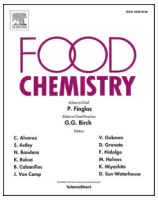
Food Chemistry 388 (2022) 132902

Contents lists available at ScienceDirect

Food Chemistry

journal homepage: www.elsevier.com/locate/foodchem



Fruit quality parameters and volatile compounds from 'Palmer' mangoes with internal breakdown

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ARTICLE INFO

Keywords:
Mango physiological disorder
Volatiles
Postharvest quality
Chemometrics

ABSTRACT

The internal breakdown (IB) is a premature and uneven mango pulp ripening physiological disorder that is noticed only when the fruit is sliced for consumption. Thus, there is a demand for analytical methods to detect IB in mangoes to avoid consumer dissatisfaction and reduce postharvest waste. In this work, physicochemical and volatile compounds were determined to evaluate the ability to predict pulp IB. Principal components analysis (PCA) and partial least squares discriminant analysis (PLS-DA) of the data show that color, firmness, and volatiles compounds are important to give some information about the physiological changes caused by IB. The volatile compounds methacrylic acid, ethyl ester, isopentyl ethanoate, limonene oxide, (E)-2-pentenal, tetradecane, and γ-elemene were identified as chemical markers of IB. Therefore, mango physical and chemical characteristics combined with PCA and PLS-DA were successfully employed for the identification of IB in mangoes, showing significant differences between healthy and IB fruits.

1. Introduction

Mango is a stone fruit from the *Mangifera* genus of Anacardiaceae family. Mango fruits vary in size, shape, peel color, flesh color, taste and aroma, depending on the cultivar (Dar et al., 2016). Mango is an increasingly important fruit in the global market (Mwaurah et al., 2020) with a production around 55.9 million of tones in 2019 (FAO, 2019). The largest producers, in decreasing order are: India, Indonesia, China, Mexico, Pakistan and Brazil (FAO, 2019).

Mangoes can be consumed as fresh fruit or used to make juices, smoothies, ice cream, fruit bars, pies, sweet chili sauce (Fasoli & Righetti, 2013) and widely used in Asian cuisine (Righetti, Esteve, D' Amato, Fasoli, Marina, & García, 2015). In Central America, mango is either eaten as ripe or as immature fruits, mixed with salt, vinegar, black pepper, and hot sauce (Righetti et al., 2015).

From a nutritional point of view, a portion of 100 g of fresh mango (cv. Palmer) gives: 72 kcal; 0.4 g of proteins; 0.2 g of lipids; 19.4 g of carbohydrates; 1.6 g of fibers; 783 ug of retinol equivalents and 65.5 mg of vitamin C (TACO, 2011). Like other fruits, its quality can be affected by biotic or abiotic factors. Among them, all physical and chemical agents stand out, such as: solar radiation, temperature, rainfall, water available, winds, soil (abiotic factors); as well as living organisms, such as pests and diseases present at a given location and which can have an effect on the quality of mangoes (Fraire-Velázquez & Balderas-Hernández, (2013); Harborne, (1999); Pavarini, Pavarini, Niehues, & Lopes, (2012). The fruit quality such as appearance, texture and flavor are important factors for consumer choice. In this respect, the quality and acceptance of mango fruits can be affected by a physiological disorder known as internal breakdown (Oldoni, Bernardo, Oliveira Filho, De Aguiar et al., 2021). This disorder is characterized by a premature and uneven pulp ripening (Raymond, Schaffer, Brecht, & Crane,1998; Gapper, Mcquinn, & Giovannoni, 2013). There is no agreement about the origin of the internal breakdown (IB), although this disorder has been associated with nutritional problems of the plant due to the

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https://doi.org/10.1016/j.foodchem.2022.132902
Received 24 October 2021; Received in revised form 11 March 2022; Accepted 3 April 2022
Available online 6 April 2022

management, especially with regard high in nitrogen and low in calcium (Wainwright & Burbage, 1989) and correction of the soil (Schaffer & Andersen, 1997; Vasanthaiah et al., 2006). Collapsed mangoes are often discarded as the disorder still remains unknown to most consumers. The disposal of fruits represents a waste of fruits that still have high nutritional value, and can be destined for other purposes, thus reducing food waste (Okawa, 2015; Parfitt, Barthel, & Macnaughton, 2010). As an alternative, broken mangoes could serve as raw material for the production of edible films (Oldoni, Bernardo, Oliveira Filho, De Aguiar, Moreira, Mattoso et al., 2021).

Mango pulp IB is difficult to detect externally and is often observed only by the final consumer when the fruit is sliced for consumption. It is possible that some pre- or post-harvest procedures can contribute to cellular collapse of the fruit, causing dark and watery areas on the pulp (Wainwright & Burbage, 1989). Although the causes of IB are still unknown there are several losses related to this disorder in all mango production areas (Krishna, Sharma, & Srivastav, 2020). The presence of IB in mangoes contributes to the problem of food waste since the affected fruits are usually discarded.

Our hypothesis for this research is that mangoes with internal breakdown (IB) and without IB (WIB) may have different physical characteristics and chemical composition. Physical analysis of mango mass, longitudinal and transverse diameters, apparent density, peel color attributes were evaluated by univariate and multivariate methods to detect the problem in intact mangoes. Mangoes firmness and pulp pH, titratable acidity, soluble solids content, and especially volatile organic compounds were determined in IB and WIB mangoes and analyzed using chemometric methods. The results show statistically significant differences between IB and WIB mangoes.

2. Materials and methods

2.1. Samples

Mango fruits (cv. Palmer) were obtained at Companhia de Entrepostos e Armazéns Gerais de Sao Paulo (CEAGESP) from a commercial orchard located in the Sao Francisco River Valley. The fruits were washed, sanitized, dried in the air, and then stored in a cold chamber at 15 °C and 85% of relative humidity (RH) until they reached maturity for fresh consumption according to the aspects of skin color, softening, and aroma (Tharanathan, Yashoda, & Prabha, 2006). Sliced fruits were used to visually determined the presence or absence of pulp IB (Brecht, 2019). Triplicate analysis of 5 fruits with internal breakdown (IB) (Fig. 1A) and 5 fruits without internal breakdown (WIB) (Fig. 1B) where used in the measurements. It is important to say that symptomatic fruits showed collapse at their most advanced level.

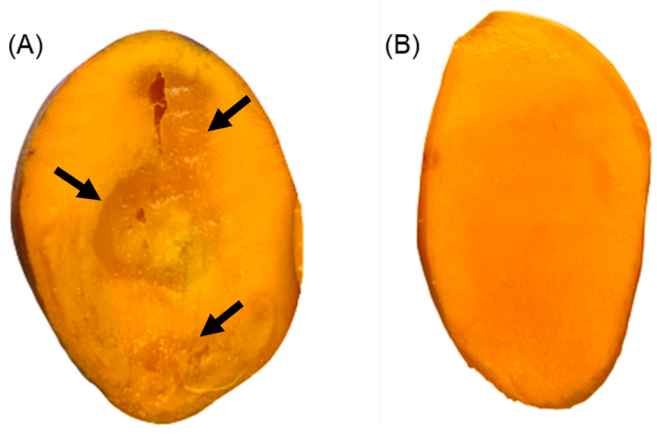

Fig. 1. Pictures of 'Palmer' mangoes pulps with IB (A) and without IB (B). Black arrows indicate the location of the internal breakdown. Photo: Fernanda, C. A. Oldoni (2019).

2.2. Physical-chemical analysis

Mass (g) of fruits was determined by a Bel S2202H semi-analytical balance (7Lab, Rio de Janeiro, Brazil). The longitudinal and transverse diameters (mm), were determined by a digital caliper (Mitutoyo Sul Americana Ltda., Suzano, Brazil). The apparent density (g cm^{-3}) was obtained by immersing the fruit in a beaker with a known volume of distilled water, at a constant temperature of 25 °C, measuring the height of the displaced water column with the aid of a digital caliper (Mitutoyo Sul Americana Ltda.) and calculating the ratio between the mass and the volume of water displaced by the fruit. The fruit firmness (F, in N) was determined with a TA.XT plus Texture Analyzer (Stable Micro Systems Ltd., England, United Kingdom), equipped with a 4 mm diameter stainless steel probe. For the analysis of dry matter (%) approximately 5.0 g of each sample was placed in Petri dishes and kept in an oven at 65 °C for 24 h. The procedure was repeated until reaching constant mass. All these physical analyses were performed in triplicate.

The color of the skin and pulp were determined using the CR 400 colorimeter (Konica Minolta, Osaka, Japan) using the CIELab system (L* - brightness, a* - red-green, and b* - yellow-blue) (Abbott, 1999; Pathare, Opara, & Al-Said, 2013). The calculation of the hue angle (h°) considered the qualitative color attribute was performed using Equation (1) (Shewfelt, Thai, & Davis, 1988; Mc Guire, 1992). The calculation of the chroma index (C*) (Pathare et al., 2013; Shewfelt et al., 1988) considered the quantitative attribute of color (Pathare et al., 2013) and was performed using Equation (2).

$$h^{\circ} = \tan - 1(b^*/a^*) \quad (1)$$

$$C^* = \left(a^{*2} + b^{*2}\right)1/2 \quad (2)$$

The hydrogen potential (pH) was determined by immersing the electrode of the QX 1500 QUALSTRON equipment (Hexis Científica, Jundiaí, Brazil) in the mango pulp. The titratable acidity (AT, in %) was determined by titration of 10 g of the homogenized pulp extract in 50 mL of distilled water, with 0.1 M NaOH solution. The total soluble solids content (SS) were quantified in an Atago RX-5000cx bench refractometer (Honcho, Itabashi-ku, Japan) by inserting a 2–3 mL aliquot of the mango pulp into the equipment. The SS/AT or ratio was obtained by the relationship between SS and AT. The physical–chemical parameters were determined in triplicate for each sample and the average data presented with standard deviations.

2.3. Organic volatile compounds by Solid-Phase microextraction (SPME) and gas chromatography and mass spectrometry (GC–MS)

Flesh of 10 mango samples (five IB and five WIB) were used for volatile analysis. The mango pulp samples (50 g) were stored in polyethylene bottles with screw caps and frozen (-20 °C) until the analysis. The mango fruit volatiles were extracted by headspace solid phase micro-extraction (HS-SPME) according to Bogusz, Tavares, Teixeira Filho, Zini, & Godoy, 2012, with minor modifications. Aliquots of the frozen pulp were grounded in a domestic blender and 1 g of the ground material was weighed into 60 mL SPME glass vial with screw cap and PTFE/silicone septa (Supelco - Bellefonte, PA, USA). After weighing the samples, 2 mL of saturated sodium chloride solution were added to the vials. The volatiles were extracted under the following optimized conditions: equilibration for 15 min, magnetic stirrer at 500 rpm, extraction time for 30 min, and temperature of extraction at 40 °C. The analyses were performed in triplicate.

The GC–MS analyses were performed on a Shimadzu GC–MS 2010 plus (Shimadzu, Kyoto, Japan), using a J & W Scientific (Agilent Technologies, USA) fused silica HP-5MS capillary column (30 m × 0.25 mm i. d. × 0.25 μm). The instrumental parameters used were as follows:

injector in splitless mode for 1.0 min at 220 °C; helium at 1.0 mL min $^{-1}$; oven, 40 °C to 250 °C at 3 °C min $^{-1}$; interface temperature, 250 °C; electron ionization at 70 eV; quadrupole mass analyzer; and mass range 35–350 *m/z*.

The Van Den Dool and Kratz linear temperature programmed retention indexes (LTPRI) of the volatile compounds were calculated using a mixture of aliphatic hydrocarbons (C_8–C_{24}) (Supelco, PA, USA) injected under the same conditions as the mango samples (Van Den Dool & Kratz, 1963). The organic volatile compounds were identified by comparing the LTPRI and the mass spectra obtained from the samples with the LTPRI and mass spectra obtained from the literature (NIST 2011), using criteria of at least 85% similarity for the mass spectra and maximum variation of the retention indices of ± 10.

2.4. Statistical analysis

Partial least squares, discriminant analysis (PLS-DA) was used to find volatile compounds whose variability was related to the fruit internal breakdown. The data set was auto scaled to minimize the influence of compounds in high concentrations on the total variance of the data. Through the analysis of the PLS-DA result, those that presented loadings below −0.15 and above + 0.15, in the first latent variable, were selected as the most important volatile compounds in the identification of the collapse, since it was responsible for the separation between the groups with the collapse of those without collapse.

After that, a principal component analysis (PCA) was carried out, also with staggering data, with the most important variables selected by the PLS-DA, to verify if these variables could be used as a fingerprint indicative of the collapse.

For the physical–chemical parameters, a PCA was initially performed with all 30 parameters. Observing the separation, the main variables were identified and a new PCA was performed with the selected variables, always using autoscaling. Both PCA and PLS-DA analysis were performed using Matlab 2011A software, using PLS_Toolbox 6.2.

Before the one-way analysis of variance (ANOVA), the equivalence of variances was tested using the Levene test. Welch-ANOVA was applied when the data were not homoscedastic. Pearson's correlation coefficient (r) was used when data were normally distributed (Shapiro-Wilk test). Statistical analyzes of the data were performed using R 3.5.2 (R CORE TEAM, 2018).

3. Results and discussion

3.1. Physical-chemical analysis of 'palmer' mango

Tables 1, 2 and 3 shows the means, standard deviations and ANOVA p values for the physical–chemical analysis of 'Palmer' mango fruits, with (IB) and without internal breakdown (WB). Table 1 shows the data for mass (M); longitudinal (LD) and transverse (TD) diameters, firmness (F), apparent density (AD) and dry matter (DM) for IB and WB mangoes. Firmness was the only parameter analyzed (Table 1) that shows significant difference $p \leq 0.05$ between the means of IB and WIB mangoes.

Mangoes firmness is an important postharvest commercial characteristic and is associated with fruit softness. During the ripening process, the occurrence of structural changes in the cell wall is widely recognized, such as the increase of softness in the fruits due to the enzymatic action (Huber, 1983). Cell walls are composed of cellulose microfibrils embedded in a hydrated matrix of non-cellulosic polysaccharides and proteins. The three main components of plant cell primary walls are cellulose, hemicellulose, and lignin, which give a high resistance to the plant structure (Cosgrove, (2005); Höfte, Peaucelle & Braybrook, (2012). In addition to these components, the cells walls have pectins (homogalacturonans, ramnogalacturonans I, and II), glycoproteins, among other differentiated components (Johnson, Gidley, Bacic, & Doblin, 2018). When the fruit reaches physiological maturity, the softening process begins, and this is due to the solubilization of pectins with the highest enzyme activity (Batisse, Fils-Lycaon, & Buret, (1994); Fischer & Bennett, (1991).

Therefore, the low firmness mean value in IB fruits (Table 1) can be related to premature or uneven ripening of the pulp by the fruit endogen enzymes. The reduction of cell wall stiffness and the rupture of hydrogen bonds between cellulose, cellulose microfibrils, and xyloglucans may be due to the action of expansive, a group of extracellular proteins with the characteristic property of cell wall loosening that regulate the extension of the cell wall during plant cell growth, disrupting the hydrogen bonds between cellulose microfibrils and xyloglucans (Cosgrove, Li, Cho, Hoffmann-Benning, Moore, & Blecker, 2002; Li, Jones, & McQueen-Mason, (2003); Rose, Catala, Gonzalez-Carranza, & Roberts, (2003). They are shown to play an important role along with other cell wall degrading enzymes (Rose and Bennet, 1999), in the fruit softening phenomenon (Rose et al., 2003). Removal of the xyloglucan causes the cellulose microfibrils to collapse, causing them to lose spacing and orientation (Hayashi 1989). Pectin-modifying enzymes also play an important role in controlling cell wall plasticity. These include polygalacturonase, pectin methylesterase, pectate lyase (Ruiz-May & Rose, 2013; Marowa, Ding, & Kong, 2016; Yashoda, Prabha, & Tharanathan, 2007; Goulao, Santos, Souza, & Oliveira, 2007). The more pronounced softening in the tissues of IB fruits indicates that the condition of the more advanced fruit maturation stage influences the expression of the

Table 1
Means, standard deviations and ANOVA p values of the data of mass (M), longitudinal (LD) and transverse (TD) diameters, firmness (F), apparent density (AD) and dry matter (DM) for IB and WIB of 'Palmer' mangoes.

Mangoes	M (g)	LD (mm)	TD (mm)	F (N)	AD (g cm^{-3})	DM (%)
IB	503.7 ± 8.9	137.17 ± 4.0	88.3 ± 3.6	2.9 ± 1.6	0.9 ± 0.1	17.0 ± 1.9
WIB	508.2 ± 61.4	138.5 ± 7.2	87.1 ± 4.1	5.4 ± 3.0	0.9 ± 0.1	17.4 ± 1.9
p-value	0.876	0.724	0.651	<0.001*	0.601	0.753

*significant difference ($p \leq 0.05$) by ANOVA and F test.

Table 2
Means, standard deviations and Welch ANOVA p values of color parameters L*, a*, b*, chroma (C*) e angle hue (°h) of peel and pulp of IB and WIB mangoes.

Mangoes	L*	a*	b*	C*	°h
			Peel		
IB	39.9 ± 3.8	25.7 ± 3.5	25.3 ± 4.9	38.0 ± 3.1	41.8 ± 6.9
WB	41.0 ± 5.9	14.9 ± 9.3	24.5 ± 10.1	30.8 ± 11.1	56.1 ± 15.0
p-value	0.724	0.040*	0.875	0.222	0.088
			Pulp		
IB	63.4 ± 2.3	15.9 ± 1.1	68.3 ± 2.5	70.2 ± 2.4	76.8 ± 0.9
WB	68.5 ± 1.9	12.4 ± 2.5	73.0 ± 3.0	74.1 ± 2.9	80.3 ± 2.1
p-value	<0.01*	0.029*	0.028*	0.049*	<0.01*

*significant difference ($p \leq 0.05$) by ANOVA and F test.

Table 3
Means, standard deviations and Welch ANOVA p values of soluble solids content (SS), hydrogen potential (pH), titratable acidity (TA) and SS/TA ratio of pulps of IB and WIB mangoes.

Mangoes	SS (°Brix)	pH	TA (%)	SS/TA
IB	16.4 ± 1.4	5.54 ± 0.3	0.11 ± 0.02	153.4 ± 16.0
WB	17.5 ± 2.1	4.82 ± 0.3	0.17 ± 0.04	100.8 ± 28.1
p-value	0.11	<0.001*	<0.05*	<0.001*

*significant difference ($p \leq 0.05$) by ANOVA and F test.

enzyme activity and, consequently, the pectin degradation.

Table 2 shows the means, standard deviations and ANOVA p values of color parameters L*, a*, b*, chroma (C*) e angle hue (°h) for the peels and pulps of IB and WB mangoes. The means of a* was the only peels parameter (Table 2) that shows significant difference $p \leq 0.05$ between IB and WIB mangoes. This result indicates that the fruits with collapse showed an increase in the red hue in the peel. The peel color is one of the main indicators of fruit quality, as well as consumer acceptance (Saranwong, Sornsrivichai, & Kawano, 2004; Vásquez-Caicedo, Sruamsiri, Carle, & Neidhart, 2005). In mango, the color of the peel, in addition to providing important elements for the recognition of the point of harvest, changes in color at the beginning of maturation. During fruit development, the color of the peel has an olive green tone, the predominant color in most varieties, later, with maturation, the green is replaced by a lighter tone, predominating a more yellowish color (Jha, Kingsly & Chopra, 2006). The change in the pigmentation of the peel is due to the chlorophyll degradation and the pigments appearance, such as carotenoids and flavonoids (Ntsoane, Luca, Zude-Sasse, Sivakumar, & Mahajan, 2019). Regarding the colorimetric parameters of the peel, there was a significant difference ($p \leq 0.05$) for the attribute a*, setting a higher value (25.7) in fruits that contained the physiological disorder (Table 2). For the other color coordinates of the peel, there was no significant difference.

The mean values of all pulp color parameters showed a significant difference ($p \leq 0.05$) between IB and WIB fruits (Table 2). The mean of L* values IB pulps was smaller (63.4) than the values of WIB pulp fruits (68.5) with $p \leq 0.05$. This reduction in L* may be associated with an increase in carotenoids content (Ornelas-Paz, Yahia, & Gardea, 2008). The L* decrease was also observed in mangoes cv. Keitt at different stages of maturation (Ibarra-Garza, Ramos-Parra, Hernández-Brenes, & Jacobo-Velázquez, 2015).

The means of a* coordinate parameter for the pulps of IB fruits showed a higher value (15.9) when compared to WIB fruits (12.4), with $p \leq 0.05$. The higher a* value related to more intense red color shows a possible increase in the metabolism of the fruits and, consequently, an increase in their ripening, since it suggests the degradation of chlorophylls and synthesis of carotenoids and flavonoids (Ntsoane et al., 2019).

The means values of b*, C* B pulps were significantly different ($p \leq 0.05$). The pulps of WIB fruits showed higher b* and C* values than in IB fruits, indicating higher intensity of the yellow color, showing a greater color saturation when perceptible to the human eye (Pathare et al., 2013; Shewfelt et al., 1988). The lower means of °h (76.8) value for the pulp of IB than WIB (80.3) fruits pulp color changes from green to yellow during ripening, indicating again this characteristic resulting from the degradation of chlorophyll, associated with the synthesis of yellow and red pigments in the flesh (Nordey, Joas, Davrieux, Génard, & Léchaudel, 2014). Red, yellow and orange carotenoids pigments are synthesized and accumulated during fruit development and have a significant increase in the final stages of maturation (Zerbini et al., 2015; Ma, Zheng, Ma, Xu, Wu, & Wang, 2018) once more indicating more advance ripening process in IB mangoes.

Table 3 shows the means, standard deviations and Welch ANOVA p values of soluble solids content (SS), hydrogen potential (pH), titratable acidity (TA) and SS/TA ratio of pulps of IB and WIB mangoes. The means of the IB and WIB solid soluble content (SS) values were the only parameter without statistical significance. The pulps of IB mangoes show higher pH and lower TA values than WIB mangoes ($p \leq 0.05$) indicating a higher consumption of organic acids in IB mangoes. The organic acids can be converted in CO_2 and H_2O in the respiratory process during the ripening, as well as conversion into sugars by gluconeogenesis (Eskin, Hoehn, & Shahidi, 2013). They are also involved in the biosynthesis of aromatic amino acids and volatiles, which further influences to fruit taste (Chen et al., 2012), which were also observed by Oliveira et al. (2017) in passion fruit at different stages of ripeness. Organic acids are considered one of the most important indices to determine the taste and quality of fruits (Cohen et al., 2014).

The means SS/TA ratio were higher in IB than WIB pulps ($p \leq 0.05$) indicating that the IB mangoes have a more advanced maturation stage. The SS/TA ratio is an important parameter of fruit quality and is commonly used to determine the palatability and ripeness of the fruits (Oldoni, Lima, Cavalcante, De Sousa, Carneiro, & De Carvalho, 2018). Although there was no statistical difference for soluble solids in mangoes without and with internal breakdown, a statistical difference was observed between the SS/TA ratio ($p \leq 0.05$). This parameter can be used as a reference for the maturity index indicating that the collapsed mangoes present a more advanced stage of maturation.

3.2. Mango volatiles compounds analysis

The GC–MS analyzes of volatile compounds (Table 4) of IB and WIB mangoes cv Palmer identified 108 volatile compounds distributed in different chemical classes: alkanes (2), halides (1), alcohols (7), aldehydes (14), ketones (3), esters (9), monoterpenes (29), sesquiterpenes (16), and unidentified compounds (27). Some of these compounds, like 3-carene, limonene; terpinolene; α-fellandrene, β-myrcene; 2-hexenal (E) and 3-hexen-1-ol (Z) have already been reported by other studies as predominant volatiles in different mango varieties (Pino, Mesa, Munoz, Marti, & Marbot, 2005; Lebrun, Plotto, Goodner, Ducamp, & Baldwin, 2008; Thiruchelvam, Landahl, & Terry, 2020).

An important result is that nine volatile compounds were found only in the group of mangos with IB, which are (E)-2-nonenal; ethyl butanoate; ethyl crotonate; butanoic acid-2-butyl ester; methyl caprylate; γ-elemene; and three unidentified compounds (41-55-69-81-109-137 and 77-79-91-107-135-150). The (E)-2-nonenal (aldehyde) was the most abundant volatile compound present only in IB mangoes. One study carried out the volatiles characterization of five mango cultivars originating in China and identified the compound (E)-2-nonenal in only one of the cultivars (Liu et al., 2020). Another study carried out on fresh and processed fruits identified the presence of the volatile compound (E)-2-nonenal at higher levels in fresh fruits than in dry fruits (Bonneau et al., 2018).

Another volatile compound identified in the present work is the ester compound ethyl butanoate which is considered responsible for the mango flavor (Lopes, Fraga, & Rezende, 1999). Some volatiles were found only in the group of WIB mangoes, which were tetradecane; (E)-2-pentenal; 4-methyl-2-heptanone; geranyl butanoate and γ-gurjunene compounds.

It is important to highlight that the ester methyl methacrylate, and the methacrylic acid, ethyl ester, and isopentyl ethanoate were found with more intense chromatogram peak areas just in the IB fruits (significant difference $p \leq 0.05$).

Three alcoholic compounds were found with areas of intense peaks in the chromatogram, with emphasis on the compound 1-butanol, 2-methyl, which was present in higher concentration in the IB fruits ($p \leq 0.05$). On the other hand, 1-pentanol and (Z)-2-penten-1-ol were found with intense chromatogram peak area in WIB fruits, statistically differing ($p \leq 0.05$) from those fruits with IB. During the ripening process, fruit metabolism converts some fatty acids into esters, ketones and alcohols (Defilippi, Manríquez, Luengwilai, & González-Agüero, 2009).

In the IB mangoes aldehyde volatile compounds like isopentanal, butanal, 2-methyl-, hexadecanal and specially (E)-2-hexenal were found with intense chromatogram peak areas. According to the literature, the presence of aldehydes occurs in significant amounts in the mango seed (Oliver-Simancas, Muñoz, Díaz-Maroto, Pérez-Coello, & Alañón, 2020). In addition, some research attributed a tendency in the increase of aldehydes in ripe fruits, (Beaulieu & Lea, 2003; Bartley & Schwede, 1987).

The presence of the volatile compound butanal, 2-methyl-, formed by branched-chain amino acids and known to have a pungent fruit aroma, increased with maturation (Narain, Galvão & Madruga, 2007) in symptomatic fruits. Regarding the biochemical formation of (E)-2-hexenal, Liu et al, (2020) report the pathway via auto-oxidation of

Table 4
Volatile compounds identified by GC–MS analyzes of mangoes cv Palmer with (IB) and without internal breakdown (WIB).

Compounds	IB	WIB	Sig
Alkanes			
tetradecane	ND	0.01 ± 0.00	
heptadecane	0.16 ± 0.24	0.06 ± 0.03	ns
Halides			
Pentane, 1-chloro-	1.06 ± 1.85	0.78 ± 0.40	ns
Alcohols			
1-penten-3-ol	2.67 ± 1.43	10.74 ± 17.73	ns
isopentyl alcohol	2.18 ± 2.91	1.60 ± 0.87	ns
1-butanol, 2-methyl-	2.67 ± 2.47	0.97 ± 0.87	*
(Z)-3-hexen-1-ol	37.08 ± 18.50	40.03 ± 19.84	ns
1-hexanol	2.91 ± 3.43	2.29 ± 2.23	ns
1-pentanol	1.04 ± 1.01	1.80 ± 0.79	*
(Z)-2-penten-1-ol	1.55 ± 3.27	9.03 ± 1.62	*
Aldehydes			
isopentanal	1.97 ± 3.04	0.31 ± 0.22	*
butanal, 2-methyl-	5.78 ± 4.57	1.22 ± 0.87	*
(E)-2-pentenal	ND	0.16 ± 0.03	
(E)-3-hexenal	2.99 ± 3.15	2.63 ± 1.73	ns
hexanal	15.45 ± 10.52	10.16 ± 3.68	ns
(E)-2-hexenal	42.95 ± 35.80	17.41 ± 15.23	*
heptanal	2.90 ± 2.11	3.14 ± 0.75	ns
(Z)-2-heptenal	3.40 ± 3.59	1.93 ± 1.50	ns
nonanal	4.95 ± 2.04	6.54 ± 1.98	*
(E, Z)-2,6-nonadienal	20.35 ± 9.81	16.38 ± 9.50	ns
(E)-2-nonenal	2.04 ± 0.24	ND	
decanal	0.97 ± 2.63	6.63 ± 3.10	*
undecanal	0.19 ± 0.09	0.24 ± 0.19	ns
hexadecanal	0.28 ± 0.20	0.12 ± 0.07	*
Ketones			
1-penten-3-one	8.79 ± 8.76	15.93 ± 6.22	*
2-heptanone, 4-methyl-	ND	0.01 ± 0.00	
sulcatone	1.96 ± 1.60	2.43 ± 1.04	ns
Esters			
methyl methacrylate	12.02 ± 12.28	0.31 ± 0.65	*
ethyl butanoate	0.21 ± 0.12	ND	
methacrylic acid, ethyl ester	24.94 ± 17.59	0.61 ± 0.70	*
ethyl crotonate	0.22 ± 0.11	ND	
isopentyl ethanoate	2.10 ± 3.22	0.16 ± 0.09	*
butanoic acid, 2-butyl ester	0.01 ± 0.00	ND	
methyl caprylate	0.03 ± 0.02	ND	
(E)-3-hexenyl valerate	0.06 ± 0.06	0.08 ± 0.17	ns
2-ethyl-3-hydroxyhexyl 2-methylpropanoate	0.52 ± 0.48	0.46 ± 0.82	ns
Monoterpenes			
α-thujene	0.25 ± 0.13	0.18 ± 0.11	ns
α-pinene	12.21 ± 5.58	11.10 ± 5.15	ns
camphene	2.62 ± 1.33	2.11 ± 1.59	ns
β-pinene	1.12 ± 0.57	1.22 ± 0.38	ns
β-myrcene	60.05 ± 37.44	49.38 ± 38.75	ns
2-carene	3.55 ± 1.85	3.80 ± 1.80	ns
α-fellandrene	11.62 ± 11.05	7.29 ± 6.13	ns
3-carene	368.33 ± 155.55	338.11 ± 152.92	ns
α-terpinene	18.26 ± 10.41	14.51 ± 9.53	ns
p-cymene	20.77 ± 11.06	18.96 ± 11.00	ns
sylvestrene	8.73 ± 4.77	8.18 ± 5.26	ns
limonene	60.20 ± 31.19	56.67 ± 32.88	ns
(Z)-β-ocimene	1.04 ± 0.69	0.96 ± 0.82	ns
(E)-β-ocimene	4.21 ± 2.84	3.34 ± 2.67	ns
p-cymenene	0.63 ± 0.34	0.50 ± 0.25	ns
terpinolene	81.79 ± 46.66	71.39 ± 45.68	ns
linalool	0.79 ± 0.37	0.71 ± 0.44	ns
1,3,8-p-menthatriene	0.87 ± 0.50	0.67 ± 0.44	ns
(Z)-allo-ocimene	0.38 ± 0.30	0.31 ± 0.32	ns
(Z)-p-menth-2,8-dien-1-ol	3.87 ± 1.96	2.95 ± 1.47	ns
limonene oxide	0.28 ± 0.16	0.13 ± 0.13	*
p-cymenol	0.37 ± 0.41	0.27 ± 0.58	ns
dihydrocarvone	0.67 ± 0.63	0.33 ± 0.21	ns
β-cyclocitral	0.34 ± 0.22	0.39 ± 0.12	ns
β-citral	0.19 ± 0.26	0.07 ± 0.15	ns
eucarvone	6.15 ± 6.00	2.29 ± 2.64	*
(E)-nerol	4.52 ± 8.16	7.00 ± 5.87	ns
geranial	0.45 ± 0.71	0.61 ± 0.61	ns
geranyl butanoate	ND	0.05 ± 0.04	
Sesquiterpenes			
α-cubebene	0.01 ± 0.02	0.01 ± 0.03	ns
α-copaene	0.95 ± 0.48	0.75 ± 0.82	ns
β-elemene	0.01 ± 0.03	0.05 ± 0.12	ns
caryophyllene	0.19 ± 0.10	0.20 ± 0.27	ns
α-gurjunene	1.62 ± 0.71	2.46 ± 2.59	ns
(E)-β-caryophyllene	15.05 ± 6.05	14.24 ± 12.75	ns
aromadendrene	0.53 ± 0.23	0.54 ± 0.69	ns
γ-elemene	0.01 ± 0.01	ND	
humulene	10.00 ± 4.07	9.37 ± 8.05	ns
γ-gurjunene	ND	0.03 ± 0.00	
β-chamigrene	0.20 ± 0.10	0.28 ± 0.54	ns
β-selinene	4.66 ± 1.80	5.72 ± 5.98	ns
valencene	0.35 ± 0.15	0.47 ± 0.62	ns
α-selinene	0.87 ± 0.42	1.40 ± 1.87	ns
delta-cadinene	0.02 ± 0.03	0.05 ± 0.11	ns
α-panasinsene	0.14 ± 0.07	0.16 ± 0.29	ns
Unidentifieds			
39-41-55-77-83-94-100	ND	0.18 ± 0.02	
39-41-42-55-68-69-104	7.17 ± 7.66	10.76 ± 2.49	ns
41-43-57-67-81-109-121	0.30 ± 0.14	0.30 ± 0.26	ns
41-55-69-81-109-137	1.16 ± 0.97	0.56 ± 0.37	*
71-55-67-79-95-123	2.10 ± 1.90	1.03 ± 0.92	ns
79-93-107-121-136	0.91 ± 0.61	0.72 ± 0.47	ns
41-79-91-105-121-136-	0.52 ± 0.35	0.43 ± 0.41	ns
41-43-57-69-82-95-123	0.48 ± 0.29	0.82 ± 0.49	*
39-41-55-67-69-82-112	1.25 ± 0.42	ND	
77-79-91-107-135-150	0.27 ± 0.21	0.14 ± 0.05	*
39-41-55-67-69-82	0.57 ± 0.79	0.98 ± 0.98	ns
39-41-55-67-69-83-132-125	0.92 ± 1.43	0.17 ± 0.23	ns
41-57-70-81-95-123	0.04 ± 0.05	0.08 ± 0.17	ns
43-57-71-85-113-150	0.02 ± 0.04	0.04 ± 0.08	ns
41-55-67-82-83-101	1.06 ± 1.19	0.68 ± 0.43	ns
41-43-56-71-89-159	0.05 ± 0.07	0.05 ± 0.11	ns
43-56-71-83-89-98-143	0.15 ± 0.35	0.22 ± 0.46	ns
41-43-55-69-83-97	0.06 ± 0.02	ND	
41-55-67-81-93-107-189	0.08 ± 0.03	0.05 ± 0.12	ns
41-79-91-93-105-161	0.02 ± 0.04	0.06 ± 0.14	ns
41-79-91-105-119-133	0.42 ± 0.18	0.46 ± 0.58	ns
41-57-71-91-105-119-161	0.29 ± 0.10	0.19 ± 0.39	ns
41-55-79-91-105-121-133	0.53 ± 0.22	0.70 ± 0.88	ns
41-81-91-105-119-161	0.17 ± 0.12	0.28 ± 0.39	ns
41-54-55-67-68-81-95	0.08 ± 0.01	ND	
91-105-119-133-161-204	ND	0.01 ± 0.00	
43-57-71-84-113	0.06 ± 0.03	0.06 ± 0.15	ns

Sig = statistical significance, ns = not significant, *, significant difference by the ANOVA and F test ($p \leq 0.05$) and ND = not detected. Results of peak area divided by 10^6. The peak area results are presented as the mean of triplicate experiments.

linolenic acid. The high intensity of the compound imparts a green aroma, increasing the perception of bitter taste in fruits with IB (Caporale, Policastro & Monteleone, 2004). Besides that, these aldehydes are recognized as potent and important contributors to the flavor of fresh mango pulp, found in different varieties of mangoes (Zhang, Dong, Lao, Liu, Liao, & Wu, 2019). Nonanal and decanal aldehydes, found in different mango varieties (Pino & Mesa, 2006) and described with floral and sweet aromas, were found with greater peak area in WIB fruits, differing statistically ($p \leq 0.05$) from fruits with IB.

On the other hand, the ketone 1-penten-3-one was found with intense chromatogram peak area in asymptomatic fruits ($p \leq 0.05$). There are several routes for the formation of ketones, and their precursors may be fatty acids, amino acids, as well as sugars (Campo, Ferreira, Escudero, Marqués, & Cacho, 2006; Câmara, Marques, Alves, & Ferreira, 2004). The 1-penten-3-one has been identified in previous studies with mango fruits and the aroma of this ketone has been described as mushroom, this compound is also among the most important contributors of mango aroma (Liu et al., 2020).

The class of volatile esters was one of the main compounds identified in the study between IB and WIB mangoes. The perception of sweet and fruity odors is assigned to the chemical class of the esters (Rita, Zanda, Daina, & Dalija, 2011). Esters, representative of fruity aromatic volatiles, typical in ripe fruits, are produced through the esterification of acyl-CoAs and alcohols during the lipoxygenase (LOX) pathway (Chen, Quek, Fedrizzi, & Kilmartina, 2020; Defilippi et al., 2009).

Three ester compounds (methacrylic acid, ethyl ester, methyl methacrylate, and isopentyl ethanoate) with intense chromatogram peak areas were identified in IB fruits. The formation of esters occurs through the action of alcohol acyltransferase (AAT) enzymes and the fermentative metabolism that can be potentiated in the fruit through stress factors, such as intrinsic factors (maturation, senescence), biotic (microbial growth) and extrinsic factors (temperature, in addition to of hypoxic conditions) (White, Blake, Taylor, & Monks, 2016; Caleb et al., 2013). Furthermore, the greater release of esters in IB fruits indicates a more accelerated ripening of the fruits, since the synthesis of these compounds is increase during ripening as shown in studies with Shelly' and 'Delta R2E2′ mango fruits (Ntsoane et al., 2019; Lalel, Singh, & Tan, 2005).

Terpenes are considered one of the largest classes of plant secondary metabolites. These compounds have defense functions against pathogens and herbivores, in addition to protection against environmental stress (Goyal, Lambert, Cluzet, Merillon, & Ramawat, 2012; Huang et al., 2010; Tholl, 2006). The monoterpenes (10 carbons) and sesquiterpenes (15 carbons) volatilize easily at room temperature and contribute with floral aromas to essential oils, vegetables, and fruits (Dudareva & Pichersky, 2008). Monoterpenes are the primary compounds that contribute to mango taste (Pino & Mesa, 2006).

The monoterpenes IB fruits with high chromatogram peak areas was eucarvone, ($p \leq 0.05$). In a study conducted in three locations (with geographic variation), it was possible to detect greater amounts of total and individual monoterpenes in mature Alphonso fruits compared to the other stages (Kulkarni, Chidley, Pujari, Giri, & Gupta, 2012).

3.3. Chemometric analysis of physical and chemical and volatiles mango fruit quality parameters

The determination of the physical–chemical parameters is essential to monitor the ripening process of the fruits, and when related to analyzes such as GC–MS, they become even more interesting for the investigation of disorders such as the internal breakdown that affects mango fruits.

The discriminant analysis by PLS-DA was performed using all physical and chemical data and the 108 volatile compounds and with the fruits classified into mangoes IB and WIB. Fig. 2 shows the score plot of the first two latent variables explained that explain 27.22% of the total variance and mangos with IB and without IB have scores >0 and scores <0, respectively. It is important to notice that the focus of the PLS-DA is not used to maximize the explanation of the variance in each component (as in principal component analysis-PCA), but rather to maximize the explanation of the variance that is correlated with the separation of assigned groups.

With the verification of the separation of the two groups by the first latent variable in the PLS-DA, an analysis of the loadings was carried out in order to select the most important volatiles (variables) in the separation of fruits with and without IB, as shown in Fig. 2. Regarding the

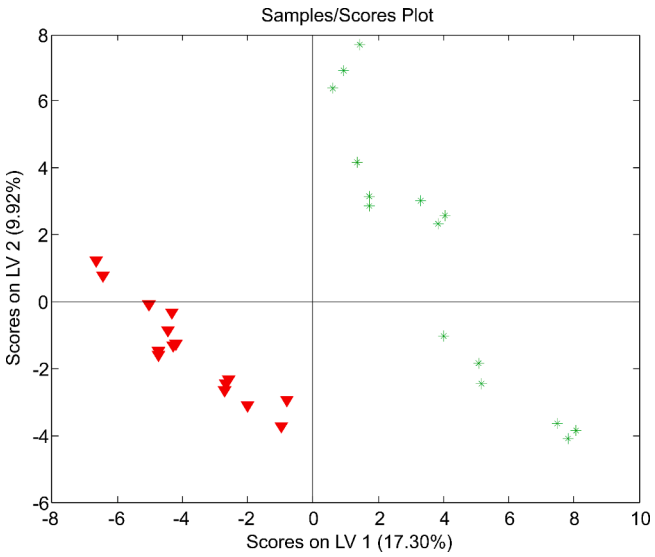

Fig. 2. Partial least square-discrimination analysis (PLS-DA) score plot of IB (*) and WIB (▼) mangoes samples, obtained with all physical and chemical data and with the 108 volatiles compounds.

physical–chemical data, there were a total of 30 variables. The analysis of these data was performed through PCA, which directly indicated the possibility of separation between groups in the first main component. This first PCA was used to identify the most important variables for the separation of the two groups using only the physical–chemical data. Of the initial 30 variables, 13 were identified as most responsible for the separation between groups, from 1 to 13 respectively: pH, titratable acidity (TA), ratio (SS/TA), firmness, a*, and C* (peel) and L*, a*, b*, C*, °h, dp a* and dp °h (pulp).

Fig. 3 shows the score (A) and loading (B) plots of the PCA for the selected variables from the physical–chemical data. Fig. 3 A shows a reasonable separation between the two classes in PC1. The fruits IB and WIB were in negative and positive score values of PC1, with the exception of a non-collapsed healthy sample. The loadings (Fig. 3B) show that the most important variables in the mangoes WIB are AT (%), firmness, mean L * and b * of the peel, mean C* and °h of the pulp. In IB mangoes, the most important variables were pH, ratio (SS/AT), mean a* and C* of the peel, mean a*, dp a* and dp °h of the pulp.

Eleven volatile compounds were selected as potential candidates for IB markers i.e. (E)-2-pentenal, (Z)-2-penten-1-ol, methacrylic acid, ethyl ester, isopentyl ethanoate, limonene oxide, (E)-2-nonenal, decanal, tetradecane, γ-elemene and two unidentifieds pics (39-41-55-77-83-94-100 and 39-41-55-67-69-82-112). In order to verify the possibility of creating a model to predict IB mango, a new PLS-DA was carried using the 11 selected variables. The model classified all samples in their respective groups using cross-validation, with a determination coefficient equal 0.969 for calibration and 0.769 for cross-validation. Such result indicates that it is possible to create a model to predict mangoes with IB using these 11 volatiles.

A PCA analysis was performed with these variables to verify whether these 11 selected volatiles compounds could generate a fingerprint in relation to the IB. Fig. 4 presents the scores and loadings plots of the PCA analysis, with the separation between the two classes clearly occurring in PC1. Fruits IB and WIB are in the positive and negative values of PC1 (Fig. 4A), respectively. Fig. 4B shows that the mangoes WIB, in negative side of PC1 have high concentration of compounds 1, 2, 3, 9 and 10, which correspond to compounds 39-41-55-77-83-94-100, (E)-2-pentenal, (Z)-2-penten-1-ol, decanal and tetradecane, respectively. On the positive side of PC1 (Fig. 4B) are the mangoes IB, which have a higher concentration of volatiles compounds 4, 5, 6, 7, 8 and 11, which correspond to the compounds methacrylic acid, ethyl ester, isopentyl

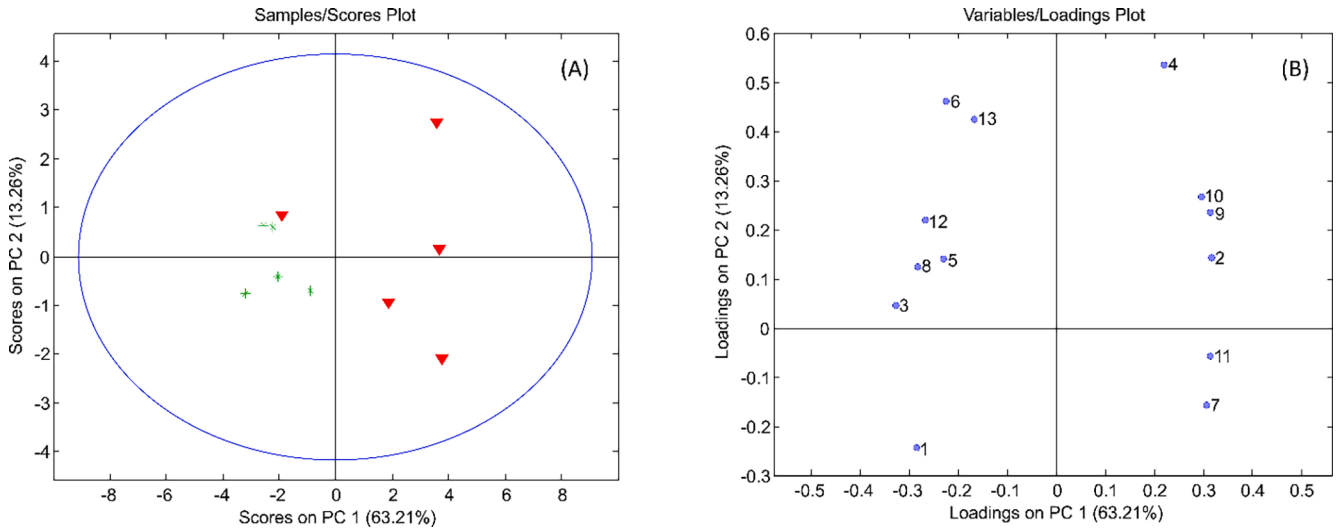

Fig. 3. Principal component analysis (PCA) of the most important physical–chemical parameters of IB and WIB. Fig. 3A shows the PCA scores plot where IB (*) and WIB (▼) mangoes. Fig. 4B shows a PCA loading plot where, 1: pH; 2: titratable acidity (TA); 3: ratio (SS/TA); 4: firmness; 5: a* (peel); 6: C* (peel); 7: L* (pulp); 8: a* (pulp); 9: b* (pulp); 10: C* (pulp); 11: °h (pulp); 12: dp a* (pulp) and 13: dp °h (pulp).

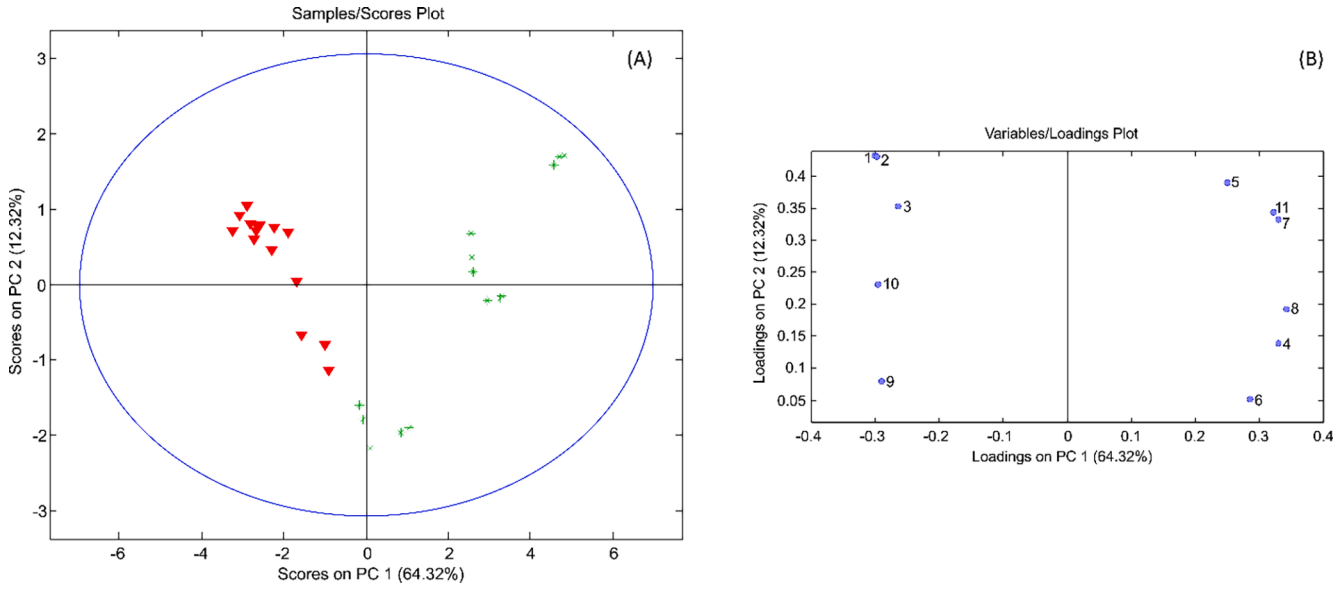

Fig. 4. Principal component analysis (PCA) or the differentiation between mangoes with and without IB from the 11 most important volatile compounds. Fig. 4A scores plot PCA where * mangoes with IB ▼ and WIB mangoes. Fig. 4B loading plot PC1 where, 1: 39-41-55-77-83-94-100; 2: (E)-2-pentenal; 3: (Z)-2-penten-1-ol; 4: methacrylic acid, ethyl ester; 5: isopentyl ethanoate; 6: limonene oxide; 7: (E)-2-nonenal; 8: 39-41-55-67-69-82-112; 9: decanal; 10: tetradecane and 11: γ-elemene.

ethanoate, limonene oxide, (E)-2-nonenal, 39-41-55-67-69-82-112 and γ-elemene, respectively.

4. Conclusions

The chemometric evaluation was adequate to identify the physical–chemical parameters and the most important volatile compounds in the differentiation of fruits with and without IB. The fruits IB have an increase in the color index (a* of the peel and pulp), softening of the pulp, enhancement of the flavor (pH and SS/TA). Quantitative differences in volatile compounds were observed for both IB and WIB mangoes. The compounds methacrylic acid, ethyl ester, isopentyl ethanoate, limonene oxide, (E)-pentenal, unidentified (39-41-55-67-69-82-112), tetradecane and γ-elemene are indicative of markers of IB fruits and (Z)-2-penten-1-ol, (E)-2-nonenal, decanal and the unidentified (39-41-55-77-83-94-100), are indicative markers for WIB fruits.

The results revealed that the detection of volatile compounds can be used for future separations between IB and WIB mangoes in the post-harvest, however, more studies are needed to understand how the expression of volatile compounds is associated with mangoes with the presence of this physiological disorder. The volatile compounds identified in sliced mangoes were initially evaluated for a better understanding of the physiological point of view between the mango groups with and without collapse. It is believed that these results may assist future studies regarding the refinement of the methodology for the identification of different volatiles in intact mango fruits.

CRediT authorship contribution statement

Fernanda Campos Alencar Oldoni: Conceptualization, Methodology, Investigation, Writing – original draft. **Camila Florencio:** Methodology, Writing – original draft. **Giovana Brait Bertazzo:**

Methodology, Writing – original draft. **Pamela Aparecida Grizotto:** Methodology, Investigation. **Stanislau Bogusz Junior:** Supervision, Writing – review & editing. **Renato Lajarim Carneiro:** Supervision, Writing – review & editing. **Luiz Alberto Colnago:** Supervision, Writing – review & editing. **Marcos David Ferreira:** Conceptualization, Funding acquisition, Supervision, Writing – review & editing.

Declaration of Competing Interest

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

Acknowledgements

The authors are grateful to Coordination for the Improvement of Higher Education Personnel (CAPES, Brazil - Finance Code 001), and FAPESP (grant no: 2019/13656-8 and 2019/05159-4) for the financial support.

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