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Vinegars from fruits of Myrciaria cauliflora (Mart.) O.Berg and Myrciaria jaboticaba (Vell.) Berg: Phytochemical, volatile and, sensory profiles, antioxidant activity and chemical characteristics

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Abstract

Jabuticaba is a tasty Brazilian fruit, with high productivity and perishability, with a short period of consumption after harvest. For a better use of its production, an alternative is the production of derivatives, such as vinegar. This study aimed to determine the phenolic, volatile and, sensory profiles, antioxidant activity and chemical characteristics of vinegars produced with fruits, with and without peel, of *Myrciaria cauliflora* (Mart.) O. Berg and *Myrciaria jaboticaba* (Vell.) Berg. Four vinegars were obtained. Fourteen phenolic compounds were identified and quantified, classified between phenolic acids and flavonoids, with emphasis on 3,4-DHB, chlorogenic acid and, sinapic acid. The highest antioxidant activity was for *M. jaboticaba* vinegar, made with unpeeled fruits. For volatile compounds, 21 esters, 7 alcohols, 5 terpenes, 1 ketone, and, 1 vinylarene were identified. Sensory analysis showed similarities in terms of taste and differences in terms of odor between Jabuticaba vinegars and commercial vinegars. Phenolic compounds, acetic acid and, esters were the main chemical groups identified. Vinegars, in general, showed differences regarding the presence and absence of peels. The jabuticaba vinegars showed characteristics suitable for the product, and several important compounds for human health.

1. Introduction

Jabuticaba is a small fruit native to Brazil, which has a sweet and slightly acidic pulp and, high levels of sugars, organic acids and, terpenes. It is grown on a small scale, with production between August and November. It has a spherical shape, with a thin (*Myrciaria cauliflora* (Mart.) O.Berg) or thick (*Myrciaria jaboticaba* (Vell.) Berg) peel, depending on the species, with a green to dark purple color, depending on the maturation stage [1–4]. The dark purple peel is rich in phenolic acids, flavonols, ellagitannins and, anthocyanins such as cyanidin and delphinidin glycosides. It is also rich in phenolic compounds that are responsible for the high antioxidant activity found *in vitro* in different assays, antioxidant effects in humans, anti-inflammatory modulation of the intestinal microbiota and, insulin resistance in rats [5, 6].

Jabuticaba is very popular throughout Brazil, however, its high perishability limits the commercialization of the fruit *in nature*. The most commonly consumed part of the fruit is the pulp. The peels and seeds, where most of the anthocyanins and phenolic compounds are found, are discarded [7]. Due to these factors, researchers have been working on technological processes for the development of products derived from Jabuticaba, such as juices, jellies, liqueurs, wines and, vinegars [2, 8].

Vinegar is produced from numerous fruits and vegetables rich in amino acids, organic acids, phenolic compounds, vitamins and, mineral substances. It is a flavoring and preservative agent for foods, used directly as a seasoning and in sauces, ketchup and, mayonnaise [9–11]. Due to the mild fermentation conditions used in production, molecules naturally present in the fruits remain in the vinegar, in addition to generating new molecules. These substances play an important role in the prevention and treatment of human diseases. This role is attributed to bioactivities and numerous pharmacological properties [11] such as antioxidant, anti-obesity, anti-diabetic, antimicrobial, anti-hypertensive and, anti-cancer activities [11–14]. Therefore, vinegar has been used as a medicine in many civilizations throughout history.

The phenolic compounds present in vinegars come from the raw material used, but changes in their composition or quantity may occur due to different processing methods and plant materials [15]. These compounds contribute to antioxidant activity and, in Jabuticaba, studies highlight the contribution of anthocyanins, a class of flavonoids present in dark-colored fruits. Jabuticaba is known as one of the richest Brazilian sources of anthocyanins [16]. The Jabuticaba fermented product has a vasorelaxant capacity, associated with the antioxidant potential of the phenolic compounds present [17].

The composition of aromatic compounds in vinegar is complex and mainly includes esters, acids, alcohols, aldehydes, phenols and, amino acids [14]. Flavor, which is the sum of taste and smell, is one of the most intuitive and important attributes that affect the quality and consumer acceptance of vinegar. The volatile compounds associated with aroma make a major contribution to flavor [18], and their unique profile represents the fingerprint of each vinegar. The aroma is considered one of the most important indicators of the quality of vinegar [19, 20].

Given this context, it is important to contribute information related to the chemical aspects of vinegar made with fruit, and how the use of different parts of the fruit may be associated with the availability of important compounds for human health. Therefore, the objective of this study was to obtain the phenolic, volatile and, sensory profiles of vinegars made with Jabuticaba with and without peel, from the species *Myrciaria cauliflora* (Mart.) O.Berg and *Myrciaria jaboticaba* (Vell.) Berg. In addition, to characterize the vinegars in terms of *in vitro* antioxidant activity and chemical aspects.

2. Material And Methods

2.1 Plant material and chemicals

The Jabuticabas, of the *Myrciaria cauliflora* (Mart.) O.Berg and *Myrciaria jaboticaba* (Vell.) Berg varieties, were harvested at the maximum stage of maturation, from plants in a rural environment in the city of Nova Erechim, west of Santa Catarina state (Latitude: 26º54'09" south, 52º54'21" west), in September 2021 (early spring in Brazil). The voucher specimen was deposited in the LUSC - Lages Herbarium of Santa Catarina State University (voucher specimen numbers of LUSC 10713 for *M. cauliflora* and LUSC 10714 for *M. jaboticaba*). Flowering was induced by irrigation, with fruit development and harvest occurring at the same time for both varieties. The fruits were selected and those that were damaged were discarded, keeping a uniform sample for each variety. The fruits were washed with a 0.1% NaClO solution, rinsed with distilled water, dried with a paper towel, and stored for no more than 24 h at 4°C.

All the chemicals used in the research were of analytical grade and the most important were: the sodium phosphate monobasic, bibasic sodium phosphate heptahydrate, Rochelle salt, *Folin–Ciocalteu* reagent, 3,5-dinitrosalicylic acid, hydrochloric acid, ethyl ether, formic acid, trichloroacetic acid, dimethyl sulfoxide, malondialdehyde, sodium hydroxide, gallic acid, Trolox, 1,1-diphenyl-2-picrylhydrazyl, thiobarbituric acid, 2,2-azinobis (3-ethylbenzothiazoline-6-sulfonic acid), 2,4,6-Tris(2-Pyridyl)-S-Triazine (TPTZ), were purchased from Sigma Aldrich (Cotia, SP, BR). The organic solvent methanol (100%) and ethanol (99.5%)

were purchased from Synth (Diadema, SP, BR). The standards of phenolic compounds and volatile compounds were purchased from Sigma-Aldrich and Merck (Cotia, SP, BR). This research is registered in SisGen (*Sistema Nacional de Gestão do Patrimônio Genético e do Conhecimento Tradicional Associado*) with the code ABB9D14.

2.2 Preparation of Jabuticaba vinegars

The Jabuticabas, of each variety, were separated into two fractions. In one of the fractions, the peels were removed manually. The Jabuticabas were crushed manually, resulting in four musts: two with peels and two without peels (Fig. S1 - supplementary material). The soluble solids content was determined (digital refractometer RFM 732, Bellingham + Stanley Ltd, UK) in each of the musts (10.9°Brix for *M. cauliflora* and 12.1°Brix for *M. jaboticaba*) and then sucrose was added to adjust to 18°Brix. The inoculum (*Saccharomyces cerevisiae* - Itaquara, Tapiratiba, SP, BR), standardized to 0.5 McFarland (10^6 log CFU/mL), was added to the must. The first stage of alcoholic fermentation was conducted at 25°C for 4 days. Subsequently, racking was performed to remove all solid material, and the second stage of alcoholic fermentation was carried out at 25ºC for 30 days. The wines obtained were used in the vinegar production stage, with the traditional fermentation of acetic acid being carried out at 25ºC for 30 days [12]. Four vinegars were obtained, coded as McP and Mc – vinegars of the *M. cauliflora* variety, made with fruits with peel and without peel, respectively; MjP and Mj - vinegar of the *M. jaboticaba* variety, made with fruits with and without peel, respectively (Fig. S2 - supplementary material). 1/4 of the final volume obtained from each vinegar was lyophilized at -60 ºC and 0.05 mTorr (Benchtop Model Freeze Dryers, ilShin, Europe, NL) for 48 h, and used in the analyzes of item 2.8. For the other tests, samples without any physical or chemical modification were used.

2.3 LC-ESI-MS/MS analysis of phenolic profile

The identification and quantification of the individual phenolic compounds were performed using Liquid Chromatography-Electrospray Ionization-Tandem Mass Spectrometry (LC-ESI-MS/MS). A liquid chromatograph was used (Agilent 1290 Series, Agilent Technologies, Wilmington, USA), coupled with a quadrupole hybrid mass spectrometer with linear quadrupole ion trap (QTRAP® 5500, Sciex, Foster City, USA) equipped with an electrospray ionization source (ESI). Identification and quantification of compounds were performed according to retention time, precursor ion, major fragment (quantitation ion) and, secondary fragment (confirmation ion), by comparison with commercial analytical standards. Chromatographic separation was obtained using an Agilent Zorbax Eclipse Plus C18 column (3.0 x 100 mm, 3.5 µm). The mobile phase consisted of water (A) and methanol (B), both with 0.1% formic acid. The following gradient mode was used: 0–3 min, 2% B; 3–10 min, 20% B; 10–11 min 90% B; 11–13 min, 2% B. The flow was 0.3 mL/min. An equilibration time of 2 min was used between runs. The injection volume was 5 µL. The acquisition and processing of data were performed in software Analyst and MultiQuant (Sciex, Framingham, MA, USA), respectively. Thirty-five phenolic compounds standards were used, as follows: 2,4-DHBA, 3,4-DHB, 2,5-DHBA, 3,5-DNB, 4-aminobenzoic acid, 4-methylumbelliferone, apigenin, benzoic acid, caffeic acid, catechin, chlorogenic acid, epicatechin, gallic acid, hesperidin, isoquercitrin, pinocembrin, quercetin, rutin, sinapaldehyde, sinapic acid, chrysin, coniferaldehyde, coumarin, ferulic acid,

galangin, isorhamnetin, kaempferol, naringenin, naringin, p-coumaric acid, pinobanksin, salicylic acid, syringaldehyde, syringic acid, vanillic acid.

2.4 Total phenolic compounds and in vitro antioxidant activity

The determination of the total phenolic compounds (TPC) of vinegars was carried out by the method that uses *Folin-Ciocalteu* and spectrophotometry (DR 3900, Hach, DE) [21], with modifications and measurements in triplicate. 0.1 mL of vinegar was diluted in 6 mL of distilled water. Next, 0.5 mL of reagent *Folin-Ciocalteu* and 2 mL of a solution of Na_2CO_3 (20%) were added. The mixture was submitted to agitation for 30 s and, later, incubated for 2 h at 25ºC. The absorbance was measured at 750 nm. The calibration curve was obtained from solutions with different concentrations of gallic acid (0, 40, 80, 120, 160, 200, 240, 280, 320, 360, and 400 µg/mL. The results were calculated by using the linear equation y = 0.0015x + 0.0294 (R^2 = 0.9925) where *y* axis is absorbance and *x* axis is gallic acid concentration and was expressed in equivalent milligrams of gallic acid per gram of dry mass (mg EAG/g MS).

The antioxidant activity was determined by the 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging, by the scavenging of the 2,2'-azino-bis(3-ethylbenzthiazoline-6-sulfonic acid) radical (ABTS) and by the ferric reducing antioxidant power (FRAP), with measurements in triplicate.

For the assay of DPPH radical scavenging [22], 0.1 mL of the sample was mixed with 3.9 mL of 0.06 mM DPPH solution, in methanol. In the control solution, methanol was used in place of the sample. The mixtures were incubated at 25°C for 1 h in the dark. The absorbance reading was performed at 515 nm, with methanol to calibrate the equipment. Quantitation was performed based on a standard curve of DPPH in methanol (at concentrations of 0 µM, 10 µM, 20 µM, 30 µM, 40 µM, 50 µM and, 60 µM) using the linear equation $y = 0.0104x + 0.0248$ (R^2 = 0.9919), where the *y*-axis is absorbance and *x*-axis is DPPH concentration. The results were expressed as EC_{50}, which is the concentration of the sample required for DPPH radical scavenging by 50%. For the ABTS radical scavenging [23], a stock solution of 7 mM ABTS was prepared. The ABTS working solution was prepared by mixing the ABTS stock solution with the 2.45 mM $K_2S_2O_8$ solution in a ratio of 1:1 (v/v). 20 µL of the sample was mixed with 980 µL of ABTS working solution. The absorbance of the mixture was measured in a spectrophotometer at 734 nm after 6 min of incubation, in the absence of light. Quantitation was performed using a standard curve of Trolox in ethanol (at concentrations of 100 µM, 500 µM, 750 µM, 1000 µM, 1500 µM and, 2000 µM), using the linear equation y=-0.000289x + 0.53447 (R^2 = 0.9176), where the *y*-axis is absorbance and *x*-axis is Trolox concentration. Results were expressed in µM Trolox/g of the sample. For the ferric reducing antioxidant power (FRAP) [24, 25], 200 µL of the sample was mixed in 200 µL of 3 mM ferric chloride solution. The mixture was allowed to stand for 30 min at 37°C. Then, 3600 µL of TPTZ solution (2,4,6-Tris(2-pyridyl)-s-triazine), prepared in the proportion of 0.078 g of TPTZ diluted to 250 mL of 0.05M HCl, were added. The absorbance of the mixture was measured in a spectrophotometer at 620 nm after 10 min of reaction, in the absence of light. Quantitation was performed based on a Trolox standard curve in ultrapure water (at concentrations 25 µM, 50 µM, 100 µM, 200 µM, 400 µM, 800 µM and, 1000 µM) using the linear equation

$y = 0.0021x + 0.0553$ ($R^2 = 0.9985$), where the *y*-axis is absorbance and *x*-axis is Trolox concentration. Results were expressed in μM Trolox/g of the sample.

2.5 GC-MS analysis of volatile compounds

The determination of volatile compounds followed the methodology described in Hendges et al. [26], with adaptations and, was carried out for fruits and vinegars. Extraction of volatile compounds was performed by solid phase microextraction (SPME) using fiber coated with dedivinylbenzene/carboxene/poly dimethylsiloxane (DVB/CAR/PDMS) (1 cm long, 50/30 μm thick, StableFlex™, Supelco, USA). 2 mL of the sample, 5 mL of ultrapure water and 3 g of NaCl were added to a 20 mL glass vial, mixed, sealed with a silicone septum and closed with a crimp cap. The flasks were kept at 45°C for 40 min in a water bath. Then, the SPME fiber was exposed for 15 min inside the flasks (headspace) and, after adsorption, the fiber was removed and the analytes were thermally desorbed in the GC injector in splitless mode at 270ºC for 10 min. The evaluation of aromatic compounds was performed by gas chromatography (GC - Perklin Elmer Clarus 680) coupled with mass spectrometry (MS - Perklin Elmer SQ8S). In the GC, a Perkin Elmer Elite-5MS capillary column, 30 mx 0.25 mm i.d., 0.25 μm thick, was used. The carrier gas was helium, with a flow rate of 1 mL/min. The oven temperature was programmed as follows: 25°C for 5 min, 1°C/min increments up to 30°C, 5°C/min increments up to 80°C, and finally 220°C for 5 min. Volatile compounds were identified by mass spectrometry (MS). The detector operated in the range of 33 to 450 m/z, the temperature in the ion source was 250°C and the temperature in the injector was 200°C. All compounds were confirmed by combining their mass spectra with the NIST Mass Spectral Library, version NIST 2.0 (National Institute of Standards and Technology, USA).

2.6 Sensory analysis: electronic tongue (E-Tongue) and electronic nose (E-Nose)

Flavor and odor profiles were obtained for Jabuticaba vinegars (McP, Mc, MjP and, Mj) and commercial vinegars, namely: white wine vinegar (WWV), red wine vinegar (RWV), apple cider vinegar (AV), alcohol vinegar (EV), balsamic vinegar (BV) and, rice vinegar (RV), totaling 10 samples.

Flavor profiles were evaluated in E-Tongue (ASTREE v5.2, Alpha MOS, Toulouse, France). The equipment contains a set of 7 flavors sensors, a silver/silver chloride (Ag/AgCl) reference electrode, and an autosampler with 16 positions for 150 mL beakers. The measurement consists of the potentiometric difference between each sensor and the reference electrode, in a steady state, at room temperature. AHS, CTS, NMS, ANS and, SCS sensors represent sourness, saltiness, umami, sweetness and, bitterness, respectively. PKS and CPS sensors represent other complex flavors [27]. The sensors were conditioned and calibrated in a standard HCl 0.01 mol/L solution. Samples were diluted in ultrapure water at a ratio of 1:100. The E-tongue data acquisition sequence was performed alternately with ultrapure water. Data acquisition time and analysis time were 120 s and 180 s, respectively. E-tongue detection results, read in triplicate, were converted into taste values using AlphaSoft v. 2021 (Alpha MOS, Toulouse, FR).

The odor profiles were obtained in E-Nose (HERACLES II, Alpha MOS, Toulouse, France) integrated with FAST-GC functionalities dual channel composed of two flame ionization detectors (FID), using columns MXT-5 and MXT − 1701. Each vial, containing 50 µL of the sample, was heated to 40°C for 20 min, and 250 µL of headspace gas was injected into the GC at 200°C. Hydrogen was used as carrier gas with a constant flow rate of 10 mL/min. The oven temperature was 50°C for 2 s, up to 80°C at the rate of 1°C/s and, 250°C at the rate of 3°C/s and held for 21 s. The temperature of the FIDs was 260°C. The acquisition time was 110 s and each sample were prepared in triplicate. For data processing, the software AlphaSoft v. 12.46 (Alpha MOS, Toulouse, FR).

2.7 Attenuated total reflection (ATR) Fourier transform infrared (FTIR) spectroscopy

The spectra of the vinegars (32 scans per sample) were acquired on an FTIR spectrometer (INVENIO-S, Bruker, Billerica, USA), equipped with a diamond crystal cell for attenuated total reflection (ATR) operation, with a resolution of 4 cm^{-1} and range from 400 cm^{-1} to 4000 cm^{-1}. The spectrum of each sample was collected twice and corrected using the spectrum of CO_2 and H_2O, in addition to baseline correction. The analysis was performed at room temperature. For data acquisition, the OPUS program (version 8.2, Bruker, Billerica, USA) was used.

2.8 X-ray fluorescence

The elemental composition of lyophilized vinegars was determined using an X-ray Fluorescence Spectrometer (EDX-720 - Shimadzu, Kyoto, JP). The sample was mixed with a spectromixture binder, forming a homogenized analytical pellet.

2.9 Statistical analysis

Statistical analysis of results was performed using R 3.5.1 [28] and Microsoft Excel, performing analysis of variance (ANOVA), and the difference between the averages was evaluated using Tukey's test, with 95% reliability ($P < 0.05$).

3. Results And Discussion

3.1 Phytochemical profile and in vitro antioxidant activities of vinegars

The phytochemical profile (Table 1) of the vinegars shows the quantification of 14 phenolic compounds, divided into phenolic acids and flavonoids. Regarding the general total of phenolic compounds, McP and MjP have the highest concentrations. Concerning phenolic acids quantified for each vinegar, the highest total concentrations are in vinegars made with peel (McP and MjP), with emphasis on 3,4-DHB, chlorogenic acid and, sinapic acid. Of all phenolic acids identified and quantified, only gallic acid was not quantified in Mj. Phenolic acids have cardioprotective, hypolipidemic, anti-obesity and, antitumor

activities. They also act to control rheumatism, and muscle and joint pain and protect cells against oxidative stress induced by hydrogen peroxide [29]. For flavonoids, isoquercitrin was the one with the highest concentrations. Pinocembrin had higher concentrations in Mc and Mj, and hesperidin and quercetin were quantified only in one of the vinegars. For the other phenolic compounds, the average concentration values were similar or even equal ($P > 0.05$), considering the statistical analysis, between vinegars made with and without the peel. In addition to the compounds already mentioned, it should be noted that other important phenolic compounds were quantified in vinegars. These same compounds, for example, rutin, catechin and, epicatechin, are reported in fruits [1]. This demonstrates the migration of compounds from the fruit to the fermented product.

Table 1
Phytochemical profile of vinegars from the fruits of *Myrciaria cauliflora* (Mart.) O.Berg and *Myrciaria jaboticaba* (Vell.) Berg.

Phenolic compound	Molecular formula	Concentration ± SD (µg/L)			
		McP	Mc	MjP	Mj
Phenolic acids					
3,4-DHB (Protocatechuic acid)	$C_6H_{14}O_8S_2$	526.73^{a} ± 4.96	121.40^{c} ± 1.39	197.47^{b} ± 2.20	91.67^{d} ± 0.31
Benzoic acid	$C_7H_6O_2$	50.07^{a} ± 4.80	47.60^{a} ± 5.25	46.47^{a} ± 3.04	49.93^{a} ± 9.07
Caffeic acid	$C_9H_8O_4$	66.33^{a} ± 0.42	65.93^{a} ± 1.27	65.80^{a} ± 1.44	66.67^{a} ± 0.31
Chlorogenic acid	$C_{16}H_{18}O_9$	272.87^{b} ± 8.08	109.87^{c} ± 0.64	386.40^{a} ± 9.75	86.87 ^{d}± 0.12
Gallic acid	$C_7H_6O_5$	42.73^{a} ± 0.61	41.73^{b} ± 0.12	43.13^{a} ± 0.42	<LQ
Sinapic acid	$C_{11}H_{12}O_5$	111.13^{ab} ± 0.12	111.27^{a} ± 0.12	111.27^{a} ± 0.12	111.00^{b} ± 0.00
Total		*1069.86*	*497.80*	*850.54*	*406.14*
Flavonoids					
Catechin	$C_{15}H_{14}O_6$	48.20^{a} ± 0.40	46.73^{b} ± 0.12	45.80^{c} ± 0.20	46.47^{b} ± 0.12
Epicatechin	$C_{15}H_{14}O_6$	75.73^{a} ± 0.12	74.33^{b} ± 0.12	73.40^{d} ± 0.00	73.93^{c} ± 0.12
Hesperidin	$C_{28}H_{34}O_{15}$	61.87 ± 0.83	<LQ*	<LQ	<LQ
Isoquercitrin	$C_{21}H_{20}O_{12}$	537.27^{a} ± 2.69	159.27^{c} ± 2.34	536.93^{a} ± 11.63	406.60^{b} ± 10.39
Pinocembrin	$C_{15}H_{12}O_4$	43.94^{c} ± 0.83	85.91^{b} ± 4.38	38.15^{c} ± 0.54	195.80 ^{a}± 3.88
Quercetin	$C_{15}H_{10}O_7$	59.40 ± 1.40	<LQ	<LQ	<LQ
Rutin	$C_{27}H_{30}O_{16}$	34.27^{a} ± 0.31	33.40^{b} ± 0.00	33.73^{b} ± 0.12	33.53^{b} ± 0.12

Phenolic compound	Molecular formula	Concentration ± SD (µg/L)			
		McP	Mc	MjP	Mj
Phenolic acids					
Sinapaldehyde	$C_{11}H_{12}O_4$	39.60^{a} ± 0.00	39.40^{b} ± 0.00	39.40^{b} ± 0.00	39.60^{a} ± 0.00
Total		*900.28*	*439.04*	*767.41*	*795.93*
General total		1970.14	936.84	1617.95	1202.07
Considering the LQ, the following phenolic compounds were not detected: **2,4-DHBA** ($C_7H_6O_4$); **2,5-DHBA** ($C_7H_6O_4$); **3,5-DNB** ($C_{16}H_{15}N_3O_7$); **4-aminobenzoic acid** ($C_7H_7NO_2$); **4-methylumbelliferone** ($C_{10}H_8O_3$); **apigenin** ($C_{15}H_{10}O_5$); **chrysin** ($C_{15}H_{10}O_4$); **coniferaldehyde** ($C_{10}H_{10}O_3$); **coumarin** ($C_9H_6O_2$); **ferulic acid** ($C_{10}H_{10}O_4$); **galangin** ($C_{15}H_{10}O_5$); **isorhamnetin** ($C_{16}H_{12}O_7$); **kaempferol** ($C_{15}H_{10}O_6$); **naringenin** ($C_{15}H_{12}O_5$); **naringin** ($C_{27}H_{32}O_{14}$); **p-coumaric acid** ($C_9H_8O_3$); **pinobanksin** ($C_{15}H_{12}O_5$); **salicylic acid** ($C_7H_6O_3$); **syringaldehyde** ($C_{11}H_{12}O_4$); **syringic acid** ($C_9H_{10}O_5$) and, **vanillic acid** ($C_8H_8O_4$).					

***** LQ is limit of quantification. **Note**: McP and Mc are the vinegars of the *M. cauliflora* variety, whose first step of alcoholic fermentation took place with fruits with and without peel, respectively; MjP and Mj are the vinegars of the *M. jaboticaba* variety, whose first step of alcoholic fermentation took place with fruits with and without peel, respectively.

As for antioxidant activity (Table 2), a trend was observed: greater activity for vinegars made with whole fruit (with peel). Mj was the one that presented the results that express the lowest antioxidant activity, with the highest EC_{50} value for DPPH (the relationship is inverse) and the lowest values of radical scavenging and inhibition for the other tests (ABTS and FRAP). Phenolic acids act as antioxidants (due to the reactivity of the phenol fraction; hydroxyl substituent on the aromatic ring). Although several mechanisms are known for the antioxidant activity of phenolic acids, it is believed that radical scavenging through the donation of hydrogen atoms is the main method [30]. For flavonoids, the antioxidant activity is the most relevant and is due to the ability to scavenge free radicals, although this ability varies according to the type of functional group and the arrangement around the nuclear structure of the molecule. The mechanisms of antioxidant action of flavonoids can be by direct elimination of ROS (Reactive Oxygen Species), inhibition of ROS formation through chelation of oligoelements, or inhibition of enzymes that participate in the generation of free radicals and activation of antioxidant defenses [31].

Table 2
Total phenolic compounds (TPC) and *in vitro* antioxidant activity of vinegars from the fruits of *Myrciaria cauliflora* (Mart.) O.Berg and *Myrciaria jaboticaba* (Vell.) Berg.

Vinegar	TPC	*In vitro* antioxidant activity			
	(mg EAG/g DS)	DPPH (EC_{50})	ABTS (% inhibition)	ABTS (µM Trolox/g sample)	FRAP (µM Trolox/g sample)
McP	1554.5 ± 124.14^{a}	0.24 ± 0.06^{b}	862.2 ± 101.3^{a}	13707.01 ± 2052.98^{a}	35677.68 ± 161.22^{a}
Mc	380.33 ± 51.96^{b}	0.45 ± 0.02^{a}	150.8 ± 85^{c}	-709.28 ± 1722.23^{c}	9123.54 ± 248.89^{c}
MjP	139.5 ± 12.58^{c}	0.40 ± 0.04^{a}	395.3 ± 30.5^{b}	4246.82 ± 618.7^{b}	26315.39 ± 2441.64^{b}
Mj	192 ± 19.25^{c}	0.54 ± 0.02^{a}	5.2 ± 17.2^{d}	-3659.15 ± 347.9^{d}	5260.11 ± 747.07^{d}

Note: McP and Mc are the vinegars of the *M. cauliflora* variety, whose first step of alcoholic fermentation took place with fruits with and without peel, respectively; MjP and Mj are the vinegars of the *M. jaboticaba* variety, whose first step of alcoholic fermentation took place with fruits with and without peel, respectively.

3.2 Volatile compounds contents in fruits and vinegars

The profile of volatile compounds of fruits of *M. cauliflora* and *M. jaboticaba* (Fig. 1a) shows an expressive number of terpenes, with 37 sesquiterpenes and 16 monoterpenes. In addition, were also detected: esters (13 compounds), alcohols (4 compounds), amides (2 compounds), and aldehyde, amino acid, ketone and, nitrile (1 compound each) (additional data is in **Table S1 - supplementary material**). The sesquiterpenes have bactericidal properties, for some chemical structures [32]. Monoterpenes are effective in the treatment of infectious diseases and early cancers [33]. Caryophyllene has strong antioxidant and antitumor activities [32]. Isocaryophyllene was not detected in peeled fruits of *M. cauliflora* and was detected in peeled fruits of *M. jaboticaba*. This demonstrates that there is a difference in the volatile compounds between the fruits of the two species. The presence of (-)-β-Pinene, responsible for the pine resin or turpentine aroma, occurs for the fruit of *M. cauliflora*, without peel, and for the fruit of *M. jaboticaba*, with and without the peel. The β-elemene was detected in fruits of *M. cauliflora*, with and without the peel. Tisserand and Young [34] report the *in vitro* inhibitory effect of β-elemene on the proliferation of leukemic cells. β-copaene was also detected in fruits of *M. cauliflora* without peel and, γ-gurjunene in fruits with and without peel, of both species. Esters are usually formed by the reaction between an alcohol and acidic compounds. They are important aromatic compounds in many fruits and derivatives [12]. Esters were the predominant compounds in the whole fruits of *M. cauliflora* and *M. jaboticaba*. Ethyl acetate, a compound identified as pineapple aroma, is present in Jabuticaba. Ethyl crotonate, also known as ethyl 2-butenoate, is found in apples, papayas, strawberries, rum, wine and,

cocoa. It has a strong fruity aroma and has many important applications in the food industry as a flavoring [35]. Ethyl crotonate was detected only for *M. cauliflora* fruits. Its isomer, ethyl 2-butenoate, was detected for *M. cauliflora* fruits, with and without peel, and for *M. jaboticaba* fruits, with peel. Of the 13 esters detected, 9 are in the whole fruits of *M. cauliflora* and 7 are in the whole fruits of *M. jaboticaba*. This profile demonstrates the contribution of the peel to the presence of these compounds.

The profile of volatile compounds in vinegars produced with the fruits of *M. cauliflora* and *M. jaboticaba*, with and without peel (Fig. 1b), shows a considerable number of esters (21 compounds). Alcohols (7 compounds), terpenes (5 compounds, 2 sesquiterpenes and 3 monoterpenes), ketone and vinylarene (1 compound each), were also detected (additional data is in **Table S2 - supplementary material**). Isoamyl acetate, banana flavor, was detected in McP and was not detected in Mc. Ethyl acetate was detected in all samples. Alcohols represent the highest percentages of detected compounds. For terpenes, compared to fruits, the compounds detected were lesser in number, which suggests the loss of these compounds during alcoholic and acetic fermentation processes. It should be noted the presence of ethyl acetate, 3-methyl-1-butanol acetate and, ethyl octanoate, in addition to other esters responsible for composing the characteristic aroma of vinegars.

3.3 Sensory profile of vinegars

The difference in flavor attributes of Jabuticaba vinegars (McP, Mc, MjP and, Mj) and commercial vinegars was detected by the E-Tongue (Fig. 2a). For sourness (AHS), there is an overlapping of points for almost all vinegars, demonstrating a similarity in this attribute between Jabuticaba vinegars and commercial vinegars. For bitterness (SCS), there is an overlap between MjP, Mj and, commercial vinegars, however, McP and Mc showed greater bitterness, which may be related to components of the pulp or seed of Jabuticaba. For sweetness (ANS), almost all vinegars showed distinct points, with greater sweetness for McP and BV, less sweetness for WWV, no sweetness for RV, and medium sweetness for the other vinegars. The sweetness brings a smoothness to the vinegar that is appreciated by the consumer. For umami (NMS), there is a greater contribution in Jabuticaba vinegars, which suggests that the flavor of these vinegars is more persistent in the mouth compared to commercial vinegars. For salinity (CTS), the profiles were close, suggesting sensory similarity in this flavor. For other complex flavors (PKS and CPS), Jabuticaba vinegars have similar profiles to RWV and BV. In general, Jabuticaba vinegars had similar flavor profiles to commercial vinegars, which makes it possible for consumers to accept them. The PCA score (Fig. 2b) shows that the E-Tongue effectively discriminates the Jabuticaba vinegars and the commercial vinegars. The first two principal components PC1 (41.57%) and PC2 (21.17%) explain 62.74% of the total system variance and all samples are differentiated. McP, Mc, and MjP are different from other vinegars. Mj overlaps with rice vinegar (RV), demonstrating similarity in terms of overall flavor. The different raw materials used in the manufacture of vinegars can explain the difference in the distribution of the data cluster.

Flash GC E-nose spectrograms of vinegars (Fig. 3a) were performed to identify correlation patterns with individual compositional variables involved in the discrimination between Jabuticaba vinegars and

commercial vinegars. Differences between samples along the abscissa axis of the 2D graphs were more significant than those along the ordinate axis. The total value of the first two PCA PCs (Fig. 3b) (PC1: 97.96% and PC2: 1.92%) was sufficient to explain the similarities between the samples. Jabuticaba vinegars showed significantly different aroma profiles compared to commercial vinegars. This indicates that the different origins of raw materials significantly affect the aroma of vinegars. Except for Mj, the other Jabuticaba vinegars are located in the same quadrant of the 2D graph, suggesting similar aroma profiles. Commercial vinegars are considerably more distant from Jabuticaba vinegars, which suggests a completely different aroma profile.

3.4 ATR-FTIR spectra and elemental composition of vinegars

The positions of the bands (considering the wavenumber) of the vinegars prepared with and without peel showed similar spectra (Fig. 4). However, some differences are observed in the intensity of some peaks. The bands 3800 – 2790 cm^{-1} and 1685 – 1550 cm^{-1}, which correspond to O–H groups of water, overlapped for the four vinegars. Phenolic compounds can be verified by the simultaneous observation of three bands: 3600 – 3200 cm^{-1} (O–H stretch), 1410 – 1320 cm^{-1} and 1260 – 1180 cm^{-1} [3]. For McP and MjP, it is verified that there is a greater stretching, but with a smaller peak compared to Mc and Mj (elaborated without the peels). Three bands corresponding to acetic acid: 3800 – 2790 cm^{-1}, 1800 – 1680 cm^{-1} and 1475 – 1230 cm^{-1} (C–H, C = O, C–O stretching and C–O–H in-plane bending) showed overlap for the first two, and maximum peak for MjP for the third, respectively. For total acids (1300 – 1000 cm^{-1}) and ethanol (1100 – 1000 cm^{-1}, C–O stretching), the maximum peaks oscillate between MjP and Mc, demonstrating that there was a difference in behavior in the fermentation process for these compounds. For esters, corresponding to bands 1700 – 1100 cm^{-1} (aliphatic and aromatic C–O and C = O stretching), there was an overlapping of peaks, indicating similarity between vinegars for these compounds. Bands 1065 – 1030 cm^{-1} correspond to sugars, fructose and, glucose (O–H, $–CH_2$) and show the highest peak of Mc [36].

As for the mineral content of the Jabuticaba vinegars, there was a predominance of potassium and calcium, about the total of minerals (Table S3 - supplementary material). However, it is necessary to consider the other micronutrients, which even with smaller representation, are important for human health, such as sulfur, phosphorus, iron, copper and, zinc, are present in vinegars.

4. Conclusion

In the present study, the phytochemical, volatile and, sensory profiles, antioxidant activity and chemical characteristics of Jabuticaba vinegars were presented. For the first time, different varieties and vinegars obtained with and without the presence of peels were compared. Vinegars showed phytochemical profiles with the same compounds, however, in different amounts. The volatile profile showed the migration of some compounds from the fruit to the vinegars, in addition to differences in the composition of the

vinegars, mainly regarding esters. The sensory profile showed similarity in flavor and difference in odor, when comparing Jabuticaba vinegars and commercial vinegars, which demonstrates that they are products with a unique aroma. A high antioxidant activity was obtained for all vinegars, which demonstrates the contribution of compounds from the pulp and peels. The vinegars presented common chemical groups for the product and the presence of important minerals for the human organism. Jabuticaba vinegars can be considered a promising alternative for the use of these fruits, which are highly perishable. In addition, they can be an economical alternative for medium and small producers, who seek to diversify the products on their farms.

Declarations

Declarations Ethics Approval and Consent to Participate: Not applicable.

Consent for Publication: Not applicable.

Conflict of Interest: The authors declare that they have no conflict of interest.

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Data Availability: All data generated and/or analyzed during this research are included in this published article and its supplementary material.

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Author Contributions

Writing—original draft preparation, methodology, validation and data curation, formal analysis and investigation, project management, A.P.K. and L.B.; methodology and validation, C.A.S., R.B.H, J.D. and, M.V.D.; validation and data curation, C.L.P., M.A.P., V.A.F.O.S. and, I.C.; writing—review and editing, C.L.P., A.P.K., L.B. and, M.V.D.; supervision and writing—review and editing, A.P.K.

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Figures

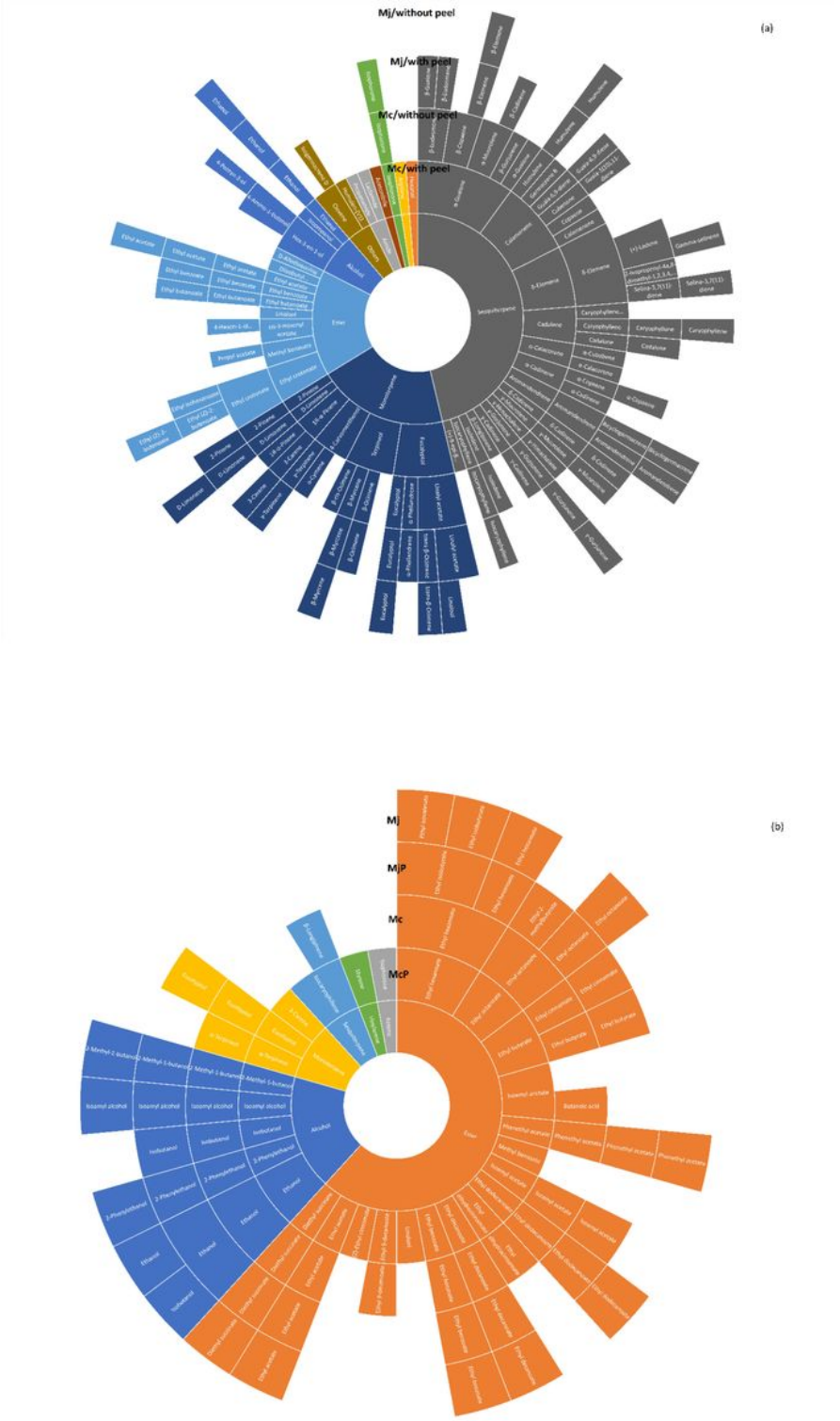


Figure 1

Sunburst diagrams showing the classification of the volatile compounds identified in fruits of *Myrciaria cauliflora* (Mart.) O.Berg and *Myrciaria jaboticaba* (Vell.) Berg(a) and, vinegars from the fruits of *Myrciaria cauliflora* (Mart.) O.Berg and *Myrciaria jaboticaba* (Vell.) Berg (b). **Note:** McP and Mc are the vinegars of the *M. cauliflora*variety, whose first step of alcoholic fermentation took place with fruits with and without

peel, respectively; MjP and Mj are the vinegars of the *M. jaboticaba* variety, whose first step of alcoholic fermentation took place with fruits with and without peel, respectively.

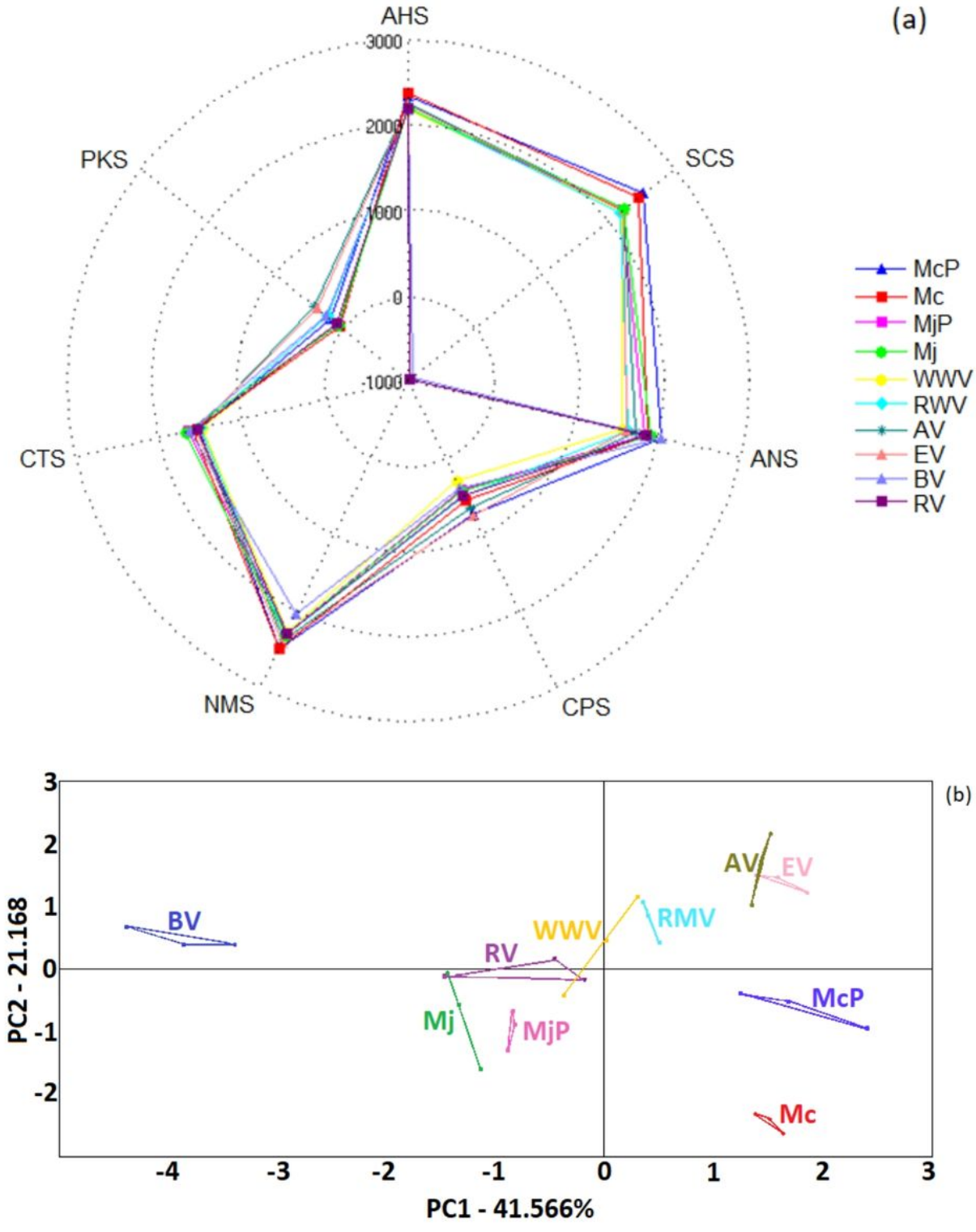


Figure 2

Flavor profiles of vinegars from the fruits of *Myrciaria cauliflora* (Mart.) O.Berg and *Myrciaria jaboticaba* (Vell.) Berg and commercial vinegars by E-Tongue (a); Principal component analysis related to the flavor

by E-Tongue of vinegars from the fruits of *Myrciaria cauliflora* (Mart.) O.Berg and *Myrciaria jaboticaba* (Vell.) Berg and commercial vinegars (b). **Note:** AHS is sourness; CTS is saltiness; NMS is umami; ANS is sweetness; and SCS is bitterness. PKS and CPS represent other complex tastes. McP and Mc are the vinegars of the *M. cauliflora* variety, whose first step of alcoholic fermentation took place with fruits with and without peel, respectively; MjP and Mj are the vinegars of the *M. jaboticaba* variety, whose first step of alcoholic fermentation took place with fruits with and without peel, respectively. WWV is white wine vinegar; RWV is red wine vinegar; AV is apple cider vinegar; EV is alcohol vinegar; BV is balsamic vinegar; and RV is rice vinegar.

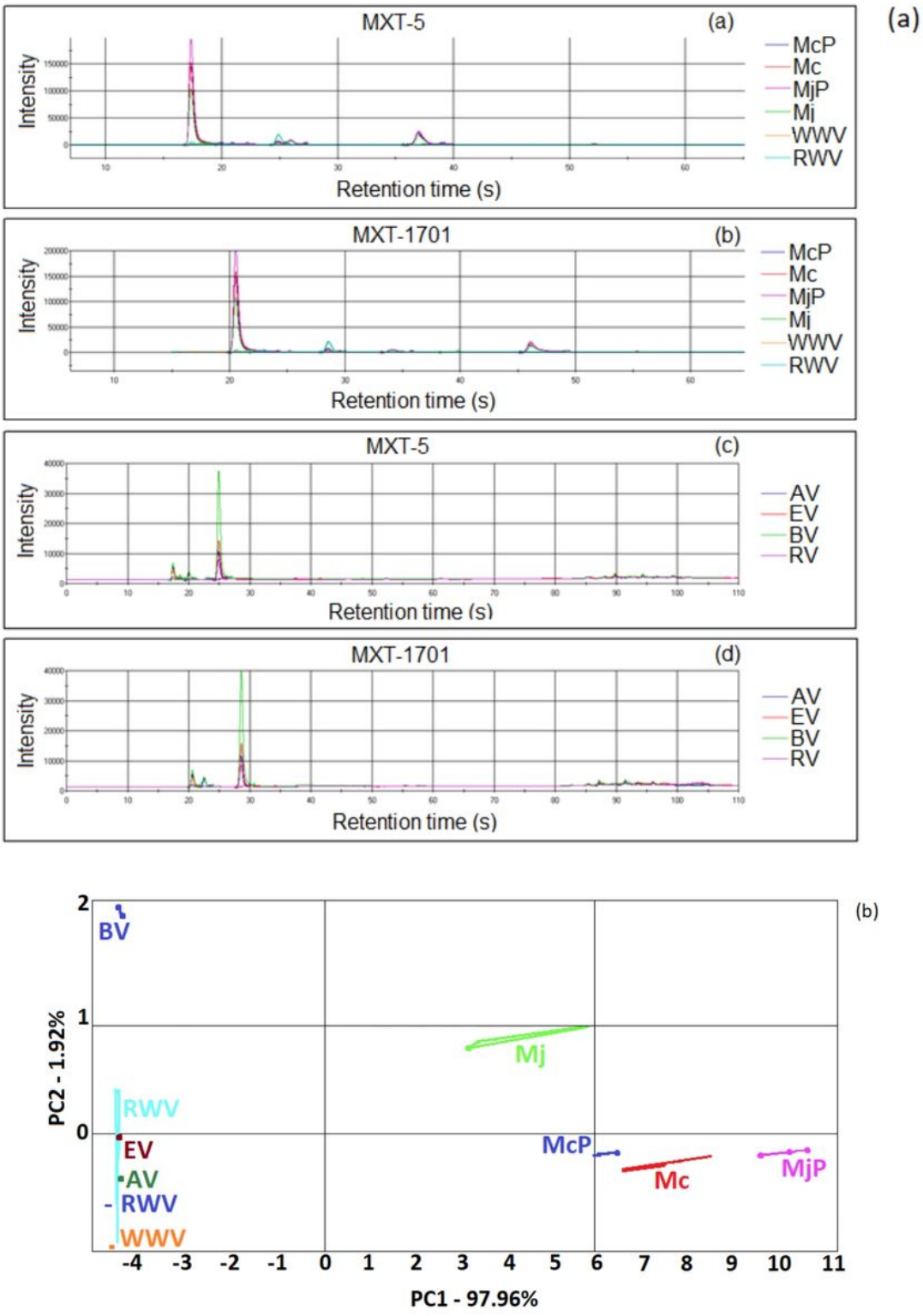


Figure 3

Overlapping of vinegars aroma detected by E-Nose (a); Principal component analysis related to the aroma by E-Nose of vinegars from the fruits of *Myrciaria cauliflora* (Mart.) O.Berg and *Myrciaria jaboticaba* (Vell.) Berg and commercial vinegars (b). **Note:** McP and Mc are the vinegars of the *M. cauliflora* variety, whose first step of alcoholic fermentation took place with fruits with and without peel, respectively; MjP and Mj are the vinegars of the *M. jaboticaba* variety, whose first step of alcoholic fermentation took place

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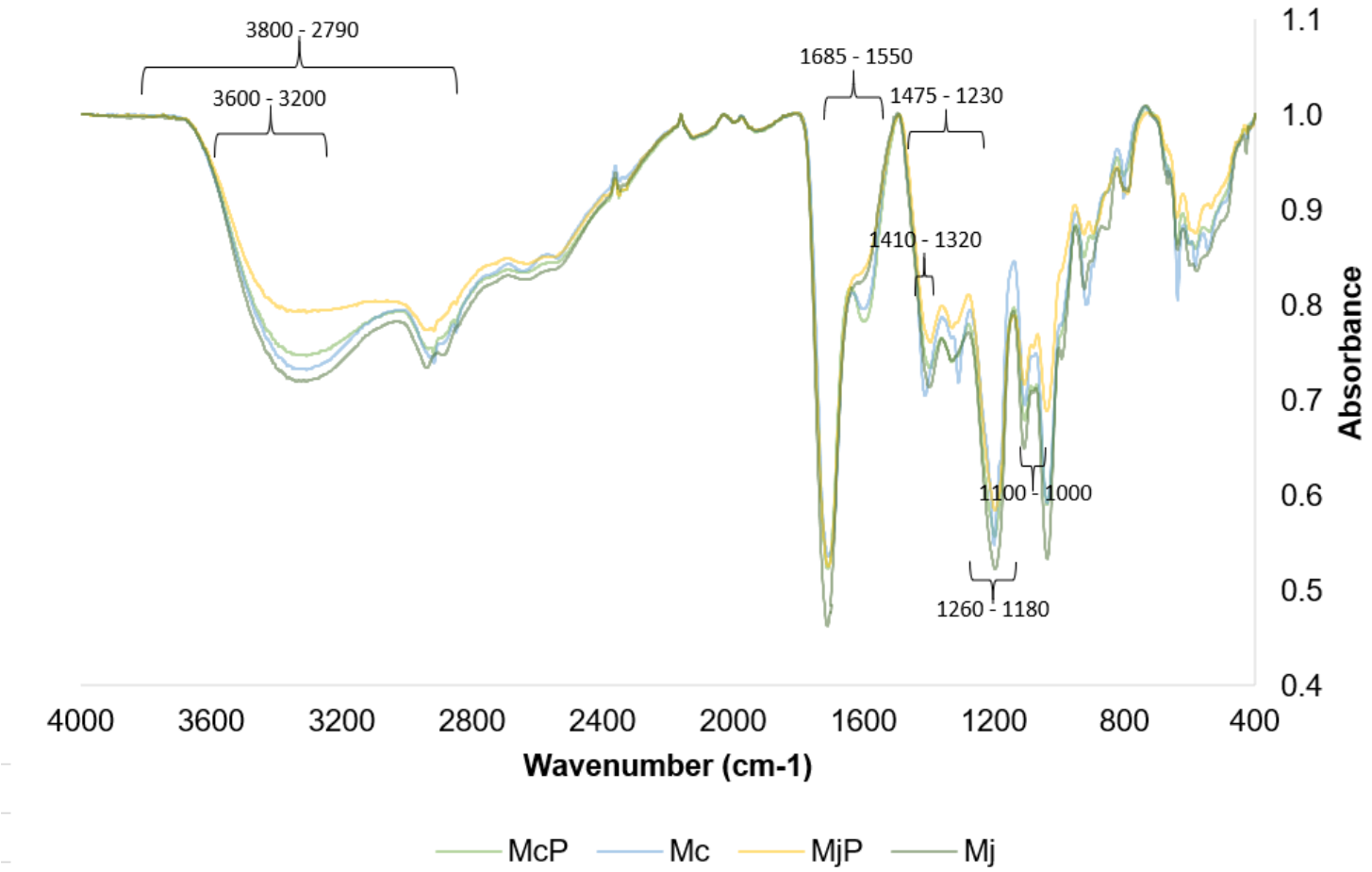


Figure 4

ATR-FTIR spectra of vinegars from the fruits of *Myrciaria cauliflora* (Mart.) O.Berg and *Myrciaria jaboticaba* (Vell.) Berg. **Note**: McP and Mc are the vinegars of the *M. cauliflora* variety, whose first step of alcoholic fermentation took place with fruits with and without peel, respectively; MjP and Mj are the vinegars of the *M. jaboticaba* variety, whose first step of alcoholic fermentation took place with fruits with and without peel, respectively.

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