Artigo

DETERMINATION OF CHEMICAL PROFILE OF *Eugenia dysenterica* ICE CREAM USING PS-MS AND HS-SPME/GC-MS

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The incorporation of Cerrado fruits in food products such as ice cream has many advantages because it represents a source of nutrients and bioactive compounds. Given the demand for less laborious methods to analyze food, the paper spray ionization mass spectrometry technique was applied for the first time for a rapid characterization of the chemical components found cagaita ice cream. PS-MS in positive and negative ionization modes were used. The profile of volatile compounds was determined by headspace solid-phase microextraction combined with gas chromatography-mass spectrometry. Fingerprints obtained through PS-MS identified various classes of compounds, such as flavones, anthocyanins, sugars, organic acids, hydroxybenzoic acids, fatty acids, hydroxycinnamic acids, lignin, and phenylpropanoid. The use of both fibers enabled the extraction and identification of 18 volatile compounds in cagaita, and 16 of them were also identified in cagaita ice cream. The most common volatile compound found in both cagaita and ice cream was 3-carene monoterpene. Considering the effect of processing on cagaita constituents, 89% of the volatile compounds remained in the ice cream. Also, 78% of the fruit chemical compounds analyzed by PS-MS were found in the product. Thus, the results indicate that most of the fruit compounds remained in the ice cream after processing.

Keywords**:** cerrado; cagaita; ice cream; paper spray; chemical profile; volatile compounds.

INTRODUCTION

The Cerrado, the richest savanna on earth, encompasses 22% of the Brazilian territory and is home to approximately 11,627 native plant species. Among the edible fruits found in this biome, cagaiteira trees (*Eugenia dysenterica*) produce fruit with low caloric value and high moisture content that are an excellent source of vitamin C containing several phenolic compounds.[1] Cagaitas are consumed fresh or used to make jellies, jams, liqueurs, and juices.[2] However, despite their social importance to inhabitants who obtain income from this natural resource, many species are at risk of extinction due to deforestation caused by the expansion of various agriculture and livestock sectors.[3]

Development of food products is a way to add value to the Cerrado fruits. According to ABIS (Brazilian Association of Industries and the Ice Cream Industry), Brazil is among the ten largest producers of ice cream in the world. In the period from 2003 to 2016, Brazilian production increased from 686 million to 1 billion liters of ice cream.[4] Ice cream is made of milk, sugars, stabilizers, emulsifiers, flavors, among others. These ingredients provide a stable emulsion when this mixture is subjected to agitation, freezing, and incorporation of air.[5-11]

The literature describes many techniques for chemical analysis of ice cream, such as spectrophotometric assay,[8,12] high-performance liquid chromatography (HPLC),[7,13] gas chromatography-mass spectrometry (GC-MS),[14] liquid chromatography coupled to mass spectrometry (LC-MS).[15] However, some of these techniques require longer analysis time with multiple sample preparation steps and generate chemical waste.

Several techniques of ambient ionization mass spectrometry have overcome these disadvantages, allowing fingerprints to be obtained through ultrafast analysis and with minimal sample preparation. Among them, paper spray ionization mass spectrometry (PS-MS) has been employed to analyze various food matrices, such as corni fructus,[16] cagaita,[2] colorings,[17] red wine,[18] olive oils[19] as well as coffee,[20] alcoholic beverages,[21,22] and teas.[23] The PS-MS ionization technique consists of applying a potential difference to a chromatographic paper containing the sample, which allows obtaining spectrum in large mass ranges. For this reason, it is a simple, fast and low-cost technique with high sensitivity, selectivity and minimal requirement for sample preparation.

This work aimed to characterize the chemical constituents of cagaita ice cream through paper spray ionization mass spectrometry and volatile compounds using headspace solid phase microextraction combined with gas chromatography coupled to mass spectrometry.

EXPERIMENTAL

Material

Solid phase microextraction fibers Polyacrylate (PA, 85 μm) and Polydimethylsiloxane/Divinylbenzene (PDMS/DVB, 65 μm) and Folin-Ciocalteu reagent were purchased from Sigma Aldrich (São Paulo, SP, Brazil). Chromatography paper 1 CHR was from Whatman (Little Chalfont, Buckinghamshire, UK) and HPLC grade methanol was supplied by J. T. Baker (Phillipsburg, NJ, USA). The other reagents were analytical grade.

Methods

Sample preparation and ice cream processing

Ripe cagaita fruits were collected in the municipality of Sete Lagoas, MG (Latitude 19° 28' 35.8'' e Longitude 44° 11' 42.4'') in December 2018. The cagaitas were transported to the Chemistry and Analytical Research Laboratory of the Universidade Federal de

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Minas Gerais. The fruits were washed in running water, sanitized for 15 min using sodium hypochlorite (200 mg L^{-1}), rinsed in running water, and stored in a freezer at -20 °C. The pulps were produced from thawed fruit. The peels and seeds were removed, and the pulp homogenized in a mixer.

The production of cagaita ice cream was performed as described by Goff and Hartel[24] with modifications. The formulation consisted of the following ingredients: cagaita pulp (40%), nonfat powdered milk (13.62%), sugar (5%), inulin (4.92%), maltitol (3.59%), sorbitol (3.15%), palm kernel oil (2.36%), glucose (0.61%), and emulsifier (0.4%). All ingredients were weighed and then mixed in a household blender (Fischer, Cook Line Turbo, São Paulo, Brazil). Next, the mix was pasteurized at 70 °C for 30 min and cooled to 4 °C. Subsequently, the mixture was placed in a domestic freezer and kept under constant agitation to incorporate air during freezing. Finally, the ice cream was packed in polypropylene jars and stored in a freezer at -20 °C.

Sample Extraction

Cagaita (n=3) and ice cream (n=3) samples were extracted in triplicate according to the method of Rufino *et al.*[25] In a 2 mL Eppendorf tube, 0.5 g of sample and 1 mL of methanol/water (50:50, v/v) were added. After incubation at room temperature for 1 h, the tubes were centrifuged at 25,406 × g for 15 min and supernatants were collected. Subsequently, 1 mL of acetone/water (70:30, v/v) was added to the tubes and a new incubation and centrifugation step was performed in the same conditions. The two supernatants obtained after the centrifugation steps were placed in a 5 mL volumetric flask and the volume completed with distilled water. The extracts were used to analyze total phenolic compounds and chemical constituents.

Total phenolic compounds

Total phenolic compounds were found using the method proposed by Singleton *et al.*[26] For this, a 150 µL volume of the sample extract, 3,850 mL distilled water and 250 µL Folin-Ciocalteu were mixed in 15.0 mL falcon tube coated with aluminum foil and incubated at room temperature for 8 min. After, 750 µl of 20% sodium carbonate was added. After 2 h incubation, the samples were read at 765 nm (Spectrophotometer Analytik Jena, model Spekol 1300, CA, USA) and the data expressed as mg of gallic acid equivalent (GAE) 100 g^{-1} sample.

Chemical Profile of the Cagaita and Cagaita Ice Cream by paper spray ionization mass spectrometry (PS-MS)

The chemical constituents of the samples were identified as described in Silva *et al.*[2] by using an LCQ Fleet ion trap mass spectrometer (Thermo Scientific, San Jose, CA, USA) with paper spray ionization (Figure 1). For this, the following experimental conditions were employed: mass range: 100 to 1000 *m/z*; PS-MS voltage: + 5.0 kV (positive ionization mode) and -3.0 kV (negative ionization mode); and capillary voltage of 40 V; tube lens voltage: 120 V.

Aliquots with 2 µL of the sample extracts were placed on the tip of a triangular-shaped chromatographic paper (1.5 cm dimensions) positioned 0.5 cm from the mass spectrometer inlet using a clamp attached to an XYZ platform. This clamp was connected to a high voltage source of the spectrometer by a copper wire. Subsequently, 40 µL of HPLC grade methanol was applied to the base of the triangular paper and the voltage source was switched on to obtain the mass spectra.

Extraction and identification of volatile compounds

Headspace solid phase microextraction (HS-SPME) and volatile compound identification were performed as described by Silva *et al.*[27]

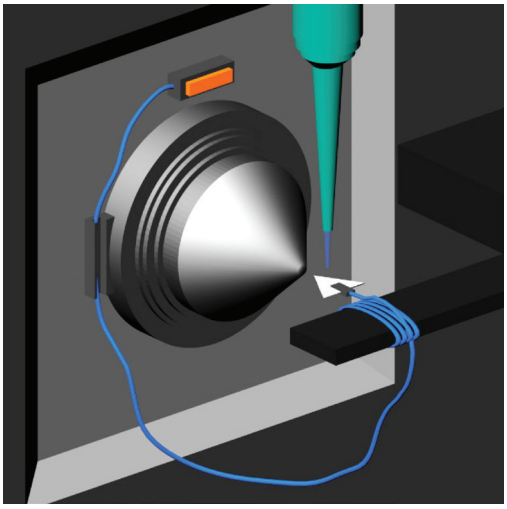

Figure 1. *Illustration of ionization source for paper spray*

For this, 0.5 g of the samples (cagaita and ice cream) were transferred to 20 mL vials, which were closed and placed inside aluminum blocks (8.5 × 10 cm). After a 5 min preheating step, the fibers (Polyacrylate (PA) or Polydimethylsiloxane/Divinybenzene (PDMS/DVB)) were inserted into these vials and kept at 60 °C for 10 min and then taken to the GC-MS injector, remaining in that equipment for 5 min at 200 ºC.

A gas chromatograph (Trace GC Ultra) equipped with a Polaris Q mass spectrometer from Thermo Scientific (San Jose, CA, USA) with an ion-trap analyzer equipped with a split/splitless injector was used in splitless mode. Helium gas (1 mL min^{-1} flow) and an HP-5 MS capillary column; 30 m × 0.25 mm × 0.25 µm (Agilent Techonolgies INC, Munich, Germany) were used. Oven temperatures were: 40 °C (1 min), subsequent heating to 110 °C (10 °C min^{-1}), then to 180 °C (15 °C min^{-1}). The conditions used in the mass spectrometer were: 35 to 300 *m/z* mass range, 70 eV electron ionization mode, 275 °C transfer line temperature, and 200 °C ion source temperature. Compounds were tentatively identified by comparing the data obtained with the mass spectra of the Nist Library (National Institute of Standards and Technology Research Library). The identification was also based in article that determined the volatile compounds of cagaitas.[27]

Statistic

All experiments were performed in triplicate. The results of the total phenolic compounds content were evaluated by one-way ANOVA and Tukey test ($p < 0.05$) used to evaluate the means. Chromatograms containing the volatile compounds were analyzed using the programs Xcalibur version 1.4 (Thermo Scientific, San Jose, CA, USA)[28] and Excel version 2013 (Microsoft, Redmond, WA, USA).[29]

Mass spectra were evaluated using Xcalibur version 2.1 software (Thermo Scientific, San Jose, CA, USA).[30] The Principal Component Analysis (PCA) model was built with data centered mean using MatLab version 7.9.0.529 software (Mathworks, Natick, MA, USA)[31] with the aid of PLS Toolbox version 5.2.2 (Eigenvectors Research, Manson, WA, USA).[32]

RESULTS AND DISCUSSION

Volatile compounds profile

Table 1 shows the volatile compounds identified in samples of cagaita pulp and cagaita ice cream.

Table 1. Relative composition (%) of volatile organic compounds found in cagaita and cagaita ice cream using PDMS/DVB and PA fibers by SPME/GC-MS

Nº	Volatile compounds	PA fiber		PDMS/DVB fiber	
		Cagaita	Cagaita ice cream	Cagaita	Cagaita ice cream
1	Pent-4-en-2-ol	0.92	8.68	0.15	0.57
2	Ethyl butanoate	-	-	0.22	0.60
3	But-2-en-1-ol, 3-methyl-, acetate	-	-	0.69	1.46
4	4-Heptenoic acid, methyl ester	0.30	-	-	-
5	Hexanoic acid ethyl ester	1.74	3.71	3.71	7.77
6	α-Pinene	0.71	-	2.08	1.54
7	1,8 cineol	0.33	-	0.79	0.94
8	3-carene	14.47	9.51	32.74	23.49
9	Ocimene	2.37	1.21	5.24	3.79
10	Linalyl acetate	2.49	3.18	2.48	2.78
11	Linalyl isobutanoate	4.01	-	0.48	-
12	Caryophyllene	4.18	0.24	2.77	-
13	Humulene	2.49	0.89	3.17	0.86
14	Muurolene	5.32	0.81	2.01	0.73
15	Guaiene	6.94	2.97	5.06	0.43
16	Cadinene	3.07	0.31	1.73	1.99
17	Copaene	3.88	0.71	1.70	0.39
18	Decanoic acid	2.08	1.86	2.97	1.94

Eighteen volatile compounds were identified in cagaita, including 16 using PA fibers and 17 using PDMS/DVB fiber. Of these, 16 compounds were also found in cagaita ice cream (PA: n=12; PDMS/DVB: n=15). It's important to note that the abundance is based on the relative response of the MS scanned in the mass range from 35 to 300 and also due the selectivity of each fiber to the disctinct analytes. The 3-carene monoterpene was the most abundant in cagaita (PA = 14.47%, PDMS/DVB=32.74%) and cagaita ice cream (PA = 9.51%, PDMS/DVB = 23.49%). The higher percentage of 3-carene found using the PDMS/DVB is problably due to the semi-polar characteristic of this fiber, which promoted a higher adsorption of this monoterpene in relation to the PA polar fiber. The use of fiber PA promoted an increase of 8.68% in the extraction of the compound Pent-4-en-2-ol in ice cream. This may be relateld to some effect by the ice cream mixture that provided a higher fiber adsorption. This can occur since the extraction of VOCs by HS-SPME is a physical-chemical equilibrium process, which depends, among other factors, on the type of fiber.[2]

Table 1 shows that most of the compounds identified in cagaita were also found in cagaita ice cream, thus the manufacturing process did not cause large losses of these volatile organic compounds in the product. The relative area of volatile compounds in ice cream generally decreased compared to cagaita pulp, which was expected because the manufacturing processing involves several steps such as homogenization of ingredients in a blender, agitation, and freezing. No articles were found in the literature that determined volatile compounds in fruit ice cream or evaluated the effect of processing on these volatile organic compounds.

The relative area of the chemical classes of volatile compounds found in the samples evaluated as a function of the fibers used are in Figure 2.

The cagaita pulp is predominantly composed of terpenes. These results are in agreement with the work done by Silva *et al.*[27] with cagaitas collected in the 2016 harvest in the municipality of Sete Lagoas, MG, which also observed a high proportion of monoterpenes (34.64%). The profile of volatile fruit compounds is known to be related to factors such as degree of ripeness, climate, and pre- and post-harvest handling.[33,34] No studies were found in the literature that evaluate changes in the relative composition of chemical classes of volatile compounds ice cream and other cold deserts.

The average results of the content of total phenolic compounds of cagaita and cagaita ice cream were 241.26 + 4.27 mg GAE 100 g^{-1} and 79.97 + 1.44 mg GAE 100 g^{-1}, respectively. The content of total phenolic compounds found in cagaita in the present study are in agreement with those reported in the literature, which ranged from 171.76 to 367.67 mg 100 g^{-1}.[2,35] The total phenolic content of the produced ice cream is also within the range described in the literature for ice creams made with various types of fruits as reported in the works of Vital et al.[7] (46 to 117 mg GAE 100 g^{-1}), Goraya and Bajwa[36] (81 to 257 mg GAE 100 g^{-1}), and Öztürk et al.[6] (7.5 to 65 mg GAE 100 g^{-1}).

The cagaita ice cream was produced with 40% pulp and the analysis found that this product had 30% of total phenolic compounds in relation to the cagaita pulp; thus, only 10% of these compounds were lost during the process, which was lower than other studies. In previous works, Goraya and Bajwa[36] evaluated the influence of the added alma (Indian gooseberry) pulp on the functional properties of ice cream. With the total phenolic values found in alma pulp (1.48 g 100 g^{-1} GAE) and in ice creams produced with 20% pulp (0.257 g 100 g^{-1} GAE), they observed a reduction of 13.18% in relation to the expected theoretical value (0.296 g 100 g^{-1} GAE). In other study, Vital *et al.*[7] when incorporating grape juice residue (2.5 to 10%) into ice cream, obtained losses of 38.36 to 54.20%.

Paper spray ionization mass spectrometry (PS-MS) fingerprints

Figure 3 shows the mass spectrum (positive and negative ionization modes) of cagaita ice cream as well as the fragmentation spectra of some characteristic ions.

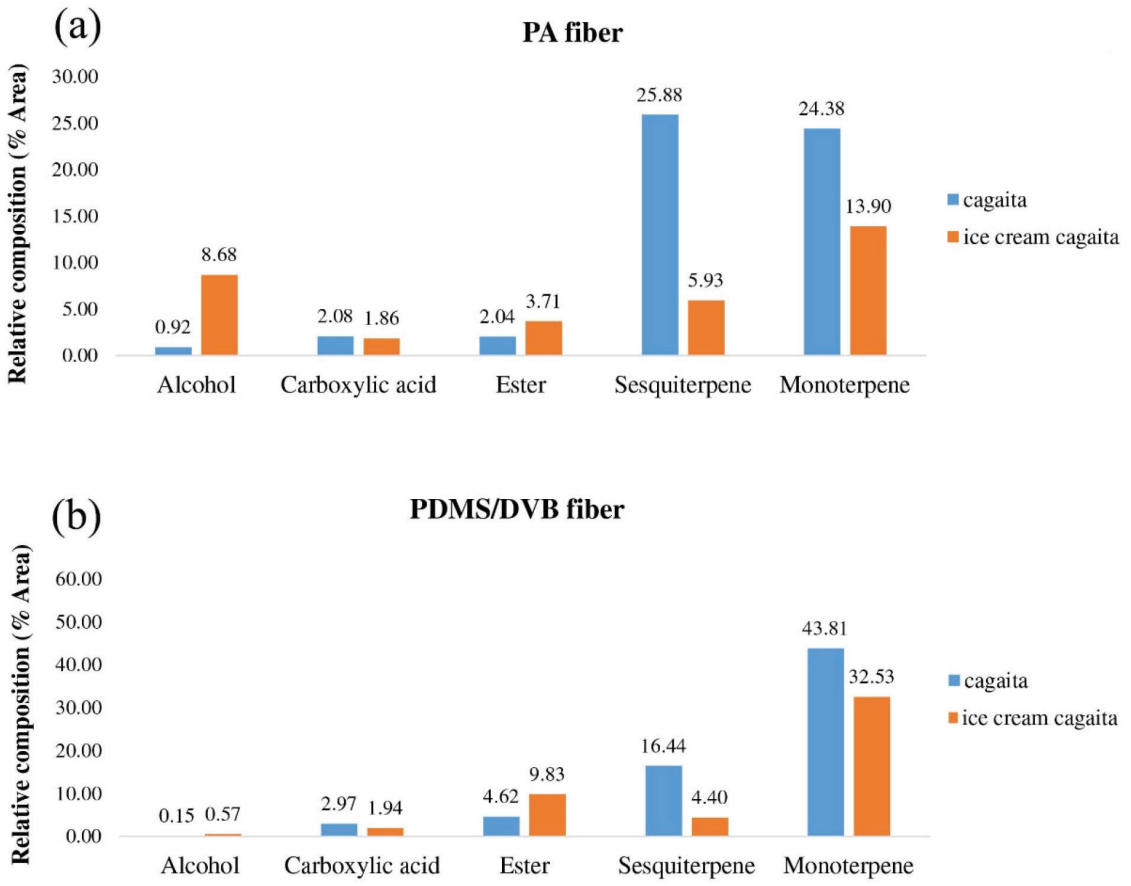

Figure 2. *Comparison of effectiveness of SPME fibers. Relative area (%) of chemical classes of volatile compounds identified in cagaita and cagaita ice cream using (a) PA and (b) PDMS/DVB fibers by SPME/GC-MS*

The PS(+)-MS identified 5 compounds of the flavone, anthocyanins, and sugars classes as in the form of sodium and potassium adducts (Table 2), which were also reported by Silva *et al.*[2] when employing PS-MS in cagaita collected in the city of Sete Lagoas, MG, Brazil.

Chrysoeriol (n = 1; 20% of the compounds) was the only compound found in cagaita that was not detected in the cagaita ice cream. Thus, 80% (n = 3) of the substances identified in the fruit remained in the product after manufacturing.

According to the ions identified using PS(-)-MS technique, a classification has been proposed as described in Table 3. The 31 compounds found included organic acids, hydroxybenzoic acids, sugars, hydroxycinnamic acids, flavone, anthocyanins, and carboxylic acids. Among them, 13 (Compounds 1, 2, 5, 7, 8, 9, 10, 12, 15, 16, 17, 22, and 26) were also described by Silva *et al.*,[2] when evaluating the chemical profile of cagaitas in different microregion using the PCA and PS(-)-MS. The observed differentiation occurred due to 15 compounds.

For the compounds identified in PS(-)-MS, the processing resulted in a 22.60% loss (n = 7; pimelic acid, shikimic acid, galloyl glucose, chlorogenic acid, syringic acid hexoside, delphinidin 3-*O*-arabinoside, and delphinidin 3-*O*-glucoside).

About 23 compounds identified in the cagaita remained in the ice cream, which corresponded to a similarity of 77.8%. This loss of only 22.22% (n = 8) may be related to the steps of homogenizing the cagaita pulp with other ice cream ingredients as well as agitating and freezing in the ice cream maker during manufacturing.

No articles were found that evaluated changes in the profile of chemical constituents (organic acids, phenolic compounds, and other secondary metabolites) of fruits during ice cream manufacturing.

Principal Component Analysis (PCA)

Effect of processing on the chemical profile of samples

The resulting PCA model was able to explain 93.20% [PS(+)-MS] and 93.80% [PS(-)-MS] of total data variability. Figures 4 and 5

Table 2. Proposed assignments for ions detected in cagaita and cagaita ice cream by PS(+)-MS

Nº	Tentative identification	*m/z*	MS/MS	Reference	Class	Cagaita	Cagaita ice cream
1	Chrysoeriol	301	258	Abu-Reidah *et al.*[37]	Flavone	+	nd[a]
2	Sucrose	365	185, 203	Guo *et al.*[16]	Sugar	+	+
3	Sucrose	381	201, 219	Silva *et al.*,[2] Yuan *et al.*,[38] Asakawa and Hiraoka[39]	Sugar	+	+
4	Pelargonidin 3-rutinoside	579	271, 519	Silva *et al.*,[40] Oliveira *et al.*[41]	Anthocyanin	+	+
5	[2 Sucrose + Na]$^+$	707	365	Furlan *et al.*[42]	Sugar	+	+

[a]nd = not detected.

Table 3. Assignments for the cagaita and cagaita ice cream ions detected by PS(-)-MS

Nº	Tentative identification	*m/z*	MS/MS	Reference	Class	Cagaita	Cagaita ice cream
1	Malic acid	115	71	Wang *et al.*,[43] Silva *et al.*[2]	Organic acid	+	+
2	Malic acid	133	89, 115	Silva *et al.*[2]	Organic acid	+	+
3	Pimelic acid	159	97, 115, 141	Wang *et al.*[43]	Organic acid	+	nd[a]
4	Shikimic acid	173	73, 111, 155	Wang *et al.*[43]	Hydroxybenzoic acids	+	nd[a]
5	[Hexose + Cl]$^-$	179	71, 89	Wang *et al.*,[43] Silva *et al.*[2]	Sugar	+	+
6	[Hexose + Cl]$^-$	181	-	-	Sugar	+	+
7	Citric acid	191	85, 111	Wang *et al.*,[43] Silva *et al.*[2]	Organic acid	+	+
8	Hexose	215	71, 89, 179	Guo *et al.*,[16] Wang *et al.*,[43] Silva *et al.*[2]	Sugar	+	+
9	Palmitic acid	255	237	Wang *et al.*[43]	Fatty acid	+	+
10	Caftaric acid	311	133	Abu-Reidah *et al.*,[37] Silva *et al.*[2]	Hydroxycinnamic acids	+	+
11	*p*-Coumaric acid hexoside	325	119, 145	Aaby *et al.*,[44] Kajdžanoska *et al.*,[45] Silva *et al.*[2]	Hydroxycinnamic acids	+	+
12	Galloyl glucose	331	169	Ramirez *et al.*[46]	Hydroxybenzoic acids	+	nd[a]
13	Conidendrin	355	337	Sanz *et al.*[47]	Lignin	+	+
14	Caffeoyl-*D*-glucose	339	159	Silva *et al.*[2]	Hydroxycinnamic acids	+	+
15	Caffeoyl-glucose	341	179	Ramirez *et al.*[46]	Hydroxycinnamic acids	+	+
16	Chlorogenic acid	353	173, 179, 191	Koolen *et al.*,[48] Wang et *al.*[43]	Hydroxycinnamic acids	+	nd[a]
17	Syringic acid hexoside	359	153, 197	Abu-Reidah *et al.*,[37] Silva *et al.*[2]	Hydroxybenzoic acids	+	nd[a]
18	Hexose or sucrose	377	215, 341	Chen *et al.*,[49] Silva *et al.*[2]	Sugar	+	+
19	Vitexin	431	341	Wang *et al.*,[43] Silva *et al.*[2]	Flavones	+	+
20	Delphinidin 3-O-arabinoside	435	303	Junqueira-Gonçalves *et al.*[50]	Anthocyanin	+	nd[a]
21	Icariside D1	439	403, 421	Jiao *et al.*[51]	Phenylpropanoid	+	+
22	Delphinidin 3-*O*-glucoside	465	303	Junqueira-Gonçalves *et al.*[50]	Anthocyanidin	+	nd[a]
23	5-pyranopelargonidin-3-glucoside	501	339	Aaby *et al.*[44]	Anthocyanidin	+	+
24	Dicaffeoylquinic acid	515	173	Catarino *et al.*[52]	Hydroxycinnamic acids	+	+
25	Hexose	521	341	Silva *et al.*[2]	Sugar	+	+
26	5′-Methoxy-demethylpiperitol-4-*O*-glucoside	533	371	Simirgiotis *et al.*[53]	Other Phenolic Compounds	+	+
27	Coumaroyl iridoid isomer 1	535	311, 491	Mikulic-Petkovsek *et al.*[54]	Hydroxycinnamic acid	+	+
28	Lithospermic acid	537	493	Wang *et al.*[55]	Carboxylic acid	+	+
29	Caffeic acid hexoside dimer	683	341	Spínola *et al.*,[56] Silva *et al.*[2]	Hydroxycinnamic acids	+	+
30	Synapic acid dihexoside hydroxy benzoyl	685	667	Silva *et al.*[40]	Phenylpropanoid	+	+
31	[Tetraose + Cl]$^-$	719	-	-	Sugar	+	+

[a]nd = not detected.

exhibit the PCA that demonstrate the effect of ice cream processing on the chemical profile of the cagaita pulp used. Using the mass spectra obtained from the sample analyzed by the positive and negative ionization modes, the PCA was built with the data mean centered with two main components.

PC 1 in the positive ionization mode (Figure 4a) recognized differences between the fruit (positive scores) and the cagaita ice cream (negative scores). Analysis of the weights of this component (Figure 4b) found that this differentiation of ice cream occurred due to the signals with *m/z* 365 and 707 related to sugars, while the cagaita differed as a function of the signals with *m/z* 206, 412, 523, and 551.

In the PCA, generated from the spectra obtained by PS(-)-MS presented in Figure 5, the composition of the cagaita ice cream (positive scores) differed from the cagaita pulp due to the ions with *m/z* 377 (sugar), 439 (icariside D1), and 683 (caffeic acid hexoside dimer), while the pulp showed more intense signs with *m/z* 115 (malic acid), 179 ([Hexose + Cl]$^-$), 191 (citric acid), and 215 (hexose).

No other articles were found that evaluated changes in the profile of compounds (organic acids, phenolic compounds, and other secondary metabolites) of fruits during ice cream manufacturing.

CONCLUSIONS

The SPME PA and PDMS/DVB fibers efficiently revealed the volatile compounds present in cagaita and cagaita ice cream. Most of the volatile compounds (89%) present in cagaita pulp were also found

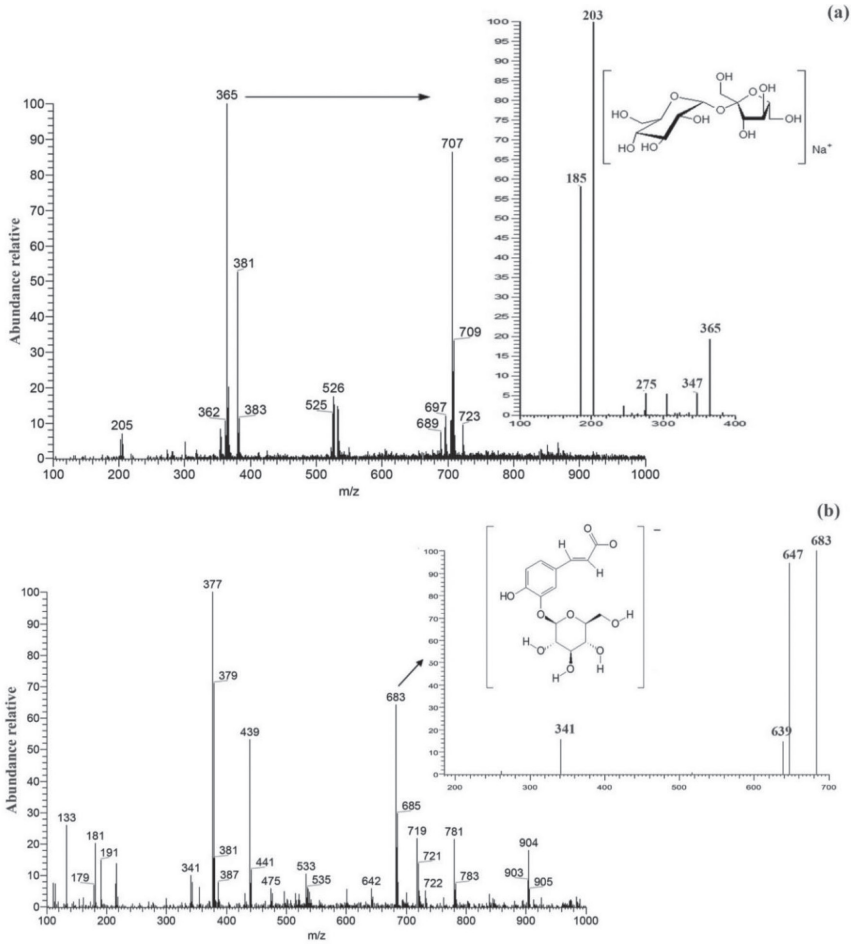

Figure 3. *Representation of (a) sucrose (m/z 365) in PS(+)-MS and (b) caffeic acid hexoside dimer (m/z 683) in PS(-)-MS of cagaita ice cream sample*

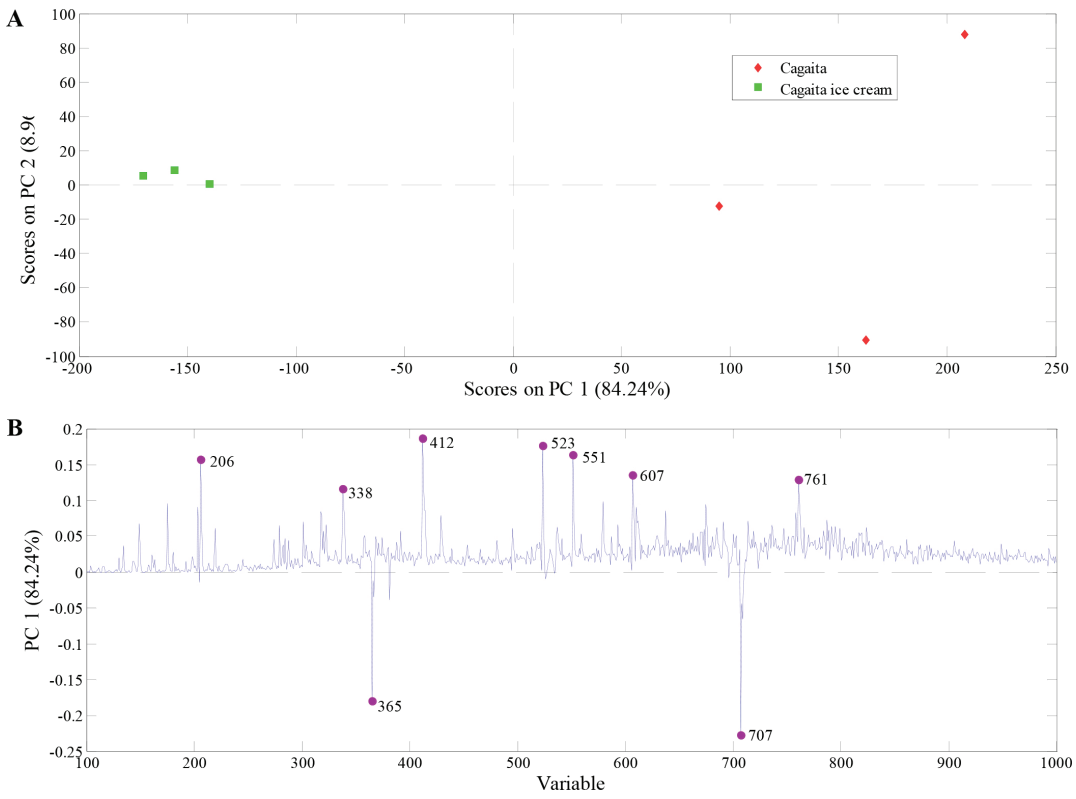

Figure 4. *PCA model built with PS(+)-MS data from cagaita pulp and cagaita ice cream samples. The upper plot (scores) split the two sets of samples into well-distinguished groups. The bottom plot (loadings) shows the main ions that account for this separation*

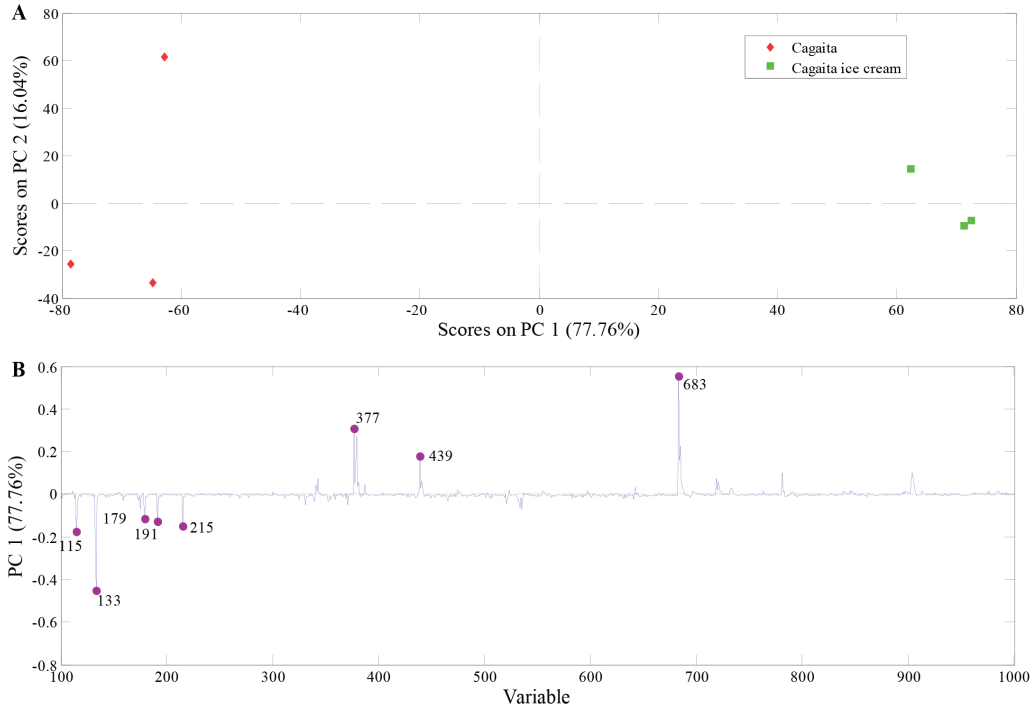

Figure 5. *PCA model built with PS(-)-MS data from cagaita pulp and cagaita ice cream samples. The upper plot (scores) split the two sets of samples into well-distinguished groups. The bottom plot (loadings) shows the main ions that account for this separation*

in ice cream. After processing the ice cream, a reduction of 10% in the content of total phenolic compounds was observed concerning cagaita pulp. Fingerprints obtained from the evaluated samples found 36 compounds, 28 of which were also present in the ice cream produced. Thus, PS-MS proved to be a simple and fast technique to determine the chemical profile of these food matrices by identifying the bioactive compounds of different chemical classes.

SUPPLEMENTARY MATERIAL

The figures contain the mass spectra of compounds identified in the cagaita ice cream by PS-MS, which are freely accessible at http://quimicanova.sbq.org.br.

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