Received: 22 August 2021 | Revised: 26 December 2021 | Accepted: 12 January 2022

DOI: 10.1111/1750-3841.16071

FOOD CHEMISTRY

Journal of Food Science WILEY

Identifying aroma-active compounds in coffee-flavored dairy beverages

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Abstract: Coffee aroma is a complex mixture of volatile compounds. This study characterized the important aroma-active compounds associated with consumer liking in formulated coffee-flavored dairy beverages. Nine coffee-flavored dairy beverages were formulated: low fat–low coffee; medium fat–low coffee; high fat–low coffee; low fat–medium coffee; medium fat–medium coffee; high fat–medium coffee; low fat–high coffee; medium fat–high coffee; and high fat–high coffee. Regular coffee consumers, (n = 231) used a nine-point hedonic scale to rate acceptance of aroma. Volatile compounds were extracted by head space-solid phase micro-extraction (HS-SPME) and analyzed by gas chromatography-mass spectrometry-olfactometry (GC-MS-O) using a modified frequency (MF) approach. Fifty-two aroma-active compounds were detected. Thirty-one aroma-active compounds were considered important compounds with MF-value ≥ 50%. The total number of aroma-active compounds and their intensity were affected because of fat and coffee concentration. Partial least squares regression (PLSR) was performed to determine the relationship between aroma-active compounds and liking. PLSR analysis identified three groups of compounds regarding liking. Twenty-five compounds were associated with positive liking, for example, 2-(methylsulfanylmethyl) furan (coffee like). Sixteen compounds were negatively associated with liking, for example, 2-methoxyphenol (bacon, medicine like). Eleven detected compounds had no association with liking, for example, butane-2,3-dione (butter, fruit like).

Practical Application: The result of this study may be applied to formulate coffee-flavored dairy beverages to maximize consumer acceptance and aroma-liking. This study suggested too low coffee concentration is not desirable. Too much fat affects aroma release and/or alters the characteristic coffee flavor which negatively affects consumer acceptance.

KEYWORDS
aroma, coffee-flavored dairy beverage, GC-MS-O, HS-SPME, PLSR

1 | INTRODUCTION

Coffee has been consumed for over 1000 years and is an important beverage that plays a major role in the economy of coffee-producing countries (de Toledo et al., 2017). Worldwide, more than 400 billion cups of coffee are consumed each year (Poole et al., 2019; Rattan et al., 2015) and demand for coffee beverages is expected to continue increasing.

Aroma is an important coffee quality attribute and a critical criterion for consumer acceptance. If aroma quality/liking can be improved, it may be possible to increase consumer acceptance of coffee products, such as coffee-flavored dairy beverages. Therefore, during the formulation of coffee products, it is important to maximize the liking. This may be supported by identifying key aroma-active compounds associated with liking. The aroma composition of coffee is influenced by numerous factors, such as processing (roasting temperature, fermentation, grinding, brewing techniques), additives (milk, fat, creamer–liquid or granular substances instead of milk), coffee species, geographical origin, ripening stage, storage condition, and so on (Caporaso et al., 2018; Parat-Wilhelms et al., 2005; Pérez-Martínez et al., 2008; Ross et al., 2006; Schenker et al., 2002; Steen et al., 2017).

A change in the formulation of foods typically results in a variation of the flavor perception. Coffee extracts are typically used as a flavoring in the development of coffee-flavored dairy beverages. Li et al. showed that liking of coffee-flavored dairy beverages increased with the increase of coffee-flavor intensity to a certain point, but further addition led to decreased liking (Li et al., 2014). Fat has a positive influence on food liking via changing mouthfeel and aroma release (Mahmud et al., 2021). The fat level in milk and lipophilicity (e.g., hydrophobicity) of aroma-active compounds affect aroma release (Frank et al., 2012; Plug & Haring, 1993). As a result, during drinking, the aroma perception and liking of a product are significantly affected by fat level. Therefore, the fat and coffee ratio needs to be optimized to retain the characteristic coffee flavor and increase the liking of coffee-flavored dairy beverages.

The aroma intensity of a compound cannot be quantified using Gas Chromatography-Mass Spectrometry (GC-MS). A low concentration compound may have high aroma intensity that could have a potential impact on flavor, whereas a high concentration compound may not be perceived. The aroma intensity of a single compound is vital to understanding its contribution to the total flavor of a sample (Brattoli et al., 2013). Gas chromatography-olfactometry (GC-O) has been widely used for the determination of important aroma-active compounds (Akiyama et al., 2008). Among different methodologies employed with GC-O, the fast and reliable Modified Frequency (MF) approach uses a group of panelists (e.g. six assessors) and combines intensity and frequency detection (Majcher et al., 2013; San-Juan et al., 2010; Ubeda et al., 2016; Zapata et al., 2018).

The aim of this study was to evaluate the effects of the fat to coffee ratio on liking of nine formulated coffee-flavored dairy beverages; to analyze the aroma-active compounds and determine their intensity by GC-O-MF method; and to correlate sensory and GC-O results using partial least squares regression (PLSR).

2 | MATERIALS AND METHODS

2.1 | Samples

The following samples were used: Nescafé Blend 43 coffee, (Nestlé, Melbourne, Australia); Bulla thickened cream, (Bulla Dairy Foods Pty. Ltd., Melbourne, Australia); skim milk, (Devondale, Murray Goulburn Co-operative Co. Ltd., Melbourne, Australia); and sucrose consisting of 100% crystal cane sugar (0% fat), (CSR, Australia).

2.2 | Sample preparation

An overview of coffee-flavored dairy beverage formulations is presented in Table 1. In brief, all the required components were homogenized at 5500 rpm (Silverson L4RT-A homogenizer, Triad Scientific, Manasquan, NJ, USA) for 10 mi. Samples were prepared on the same day of sensory evaluation and stored in refrigerator at 4°C until use. Samples were prepared on the same day for volatile compounds extraction.

2.3 | Sensory evaluation

The panel consisted of 231 consumers (191 females and 40 males) of age 19–63 years ($\bar{x} = 24.7$ and $s = 6.5$). Consumers attended one session (60 min) at the CASS Food Research Centre sensory laboratory, Deakin University, Australia. Consumers were instructed to sniff and consume the sample, then, rate the aroma-liking of each sample on a nine-point hedonic scale, where 1 = extremely dislike, 5 = neither like nor dislike, and 9 = extremely like. To avoid the carry over effect and/or refresh the olfactory, consumers were instructed to sniff roasted coffee beans and rinse their mouth with filtered deionized water for 5 s in between samples. All data collection was conducted

TABLE 1 Coffee-flavored dairy beverages formulation. Mean value and standard deviation of aroma liking as evaluated by the 231 consumers

Sample	Variables		Total fat from cream (g/100 ml)	Sucrose (g/100 ml)	Aroma liking $\bar{x}$ (s)
	Cream (g/100 ml)	Coffee (g/100 ml)			
LF-HC	0.00	6.00	0.00	5.00	4.72 (2.3)
MF-HC	10.50	6.00	3.70	5.00	5.50 (2.0)
HF-HC	21.20	6.00	7.40	5.00	5.65 (2.0)
LF-MC	0.00	2.00	0.00	5.00	5.39 (1.8)
MF-MC	10.50	2.00	3.70	5.00	5.68 (1.6)
HF-MC	21.20	2.00	7.40	5.00	5.68 (1.6)
LF-LC	0.00	0.67	0.00	5.00	5.13 (1.5)
MF-LC	10.50	0.67	3.70	5.00	4.74 (1.8)
HF-LC	21.20	0.67	7.40	5.00	4.63 (1.9)

Note. the volume was adjusted by adding skim milk to make up the volume to 100 mL.
LF-HC = low fat-high coffee; MF-HC = medium fat-high coffee; HF-HC = high fat-high coffee; LF-MC = low fat-medium coffee; MF-MC = medium fat- medium coffee; HF-MC = high fat- medium coffee; LF-LC = low fat - low coffee; MF-LC = medium fat- low coffee; and HF-LC = high fat - low coffee.

in computerized and individual partitioned sensory booths in the CASS lab using Compusense Cloud Software as part of the Compusense Academic Consortium (Compusense Inc., Guelph, ON, Canada). Refrigerated (4°C) samples were poured (15–20 ml) in plastic cups and served at room temperature (20 ± 2°C) with three-digit blinded code cup in a randomized order. All consumers were instructed to refrain from teeth brushing, eating, drinking (except water), and smoking for 2 h prior to evaluations to prevent potential influences on sensory perception. Furthermore, all consumers were urged to avoid exposure to cosmetics or strong fragrance on the testing day. This sensory study was approved by the human ethics advisory group, Deakin University (ID:2012_162).

2.4 | Extraction of volatile compounds

Manual Head-Space Solid-Phase Micro-Extraction (HS-SPME) was used to extract volatile aroma-active compounds. A 5 ml aliquot of sample was transferred to a 20 ml head-space vial and sealed with an 18 mm Teflon lined magnetic cap (Agilent technologies, Santa Clara, CA, USA). A divinyl benzene/carboxen/ polydimethylsiloxane (DVB/CAR/PDMS, gray, 50/30 μm, length 1 cm, Agilent technologies) coated SPME fiber was used for the extraction of volatiles. The equilibrium and extraction time was 20 and 30 min, respectively. Throughout the equilibrium and extraction time, the vial temperature was maintained at 35 ± 1°C in a water bath with an appropriate hot plate and thermometer. During equilibrium and extraction time, a magnetic stir bar was used to release the volatiles. After the extraction process the fiber was desorbed in the GC inlet for 5 min at 250°C, followed by oven temperature program described below.

2.5 | Analysis of volatile compounds using GC-MS-O

The analysis was carried out using an Agilent 7890B gas chromatograph equipped with Agilent 5977B Mass Selective Detector (Agilent, Mulgrave, Australia) and Gerstel ODP-3 Olfactory Detector Port (Gerstel, Lasersan Australasia Pty. Ltd., Australia). The separation was conducted using BP-5MS capillary column (30 m × 0.250 mm × 0.25 μm), (Trajan Scientific and Medical, Australia). The split/splitless inlet was fitted with a Merlin Microseal (Agilent, Santa Clara, CA, USA), and a splitless SPME liner (i.d. 0.75 mm, Agilent, USA), and operated in splitless mode. High purity helium (99.999 %) was used as a carrier gas under a constant flow of 1.4 ml/min. The column oven temperature started at 40°C with a 4 min hold time, and then ramped at 8.6°C/min to 200°C with an 8 min hold time (total analysis time 30.6 min). MS conditions were scan range 35–450 m/z., solvent delay time 0 min, electron impact mode at 70 eV, MS source 230°C, and MS quad 150°C. For ODP, the column was connected with splitter and the effluent was split 1:1 using two deactivated fused silica capillary tubes (1.43 m × 0.10 mm i.d. to MS and 0.57 × 0.10 mm i.d. to ODP, Trajan Scientific and Medical, Australia). The ODP transfer line was maintained at 250°C and the makeup gas was nitrogen.

2.6 | GC-O data collection method

MF method (Dravnieks, 1985) was used for GC-O data collection. A panel composed of six sniffers (three female and three male) were trained over the 3 months and used to carry out the analysis. Each extract was smelled once by

each sniffer. Each sniffer carried out one session per day, and each session was approximately 25 min. Panelists were asked to press the olfactory pad, describe the aroma, and score the intensity of each aroma-active compound while sniffing the effluent from ODP. The computer recorded the retention time and sniffing time of each aroma-active compound. The aroma-intensity was evaluated using a six-point scale (1 = very weak, 2 = weak, 3 = clear, 4 = very clear, 5 = intense, and 6 = very intense). All panelists were urged to avoid exposure to cosmetics and fragrance on the sniffing day to prevent potential carryover effect.

2.7 | Retention index

An alkane solution C7–C40 (49452 U, Supelco, USA) of 1000 µg/ml in hexane was employed to calculate the Linear Retention Index (LRI) of each analyte on BP-5MS column.

2.8 | HS-SPME, GC-MS-O performance, and retention time stability evaluation

The quality control (QC) sample was prepared using 2.0 g of Nescafé Blend 43 coffee into 100 ml deionized water. The QC sample and n-alkane mix were injected prior to starting and after finishing each day's sniffing. Extraction of volatile compounds of the QC sample was same as coffee-flavored dairy beverage samples. The GC analytical conditions for the QC sample and n-alkane were the same as coffee-flavored dairy beverages. The repeatability of the method or consistent performance of HS-SPME and GC-MS-O was evaluated by monitoring the total peak area of the QC sample. The coefficient of variation (CV) of the total peak area of the QC sample was ≤ 9.4% throughout the study. The stability of retention time (RT) was monitored by n-alkane. The CV % of n-alkane's RT was ≤ 0.008.

2.9 | Data analysis

Repeated measure analysis of variance (ANOVA) determined the effects of fat and coffee concentration on overall aroma-liking. The factorial design feature of the experiment was used to estimate the two-way interaction effects of fat and coffee concentration on overall aroma-liking through linear mixed models. Margins and box plot were extracted to visualize the effects of fat and coffee interaction on aroma-liking (Mahmud et al., 2021).

The MF value of each detected aroma-active compounds was calculated using the following formula:

$$\mathrm{MF}\,(\%) = \sqrt{F\,(\%) \times I\,(\%)} \tag{1}$$

where F (%) is the detection frequency of an aromatic attribute expressed as percentage of maximum detection $\left(\frac{\text{number of detections}}{6} \times 100\,\%\right)$ and I (%) is the sum of aroma intensities expressed as percentage of maximum sum of intensity $\left(\frac{\text{sum of intensities from 6 sniffers}}{30} \times 100\%\right)$ (Kortesniemi et al., 2018). MF (%) represents the importance of an aroma-active compound in a sample. The effects of different level of fat and coffee interaction on total intensity or total MF values of different samples and chemical groups were visualized using Microsoft Excel 2016.

PLSR was run on the data matrix considering GC-O data as X variables (as explanatory variables) and consumer liking data from consumer liking test as Y variables (as a dependent variable) (Yu et al., 2019).

The statistical analysis program STATA/IC 15.0 (Stata Corp LLC, 4905 Lakeway Drive, College Station, Texas 77845, USA) was used to analysis the sensory data and PLSR was constructed using XLSTAT (ver. 2016.01.26779, Addinsoft, NY, USA).

3 | RESULTS AND DISCUSSION

3.1 | Sensory evaluation

During food consumption, volatile aroma-active compounds reach the olfactory epithelium and affect food flavor liking (Yin et al., 2017). The current study found that the aroma-liking of coffee-flavored dairy beverages was significantly affected ($p < 0.001$) by fat and coffee concentration. The aroma intensity or aroma quality can alter with fat concentration (Bücking & Steinhart, 2002) which may affect the intensity and aroma-liking of coffee-flavored dairy beverages. A recent study also stated that fat concentration has effects on aroma intensity and liking of milk (Pirc et al., 2022).

The mean and standard deviation of aroma-liking ratings for tasted coffee-flavored dairy beverages are presented in Table 1. The effects of fat and coffee level and their interaction on overall aroma-liking are presented in Table 2. The result showed that the overall aroma-liking increased around 0.24 mean unit at MF and HF as compared to the LF. This study noticed that fat had a moderately flat function on aroma-liking, while coffee concentration is more important for coffee-flavored dairy beverages aroma-liking. Compared to the LC, aroma-liking increased 0.75 and 0.45 mean units at MC and HC, respectively. The combined effect of fat and coffee on overall aroma liking was determined by estimating two-way interaction between fat and coffee concentration (Table 2). For overall aroma liking outcome, LF-LC was considered as a reference group. Compared to the reference (LF-LC) group, the overall aroma-liking increased more than 0.50 mean unit at MF-MC and HF-MC, while it was increased

TABLE 2 Effects of fat and coffee level, and their interaction on overall aroma liking as evaluated by the consumers ($n = 231$)

	Mean difference	*Z*-Value	*p*-Value	95 % CI
Fat label				
LF	Reference	Reference	Reference	Reference
MF	0.23	2.79	<0.001	0.07, 0.39
HF	0.24	2.88	<0.001	0.08, 0.40
Coffee label				
LC	Reference	Reference	Reference	Reference
MC	0.75	7.29	<0.001	0.55, 0.95
HC	0.45	2.87	<0.001	0.14, 0.77
Fat by coffee interaction				
LF-LC	Reference	Reference	Reference	Reference
MF-MC	0.66	3.96	<0.001	0.33, 0.98
MF-HC	1.17	6.70	<0.001	0.83, 1.51
HF-MC	0.77	4.28	<0.001	0.42, 1.12
HF-HC	1.43	6.87	<0.001	1.02, 1.84

Note. LF = low fat; MF = medium fat; HF = high fat; LC = low coffee; MC = medium coffee; HC = high coffee; LF-LC = low fat - low coffee; MF-MC = medium fat -medium coffee; MF-HC = medium fat - high coffee; HF-MC = high fat - medium coffee; and HF-HC = high fat - high coffee.

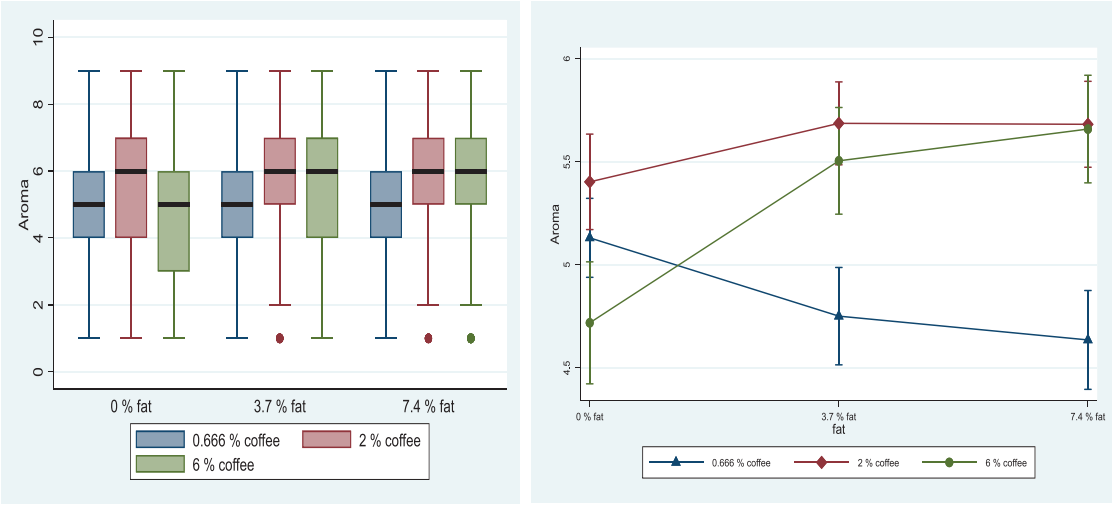

FIGURE 1 A box plot and margins plot show the effects of different fat and coffee label interaction on aroma liking of coffee-flavored dairy beverages. *X*-axis represents fat level and *Y*-axis represents aroma liking as evaluated by consumers ($n = 231$). Box plot shows the median value along with upper and lower quartile. Estimated mean and 95 % Confidence Interval (CI) are illustrated in Margin plot

more than 1.0 mean unit at MF-HC and HF-HC. High coffee concentration may increase the liking of coffee-flavored dairy beverages, but excessive coffee concentration increases the bitterness and intensity, which decrease the liking of coffee-flavored dairy beverages (Li et al., 2014). The margins and box plot illustrate the combined impacts of fat and coffee interaction on the overall aroma liking in Figure 1. The margin plots clearly show that the MF-MC is the optimum ratio to maximize the aroma-liking.

3.2 | Gas Chromatography-Olfactometry (GC-O) analysis

A total of 52 aroma-active compounds were detected by GC-O analysis, as shown in Table 3. This list comprises one acid, tow alcohols, five aldehydes, one aromatic hydrocarbon, two bases, one ester, five furans, four phenols, eight pyrazines, two pyrroles, eight ketones, five sulfurs, and eight others. For the sake of confirmation or simplicity, those aroma-active compounds not reaching a

TABLE 3 List of detected aroma-active compounds along with Modified Frequency (MF) value of nine formulated coffee-flavored dairy beverages as determined by GC-MS-O. According to the Partial Least Square Regression (PLSR) analysis, compounds are divided into three groups: (a) positive, (b) Negative, and (c) Neutral to liking

No.[1]	Compounds (IUPAC)	Aroma descriptions	LRI[2] (Cal.)	LRI[3] (Ref.)	Chemical Group	MF[4] LF-HC	MF-HC	HF-HC	LF-MC	MF-MC	HF-MC	LF-LC	MF-LC	HF-LC	Ident.[5]
(A) Positive to liking															
1	2-Methylpropan-1-ol	caramel, cocoa, green, malt, nut			Aldehyde	30	29	26	36	30	0	0	0	0	MS, AD, Tent
3	Butan-2-one	fragrant, fruit, pleasant, sweet			Ketone	**59**	**59**	**65**	47	43	**57**	0	0	0	MS, AD, Tent
4	2-Methylbutanal	almond, cocoa, malt, pungent, fermented	660	654	Aldehyde	**66**	**78**	**68**	**78**	**75**	**50**	0	0	0	MS, AD, LRI, ST
5	Pentane-2,3-dione	butter, caramel, fruit, sweet	697	699	Ketone	41	49	**59**	0	30	29	0	0	0	MS, AD, LRI, ST
8	Hexanal	grass, green	797	801	Aldehyde	41	38	0	45	26	0	0	0	0	MS, AD, LRI, ST
11	2-Methylpyrazine	cocoa, green, hazelnut, popcorn, roasted	819	821	Pyrazine	**61**	43	45	**56**	35	45	0	0	0	MS, AD, LRI, Tent
12	Furan-2-carbaldehyde	almond, baked potatoes, bread, candy, floral	828	835	Furan	0	38	**59**	0	33	31	0	0	0	MS, AD, LRI, ST
13	2,4,5- Trimethyl-1,3-oxazole	dairy, butter, aged cheeses, yogurt, caramel	844	848	Oxazol(in)es	37	**59**	**78**	45	45	26	0	0	29	MS, AD, LRI, Tent
15	Heptan-2-ol	citrus, coconut, fried, mushroom, oil	899	899	Alcohol	**71**	**66**	**70**	**75**	**63**	**51**	0	45	0	MS, AD, LRI, ST
16	1-(Furan-2-yl) ethanone	balsamic, cocoa, coffee, smoke, tobacco	904	913	Furan	**51**	**82**	**85**	**65**	**80**	**78**	35	0	0	MS, AD, LRI, ST

(Continues)

TABLE 3 (Continued)

No.[1]	Compounds (IUPAC)	Aroma descriptions	LRI[2] (Cal.)	LRI[3] (Ref.)	Chemical Group	MF[4] LF-HC	MF-HC	HF-HC	LF-MC	MF-MC	HF-MC	LF-LC	MF-LC	HF-LC	Ident.[5]
17	2,5-Dimethylpyrazine	burnt plastic, cocoa, roast, roasted nut	907	912	Pyrazine	**65**	**78**	**90**	**80**	**82**	**80**	**63**	**78**	29	MS, AD, LRI, ST
18	2-Ethylpyrazine	green, iron scorch, must, peanut butter, roasted	911	915	Pyrazine	**65**	**59**	**68**	47	**65**	**59**	0	31	38	MS, AD, LRI, ST
19	5-Methylfuran-2-carbaldehyde	almond, caramel, cooked, roasted garlic, spice	957	961	Furan	**53**	33	45	**57**	**57**	33	0	0	26	MS, AD, LRI, Tent
20	(Methyltrisulfar	cabbage, fish, onion, sulfur	968	968	Sulfur	**75**	36	38	**71**	**55**	**55**	**53**	0	0	MS, AD, LRI, ST
22	Furan-2-ylmethyl acetate	roast, fruity, sweet	988	990	Furan	43	26	33	31	43	0	0	0	0	MS, AD, LRI, ST
24	2-(Methylsulfanyl furan	coffee	996	995	Sulfur	**76**	**73**	**82**	**63**	**78**	**71**	**57**	38	38	MS, AD, LRI, Tent
25	2-Ethyl-3-methylpyrazine	green, must, nut, potato, roasted	998	999	Pyrazine	**65**	**63**	**76**	45	**73**	35	0	0	0	MS, AD, LRI, Tent
27	2-Phenylacetaldeł	pungent, fermented, earthy	1037	1038	Aldehyde	**53**	**53**	**53**	**66**	**54**	**59**	0	0	0	MS, AD, LRI, ST
28	1-Ethylpyrrole-2-carbaldehyde	burnt, roasted, smoky	1045	1046	Bases	**65**	**75**	**68**	**55**	35	35	48	33	0	MS, AD, LRI, Tent
31	3-Ethyl-2,5-dimethylpyrazir	earth, potato, roast	1076	1079	Pyrazine	47	**75**	**83**	**76**	**67**	**55**	0	0	0	MS, AD, LRI, Tent
34	Unknown	cereal, nutty, musty, roasted	1088	–	–	**59**	49	**59**	37	35	49	0	0	0	

(Continues)

TABLE 3 (Continued)

No.[1]	Compounds (IUPAC)	Aroma descriptions	LRI[2] (Cal.)	LRI[3] (Ref.)	Chemical Group	MF[4]									Ident.[5]
						LF-HC	MF-HC	HF-HC	LF-MC	MF-MC	HF-MC	LF-LC	MF-LC	HF-LC	
35	Nonanal	citrus, fat, green, paint, pungent	1101	1104	Aldehyde	0	**65**	**54**	**57**	**63**	**51**	0	38	0	MS, AD, LRI, ST
36	Unknown	roast, earth, garden	1128	–	–	0	43	37	0	41	0	0	0	0	
41	2-[(Methyldisulfanyl)methyl] furan	Smoke	1213	1222	Sulfur	**73**	41	39	**71**	**53**	31	**71**	0	0	MS, AD, LRI, Tent
48	1-(2,6,6-Trimethylcyclohexa-1,3-dien-1-yl) but-2-en-1-one	boiled apple, floral, fruit, grape, tea	1385	1388	Ketone	**60**	48	0	**55**	43	29	0	0	0	MS, AD, LRI, Tent
B) Negative to liking															
6	2-Methylthiophen	Sulfur	768	771	Sulfur	46	29	0	0	0	0	0	0	0	MS, AD, LRI, ST
9	1-Ethylpyrrole	chemical, roast	809	810	Pyrrole	35	0	0	33	0	0	0	0	0	MS, AD, LRI, Tent
10	4-Methyl-1,3-thiazole	green, nut, roasted meat	812	814	Sulfur	**57**	0	0	**57**	0	0	0	0	0	MS, AD, LRI, Tent
14	Furan-2-ylmethanol	burnt, cooked, solvent	853	854	Furan	**65**	45	0	**61**	0	33	**55**	**55**	0	MS, AD, LRI, ST
23	2-Ethyl-6-methylpyrazine	green, nut, roasted	994	997	Pyrazine	39	0	0	0	0	0	0	0	0	MS, AD, LRI, ST
29	1-(1H-pyrrol-2-yl) ethanone	bread, cocoa, hazelnut, walnut	1059	1063	Ketone	**53**	0	0	0	0	0	0	0	0	MS, AD, LRI, Tent
30	Unknown	musty, bread	1062	–	–	41	0	0	0	0	0	0	0	0	
32	2-Methoxyphenol	bacon, medicine, phenol, smoke, wood	1084	1089	Phenol	**68**	**78**	**58**	**61**	47	**65**	**66**	**78**	**61**	MS, AD, LRI, Tent

(Continues)

TABLE 3 (Continued)

No.[1]	Compounds (IUPAC)	Aroma descriptions	LRI[2] (Cal.)	LRI[3] (Ref.)	Chemical Group	MF[4] LF-HC	MF-HC	HF-HC	LF-MC	MF-MC	HF-MC	LF-LC	MF-LC	HF-LC	Ident.[5]
37	2,3-Diethyl-5-methylpyrazine	earth, meat, potato, roast	1149	1151	Pyrazine	**73**	**69**	**53**	**60**	**67**	41	**78**	**71**	**67**	MS, AD, LRI, ST
38	3,5-Diethyl-2-methylpyrazine	baked, cocoa, roast, rum, sweet	1153	1161	Pyrazine	47	0	0	0	0	0	0	0	0	MS, AD, LRI, Tent
39	Octanoic acid	fat, cheese, rancid	1171	1174	Acid	**73**	**54**	**63**	**76**	**57**	29	**80**	**76**	0	MS, AD, LRI, ST
43	4-Ethyl-2-methoxyphenol	medicine, smoke, woody	1274	1281	Phenol	38	0	0	0	0	0	0	0	0	MS, AD, LRI, ST
44	Undecan-2-one	fatty, cheese, butter, nut, fruit, floral	1289	1295	Ketone	38	0	0	0	0	0	0	0	0	MS, AD, LRI, Tent
46	Unknown	roasted, smoke, nutty	1333	–	–	34	0	0	0	0	0	0	0	0	
49	Unknown	roast, smoky	1453	–	–	46	0	0	0	0	0	0	0	0	
51	Dodecan-1-ol	fat, wax	1475	1473	Alcohol	0	0	0	0	0	0	0	33	29	MS, AD, LRI, ST
C) Neutral to liking															
2	Butane-2,3-dione	butter, caramel, fruit, sweet, yogurt	–	–	Ketone	38	31	**51**	31	45	38	38	47	26	MS, AD, Tent
7	Methyl 3-methylbutanoate	apple, fruit, pineapple	775	773	Esters	0	0	0	0	36	38	0	0	0	MS, AD, LRI, Tent
21	Phenol	medicine, phenol, smoke, spice	978	984	Phenol	0	31	0	0	0	0	0	0	0	MS, AD, LRI, Tent
26	3-Methylcyclopentane-1,2-dione	coffee, burnt, sugar	1030	1021	Ketone	**55**	**60**	**76**	**69**	47	0	35	**57**	0	MS, AD, LRI, ST
33	Nonan-2-one	pleasant, hot milk, fragrant, fruit, green	1087	1091	Ketone	**71**	**78**	**82**	**68**	**51**	47	**83**	**53**	0	MS, AD, LRI, ST

(Continues)

TABLE 3 (Continued)

No.[1]	Compounds (IUPAC)	Aroma descriptions	LRI[2] (Cal.)	LRI[3] (Ref.)	Chemical Group	MF[4] LF-HC	MF-HC	HF-HC	LF-MC	MF-MC	HF-MC	LF-LC	MF-LC	HF-LC	Ident.[5]
40	1-(Furan-2-ylmethyl) pyrrole	cocoa, green, roast	1176	1182	Pyrrole	**82**	**62**	**51**	**69**	**56**	**71**	**87**	0	0	MS, AD, LRI, ST
42	Unknown	cocoa, green, mint	1239	–	–	0	39	0	0	26	29	0	33	0	
45	4-Ethenyl-2-methoxyphenol	clove, curry, smoke, spice	1309	1318	Phenol	37	45	45	35	45	0	0	0	31	MS, AD, LRI, ST
47	Unknown	dairy, milky, cheese, pleasant	1345	–	–	0	37	0	0	0	0	0	29	31	
50	3,3,7-Trimethyl-8-methylidenetricyclo[5.4.0.02,9] undecane	sweet, woody, rose, vegetable, flower	1461	1451	Aromatic Hydrocarbon	0	0	0	0	0	0	0	0	35	MS, AD, LRI, Tent
52	Unknown	fruity, sweet	1596	–	–	0	0	0	0	0	0	0	0	36	

Note. LF-HC = low fat-high coffee, MF-HC = medium fat-high coffee, HF-HC = high fat-high coffee, LF-MC = low fat-medium coffee, MF-MC = medium fat-medium coffee, HF-MC = high fat-medium coffee, LF-LC = low fat-low coffee, MF-LC = medium fat-low coffee, and HF-LC = high fat-low coffee

[1]Corresponding number (i.e., 1–52) of each compound is presented in Figure 3.

[2]Calculated LRI in BP-5MS column.

[3]Reference LRI in DB-5MS column.

[4]MF: modified frequency, the bold MF-value (MF% ≥ 50) indicates an important aroma-active compounds.

[5]Identification: MS = matching mass spectra of GC-MS analysis with those from the NIST 2017 library (library match: ≥ 70 %); AD = coincidence of aroma description reported in online data base (http://www.odour.org.uk; http://www.thegoodscentscompany.com/; and http://flavornet.org) or literature; LRI = coincidence of Linear Retention Index (LRI) reported in online data base (e.g. https://pubchem.ncbi.nlm.nih.gov/ and https://www.pherobase.com/) or literature; ST = coincidence of LRI with standard. Tent = Tentative, when only MS or LRI or AD is present for the identification of an aroma-active compounds, it is regarded as an attempt of identification (Ayseli et al., 2021; Sertkaya et al., 2021).

maximum GC-O intensity of 25% (maximum = 100 %) and not perceived by three sniffers (maximum = six sniffers) in any of the nine formulated iced-coffee samples were eliminated and considered as noise. Therefore, the absence of a specific aroma-active compound in some of the samples means that the MF-value did not reach GC-O intensity of 25% and the perceived frequency was below 3, it still might occur in the sample, but the aroma-intensity was under the threshold level for the GC-O panelists. Thus, the GC-O analysis detected 42 aroma-active compounds in LF-HC, 38 in MF-HC, 35 in MF-MC, 33 in LF-MC, 31 in HF-HC, 30 in HF-MC, 16 in MF-LC, 14 in LF-LC, and 13 in HF-LC. Based on these results, the total number of detected aroma-active compounds or perception of aroma-active compounds was fewest in lower coffee concentrations combined with different fat levels. Previous study suggested that dairy or dairy products altered the aroma quality in coffee beverages (Bücking & Steinhart, 2002) and the release of lipophilic compounds decrease with the increase of fat concentration (Frank et al., 2011, 2012). The present investigation confirms that fat-influenced aroma release may be compensated by increasing the coffee concentration thereby maintaining or increasing the liking.

3.3 | Most important aroma-active compounds

Thirty-one compounds had the highest aroma activities (MF % = ≥ 50) (Table 3). Among all the samples, LF-HC (n = 25), HF-HC (n = 23), and LF-MC (n = 21) presented maximum number of important aroma-active compounds, while LF-LC (n = 10), MF-LC (n = 7), and HF-LC (n = 2) presented the lowest numbers. Among 31 compounds, "2-methoxyphenol" and "2,3-diethyl-5-methylpyrazine" showed the highest aroma activities in all samples. "2, 5-Dimethylpyrazine" reached the highest MF-value (90%) in HF-HC. The compounds, "1-(furan-2-yl) ethenone" and "2-(methylsulfanylmethyl) furan" reached MF-value above 50% in most of the samples and they have been reported as an important aroma-active compound in roasted or brewed coffee (Rattan et al., 2015; Blank et al., 1992; Czerny et al., 1999; Flament, 2002; Kıvançlı & Elmacı, 2016).

3.4 | Effects of fat and coffee ratio on aroma intensity

The MF-value of all aroma-active compounds and major chemical groups is summarized in Figure 2. Overall, the total intensity of each sample and different chemical groups of aroma-intensity was affected by fat and coffee ratio. The changes in intensity can be caused by different factors, for example, fat retains most volatiles. Further, along with fat, dairy products contain protein and carbohydrates that can interact by adsorption, entrapment, and encapsulation which affect volatile compounds release (Kinsella, 1990). Therefore, a simple correlation between the fat level and aroma release cannot be established. However, in all samples, a higher fat content had a negative impact on aroma intensity compared to zero fat. For example, the total intensity and different chemical groups' aroma intensity were lower in HF. The possible reason could be the complex matrices effect of fat and coffee combination such as lipophilic compounds are not released or remained below the detection limit in combination with fat (Frank et al., 2011; Frank et al., 2012).

3.5 | Correlation of GC-O and sensory results using PLSR

In the PLSR model, the 52 aroma-active compounds were specified as the X-matrix, and the mean overall aroma liking of the nine formulated iced-coffee was the Y-matrix. The cumulated R^2Y and R^2X values were 0.99 and 0.69, respectively, and the Q^2 cumulated index was 0.86, indicating the three components generated by PLSR are well summarized with the explanatory (X) and dependent (Y) variables (Kortesniemi et al., 2018). Table 3 shows which compounds were unique to which samples. The PLSR correlation plot in Figure 3 shows the strength of the association of predicted to observed for the correlation of the sensory and chemical analysis data. The following compounds were found as unique aroma-active compounds: "2- ethyl-6-methylpyrazine" "1-(1H-pyrrol-2-yl) ethenone" "unknown (LRI = 1062, musty, and bread like)" "3, 5-diethyl-2-methylpyrazine" '4- ethyl-2-methoxyphenol" "undecan-2-one" "unknown (LRI = 1333, roasted, smoke, and nutty like)" and "unknown (LRI = 1453, roast, and smoky like)" in LF-HC. For MF-HC, HF-HC, MF-MC, and HF-MC, "methyl 3-methylbutanoate" and "phenol" were found as a unique aroma-active compounds. "3,3,7-trimethyl-8-methylidenetricyclo [5.4.0.02,9] undecane" and "unknown (LRI = 1596, fruity and sweet like)" were found as a unique aroma-active compounds for HF-LC.

The PLSR analysis revealed three groups of aroma-active compounds corresponding to positive, negative, and neutral liking. Twenty-five compounds were positively related to liking, among them, "2,5-dimethylpyrazine (burnt plastic, cocoa, medicine, roast, and roasted nut like)" and "2-(methylsulfanylmethyl) furan (coffee like)" were positive to liking in all the samples (Table 3). "2-(methylsulfanylmethyl) furan" has a coffee-like quality

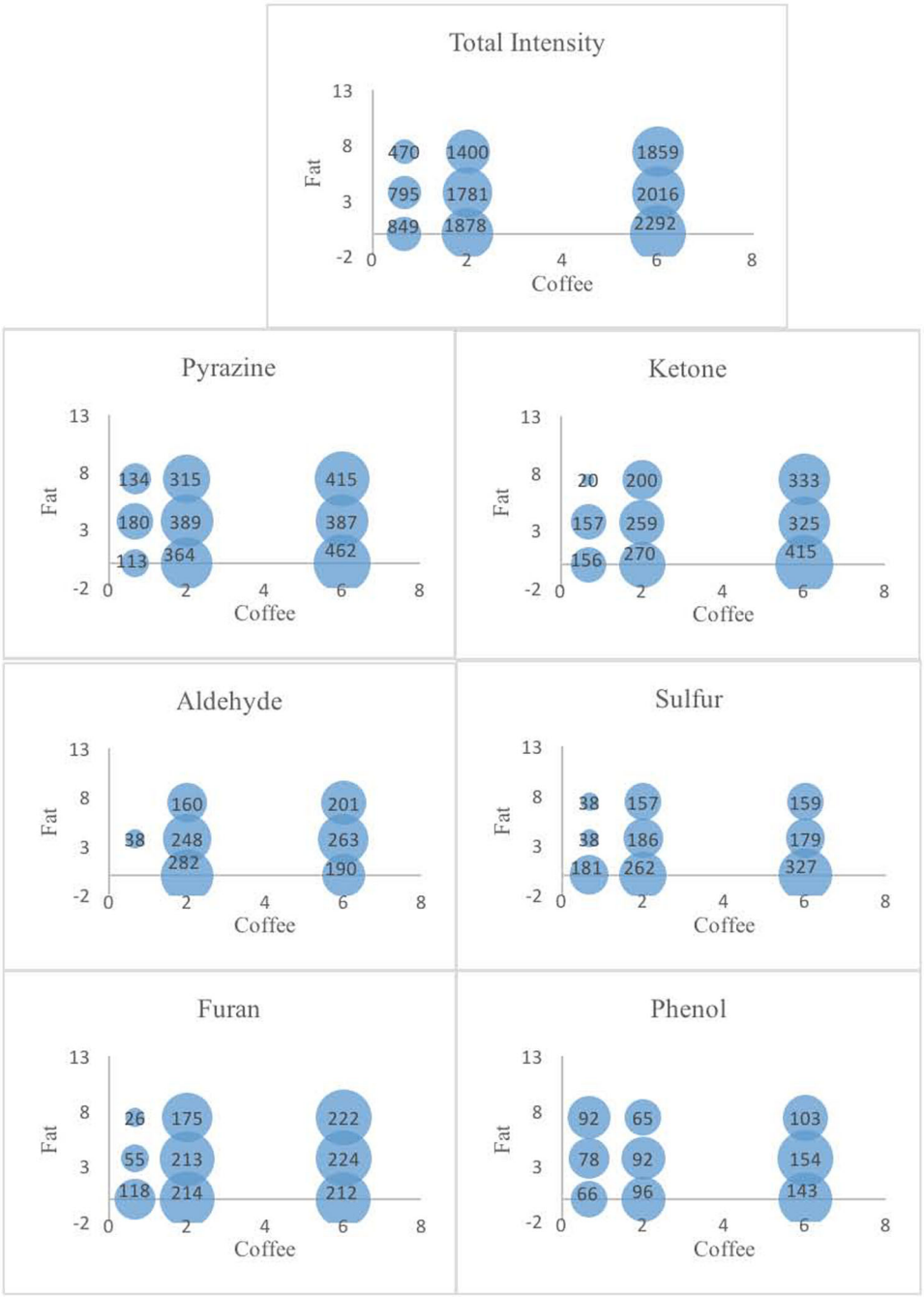

FIGURE 2 Effects of fat and coffee concentration on the total intensity and different chemical groups (e.g., pyrazine, ketone, aldehyde, sulfur, furan, and phenol). The total intensity and intensity of different chemical groups were calculated by summing-up the modified frequency (MF) value of detected aroma-active compounds as presented in Table 3. The *X*-axis represents the coffee level and *Y*-axis represents the fat level

which supports previous research showing the amount of "2-(methylsulfanylmethyl) furan" is higher in Robusta compared to Arabica coffee (Toledo et al., 2016). Therefore, a high amount of Robusta in Nescafé blend 43 coffee was the presumptive reason for the presence of "2-(methylsulfanylmethyl) furan" compounds in all samples. "2-methylbutanal (almond, cocoa, malt, pungent, fermented like)" "1-(furan-2-yl) ethanone (balsamic, cocoa, coffee, smoke, tobacco like)" "2-phenylacetaldehyde (pungent, fermented, earthy like)" "pentane-2,3-dione (butter, caramel, fruit, and sweet like)," and "3-ethyl-2,5-dimethylpyrazine (earth, potato, roast like)" had the highest intensity values and were associated with liking. All the above-mentioned compounds were presented

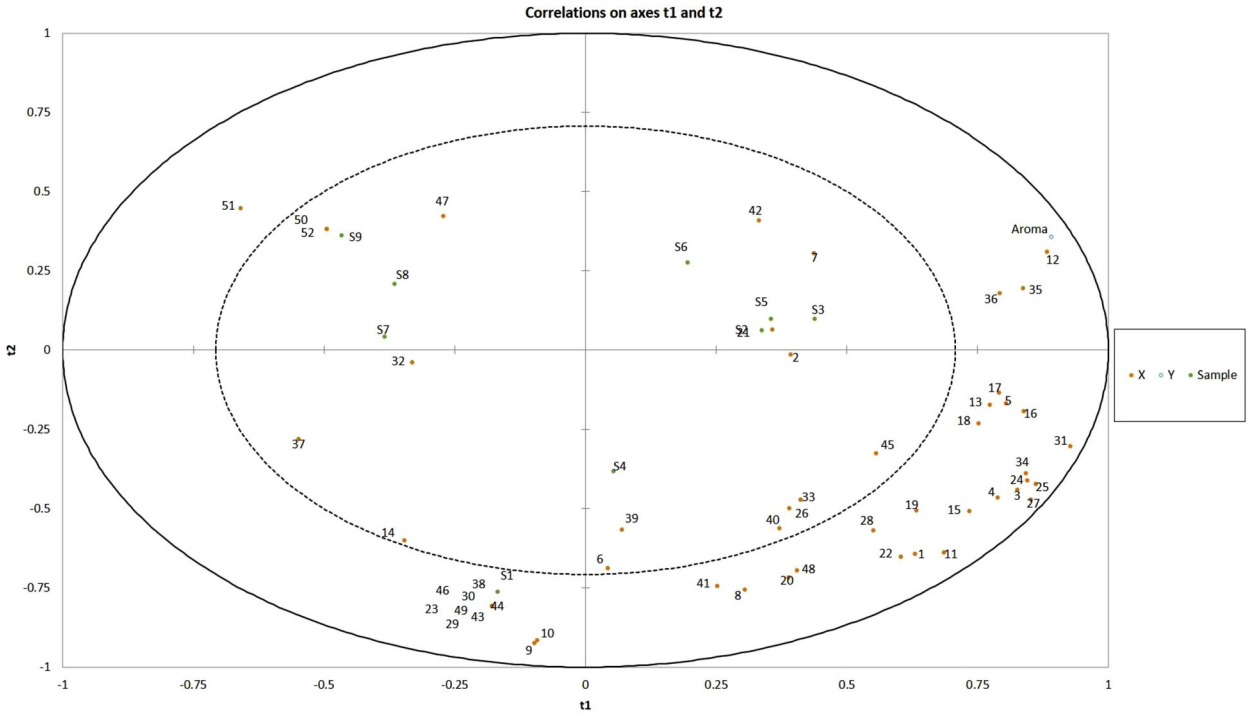

FIGURE 3 Partial Least Square Regression (PLSR) correlation plot for coffee-flavored dairy beverages. The model was established by 52 aroma compounds of GC-MS-O measurements as *X* and *Y* for the mean value of overall aroma liking as evaluated by 231 regular coffee consumers. S1 = low fat-high coffee, S2 = medium fat-high coffee, S3 = high fat-high coffee, S4 = low fat-medium coffee, S5 = medium fat-medium coffee, S6 = high fat-medium coffee, S7 = low fat-low coffee, S8 = medium fat-low coffee, and S9 = high fat-low coffee. The numbers (i.e.,1–52) are representing the aroma-active compounds name as presented in the Table 3

in HC and MC level samples (LF-HC, MF-HC, HF-HC, LF-MC, MF-MC, and HF-MC) and have been previously reported as potent aroma-active compounds for coffee-beverages (Blank et al., 1992; Czerny et al., 1999; Rattan et al., 2015; Toledo et al., 2016). Therefore, the coffee concentration is important for the aroma-active compounds release and aroma-liking of coffee-flavored dairy beverages.

Sixteen compounds were negatively associated with liking among which, "2-methoxyphenol (bacon, medicine, phenol, smoke, wood like)" and "2, 3-diethyl-5-methylpyrazine (earth, meat, potato, roast like)" were common in all samples. These two compounds were also rated as intense in all samples. Further, except HF-LC, all samples had the high intensity of "octanoic acid (fat, cheese, and rancid like)" and "furan-2-ylmethanol (burnt, cooked, and solvent like)" compounds. "Dodecan-1-ol (fat, wax like)" was only identified in LC samples but not in HC samples. The reason could be the effect of milk and fat in LC, as this compound has not previously been reported in coffee, but it is a known compound in milk products (Coppa et al., 2011; Shiratsuchi et al., 1994). In contrast, in HC sample with added milk, this compound may be suppressed by the high intensity compounds of coffee volatiles or remain under the detection limit because of the complex matrices effect of coffee volatiles.

Eleven compounds were identified as neutral to liking. Among them, only "butane-2,3-dione (butter, caramel, fruit, sweet, yogurt like)" was present in all samples. "3-methylcyclopentane-1,2-dione (coffee, burnt, sugar like)" "nonan-2-one (pleasant, hot milk, fragrant, fruit, green like)," and "1-(furan-2-ylmethyl) pyrrole (cocoa, green, roast like)" were also common neutral compounds to liking. The volatiles released or intensity of aroma-active compounds were influenced by the fat and coffee concentration. Overall fewer aroma-active compounds were released/detected in the formulated iced-coffee with fat addition. The least number of aroma-active compounds were detected or associated with liking in HF-LC sample. As a result, the perceived coffee flavor altered, and consumers scored low for HF-LC combination. Therefore, HF-LC was the least liked sample.

Aroma description of a chemical compound can be varied with concentration and/or in combination with other compounds. For example, a recent study showed

that the chemical compound "skatole" gives a "flowery like" aroma at low concentration but at high concentration, it gives a "fecal like" aroma (Regueiro et al., 2017). Further, a combination of "ethyl isobutyrate" "ethyl maltol," and "allyl-α-ionone" compounds give a distinctive "pineapple like" aroma (Thomas-Danguin et al., 2007). In this study, looking at the aroma description of each aroma compound, there was no specific trend among the three groups. However, each aroma compound has a specific aroma description, but in combination/interaction with other chemical compounds, the overall perceived aroma quality or aroma description of a compound could be altered which could affect the consumer liking (Mahmud et al., 2020).

There are limitations which must be considered when discussing these results. The effects of protein and carbohydrates were not accounted for in this study so future research should consider fixing protein and carbohydrate concentration. This study only considered intensity but not concentration. Therefore, future study should determine the concentration of each important compound. Furthermore, this study used dried coffee as a source of coffee. The dried coffee process removes almost all the coffee oil and usually replaces a small fraction back into the final blend to carry aroma and mouthfeel. As such, aroma-active compounds found in this study could be different compared to expresso with the full coffee oil content.

4 | CONCLUSIONS

This is the first time that the effect of fat and coffee ratio on liking and volatile aroma profiling and liking of the coffee-flavored dairy beverage is investigated. Sensory and instrumental results were combined using PLSR to identify the important compounds that drive consumer liking either positively or negatively. Fat and coffee ratio influences aroma release and liking of coffee-flavored dairy beverages. High fat had a negative impact on aroma-active compounds release or aroma intensity while it was opposite with coffee content. PLSR analysis identified twenty-five compounds positive to liking, sixteen compounds negative to liking, and eleven compounds neutral to liking. The positively or negatively identified compounds from this study can be used as flavor-modifiers in coffee-flavored dairy beverages. For example, this study suggests to enhance the intensity or concentration of aroma-active compounds such as "Butan-2-one" "1-(Furan-2-yl) ethanone" "2,5-Dimethylpyrazine" "2-(Methylsulfanylmethyl) furan" while reducing the intensity or concentration of aroma-active compounds such as "2-Methoxyphenol" "Furan-2-ylmethanol" "Octanoic acid" in coffee-flavored dairy beverages. Therefore, this study provides valuable information for coffee-flavored dairy beverages manufacturers wanting to increase consumer acceptance.

ACKNOWLEDGEMNTS

This research is supported by PhD scholarship, Deakin University Postgraduate Research Scholarship (DUPRS), Deakin University, Australia. Open access publishing facilitated by Deakin University, as part of the Wiley - Deakin University agreement via the Council of Australian University Librarians.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHOR CONTRIBUTIONS

M M Chayan Mahmud: Conceptualization, Data curation, Formal analysis, Methodology, Software, Validation, Writing - original draft, Writing - review & editing. Russell Keast: Conceptualization, Supervision, Writing - review & editing, Mohammadreza. Mohebbi: Software, Validation, Writing - review & editing. Robert A. Shellie Conceptualization, Data curation, Software, Supervision, Writing - review & editing - Equal.

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How to cite this article: Mahmud, M. M. C., Keast, R., Mohebbi, M., & Shellie, R. A. (2022). Identifying aroma-active compounds in coffee-flavored dairy beverages. *Journal of Food Science*, *87,* 982–997.
https://doi.org/10.1111/1750-3841.16071