51:388–396
- Poltronieri P, Rossi F (2016) Challenges in specialty coffee processing and quality assurance. *Changelles* 7:19–40
- Giacalone D, Kreuzfeldt Degn T, Yang N, Lui C, Fisj I, Münchow M (2019) Common roasting defects in coffee: aroma composition, sensory characterization and consumer perception. *Food Qual Prefer* 71:463–474
- Lyman DJ, Benck R, Dell S, Merle S, Murray-Wijelath J (2003) FTIR-ATR analysis of brewed coffee: effect of roasting conditions. *J Agric Food Chem* 51(11):3268–3272
- Beauchamp J, Herbig J, Dunkl J, Singer W, Hansel A (2013) On the performance of proton-transfer-reaction mass spectrometry for breath relevant gas matrices. *Meas Sci Technol* 24:125003
- Özdestan Ö, van Ruth SM, Alewijn M, Koot A, Romano A, Cappellin L, Biasioli F (2013) Differentiation of specialty coffees by proton transfer reaction-mass spectrometry. *Food Res Int* 53:433–439
- Yener S, Romano A, Cappellin L, Märk TD, del Pulgar JS, Gasperi F, Navarini L, Biasioli F (2014) PTR-ToF-MS characterisation of roasted coffees (*C. arabica*) from different geographic origins. *J Mass Spec* 49:929–935
- Yener S, Romano A, Cappellin L, Granitto PM, Aprea E, Navarini L, Märk TD, Gasperi F, Biasioli F (2015) Tracing coffee origin by direct injection headspace analysis with PTR/SRI-MS. *Food Res Int* 69:235–243
- Yener S, Navarini L, Lonzarich V, Cappellin L, Märk TD, Bonn GK, Biasioli F (2016) Monitoring single coffee bean roasting by direct volatile compound analysis with proton transfer reaction time-of-flight mass spectrometry. *J Mass Spec* 51:690–697
- Avelino J, Barboza B, Carlos AJ, Carlos F, Fabrice D, Guyot B, Cilas C (2005) Effects of slope exposure, altitude and yield on coffee quality in two altitude terroirs of Costa Rica. Orosi and Santa Maria de Dota. *J Sci Food Agric* 85:1869–1876
- Dold S, Lindinger C, Kolodziejczyk E, Pollien P, Ali S, Germain JC, Perin SG, Pineau N, Folmer B, Engel K-H, Barron D, Hartman C (2001) Influence of foam structure on the release kinetics of volatiles from espresso coffee prior to consumption. *J Agric Food Chem* 59:11196–11203
- Flament I (2002) Coffee flavor chemistry. Wiley, New York
- Bytof G, Knopp SE, Kramer D, Breitenstein B, Bergervoet JH, Groot SP, Selmar D (2007) Transient occurrence of seed germination processes during coffee post-harvest treatment. *Ann Bot* 100:61–66

**Publisher's Note** Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.