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ORIGINAL PAPER

Composition and sensory descriptors of pequi oil (*Caryocar brasiliense* Camb.)

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Abstract
Pequi (*Caryocar brasiliense* Camb.) is a native species of the Brazilian Cerrado whose oil exhibits recognized bioactive potential and relevance for traditional communities engaged in its artisanal extraction. Despite reported health benefits, the oil's specially food application is limited due to low sensory acceptance, attributed to the presence of volatile compounds with unfavorable organoleptic properties. This study aimed to characterize the chemical profile of pequi oil, focusing on its fatty acid composition, volatile constituents, and carotenoid content. Oleic and palmitic acids were the predominant fatty acids. A total of 50 volatile compounds were identified, primarily esters, with hexanoic acid as the most abundant. Additionally, 34 carotenoid peaks were detected, with lutein and β-carotene as the major compounds. Most volatile constituents identified have been previously associated with negative sensory attributes in literature. These findings provide a chemical basis for the oil's sensory limitations and support future strategies to enhance its functional applications.

Keywords Pequi oil · Volatile compounds · Chromatography · Carotenoids · Fatty acids · Headspace · Aroma

Introduction

The Cerrado is a Brazilian biome in the central region of the country and is the most biodiverse tropical savanna in the world. It has a high number of endemic plant species, results from fire and drought, which has led to a gradual reduction of its vegetation cover [1]. Therefore, studies on Cerrado species are essential for its conservation and preservation. The pequi (*Caryocar brasiliense* Camb.), the main fruit of the Brazilian cerrado, is a drupaceous, globose, rough, grayish-green fruit characterized by a lobed appearance resulting from the presence of up to four large seeds, which are surrounded by a woody endocarp and adorned with thin, sharp spines. Its mesocarp is thick and divided into an outer layer and an inner layer, which is yellowish in color and exhibits a distinct aroma [2, 3]. The fruit is renowned as the "*Gold of the Cerrado*" [4].

The fruit is primarily consumed by cooking the pulp and incorporating it into traditional regional dishes. In addition to its fruit, the primary product of this species is oil. The oil extracted artisanally from its pulp and/or kernel is a source of income for local communities; however, these communities lack knowledge about the use and management of the species [5]. The commercialization of the oil, still very limited, is due to the organization of extractors into associations and cooperatives created in some regions of the country [6]. Therefore, this species is a valuable source of cultural and socioeconomic resources for several communities [7].

Pequi oil offers health benefits due to its nutritional composition, including antioxidants, anti-inflammatory, cardioprotective, hepatoprotective, antigenotoxic and anticarcinogenic activities [8–10]. Due to the numerous benefits associated with consuming pequi oil, there is a growing interest in using it for the development of new products. However, food products formulated with pequi oil have low sensory acceptance among consumers, which has become a limiting factor for the commercial expansion of these products. In a sensory evaluation of yogurts and kefir formulated with the addition of pequi oil, a prominent color and aroma characteristic of the fruit were observed, which led to low product acceptance [11]. Beers supplemented with pequi oil received a score of 6.0 (corresponding to "I liked it a little") on the 9-point hedonic scale across all evaluated parameters [12]. In a discriminative sensory assessment comparing

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traditional cheese with cheese infused with pequi oil, the formulation containing pequi oil was the least accepted, with scores of 6.7 ("I liked it a little" and "I liked it") on a 9-point hedonic scale [13].

The sensory characteristics of pequi oil are formed of several volatile compounds that contribute to negative sensory descriptors, most of which belong to the ester class, including ethyl hexanoate, ethyl octanoate, α-ocimene, and β-ocimene [14]. In this context, further studies are necessary to understand the composition of pequi oil and identify which compounds affect its sensory acceptance. Therefore, the present work aimed to obtain the composition of pequi oil to determine which compounds are responsible for the sensory descriptors present.

Materials and methods

Chemicals

The (all-E)-β-carotene (99.5%), (all-E)-β-cryptoxanthin (99.0%), (all-E)-lutein (98.0%) standards were purchased from Sigma-Aldrich (Darmstadt, Germany). The (all-E)-zeaxanthin standard was supplied by DSM Nutritional Products (Basel, Switzerland). All standards were at least 95% pure, as determined by HPLC-DAD. All other chemical salts and analytical-grade solvents were purchased from Synth (São Paulo, Brazil) or Merck (Darmstadt, Germany). For chromatographic analyses, samples and solvents were filtered using 0.22 and 0.45 µm membranes, respectively, both from Millipore.

Materials

Pequi oil was purchased from the Central do Cerrado brand, extracted in Chapada Gaúcha – MG, using the cooking method in February 2024. It was then received in an amber bottle and transported to the Sensory Analysis and Quality Control Laboratory (LASCQ) at the Federal University of Rio Grande, Rio Grande - RS, where it was stored under refrigeration (4 °C) away from light until analysis that started in June 2024.

Quality parameters

The acidity index (mg KOH/g) and peroxide index (mEq O_2/kg) of pequi oil were determined following the methodology described in the Official Methods of the American Oil Chemists' Society (American Oil Chemists Society, 1995). The iodine and saponification indexes were measured using a nuclear magnetic resonance (NMR) spectrometer (Bruker High Field, model 400 MHz Ascend, Rheinstetten, Germany) equipped with a 9.4 T magnet, corresponding to 400 MHz for ^{1}H, and a 5 mm diameter probe. To acquire the NMR spectra, 20 mg of the lipid was dissolved in 0.7 mL of $CDCl_3$ and placed into the spectrometer. A ^{1}H standard sequence was used, consisting of a 90° pulse, with an acquisition time of 9.109 s, 2.000 scans, and a spectral window of 24.03 Hz [15].

Fatty acids profile

Fatty acids were derivatized into methyl esters using the method of Metcalfe [16]. Methyl esters were analyzed using a gas chromatograph (Shimadzu, model 2010AF, Tokyo, Japan) equipped with an SP-2560 capillary column (100 mm × 0.25 mm i.d. × 0.20 µm) [17, 18]. The injector temperature was set at 250 °C, and the flame ionization detector temperature was 255 °C. The carrier gas used was N_2. The column temperature was maintained at 100 °C for 15 min, then increased to 250 °C at a heating rate of 4 °C/min and held there for 45 min. Peaks were identified by comparing the retention times of the samples with those of the fatty acid methyl ester standards (Supelco 37-component FAME Mix, Sigma-Aldrich) and quantified based on peak areas.

Profile of volatile compounds

The solid-phase microextraction (HS-SPME) [19] technique was used to extract the volatile compounds, where 2.0 g of pequi oil was weighed and stored in 25 mL headspace vials sealed with aluminum and rubber septa, then kept in a freezer at −18 °C until analysis. Subsequently, polydimethylsiloxane-divinylbenzene (PDMS-DVB, 65 µm) SPME fibers (Supelco Co., Bellefonte, PA, USA) were used to collect and concentrate the volatile compounds from the headspace of the pequi oil. The analysis was performed on a GC-2010-Plus gas chromatograph coupled with a GCMS-TQ8050 mass spectrometer (Shimadzu), equipped with a split/splitless injector, flame ionization detector, and a 30 m × 0.25 mm (i.d.) × 0.25 µm thick TRACE TR-1MS fused silica capillary column (Thermo Scientific, San Jose, CA). Helium was used as the carrier gas at a flow rate of 1.0 mL/min. The oven temperature was initially set at 40 °C (held for 3 min), then increased at 2.5 °C/min to 125 °C, followed by a temperature increase of 10 °C/min to 245 °C, which was maintained for 2 min. Mass spectra were obtained by electron impact ionization (EI) at 70 eV and scanned in full scan mode over the 30–400 m/z range. The ion source temperature was set at 200 °C. Identification of volatile compounds was achieved by comparing the mass spectra with the NIST library (2005) and calculating retention indices (IR) using n-alkane standards (C8–C40).

Table 1 Quality parameters of pequi oil

Parameter	Result
Acidity index (mg KOH/g)	4.11 ± 0.15
Peroxides value (mEq O_2/kg)	2.94 ± 0.08
Saponification value (mg KOH/g)	275.00
Iodine index (gI/100 g)	89.00

Table 2 Fatty acids profile of pequi oil

Fatty acid	Composition (%)
Myristic acid (C14:0)	0.07 ± < 0.01
Palmitic acid (C16:0)	37.21 ± 0.91
Palmitoleic acid (C16:1)	0.72 ± 0.03
Margaric acid (C17:0)	0.06 ± < 0.01
Margaroleic acid (C17:1)	0.07 ± < 0.01
Stearic acid (C18:0)	1.60 ± 0.08
Elaidic acid (C18:1 *trans*)	0.04 ± < 0.01
Oleic acid (C18:1 Cis)	58.27 ± 0.78
Linoleic acid (C18:2 *cis*)	1.18 ± 0.02
Eicosanoic acid (C20:0)	0.15 ± < 0.01
Eicosenoic acid (C20:1)	0.24 ± < 0.01
Linoleic acid (C18:3)	0.23 ± < 0.01
Docosanoic acid (C22:0)	0.05 ± < 0.01
11,14,17-Eicosatrienoic acid (C23:3)	0.04 ± < 0.01
Lignoceric acid (C24:0)	0.07 ± < 0.01
Total of unsaturated fatty acids	60.79
Total of saturated fatty acids	39.21

Carotenoids profile

Carotenoid extraction was performed using 1.2 g of sample added to 5 mL of hexane and vortexed for 1 min [20]. Next, the extract was partitioned into a mixture of ethyl ether and petroleum ether (1:1), and subjected to saponification with a 10% methanolic KOH solution for 16 h, with stirring at 84 rpm at room temperature. The saponified extract was then transferred to a mixture of ethyl ether and petroleum ether (1:1) in a separating funnel, washed with distilled water until neutral pH, and the solvent evaporated. The dry extract was stored in a nitrogen atmosphere until analysis. Carotenoid analysis by HPLC-DAD-MS/MS was conducted following the method described [21]. Carotenoid quantification was achieved through external standardization using (all-E) -lutein, (all-E) -β-carotene, (all-E) -zeaxanthin, and (all-E) -β-cryptoxanthin. Identification was performed based on UV-visible spectra, mass spectral data, comparison with standards, and literature data [22, 23].

Statistical analysis

The analysis was carried out in triplicate ($n = 3$) and expressed as mean and standard deviation. Data was treated by the Statistica 5.0 program (StatSoft Inc., Tulsa, OK, USA).

Results and discussion

Quality parameters of pequi oil

The pequi oil evaluated in this study (Table 1) had an acidity index of 4.11 mg KOH/g, which is within the recommended limit of 4 mg KOH/g for high-quality crude oils codex [24]. The oil extraction method is a key factor influencing its acidity content [25]. The peroxide index of the sample was 2.94 mEq O_2/kg, below the maximum limit of 15 mEq O_2/kg established for vegetable oils to be considered suitable for consumption [24]. These results are satisfactory, considering that the oil was obtained through cooking, an artisanal method.

The saponification index of the sample was 275 mg KOH/g, indicating that pequi oil contains a high proportion of low molecular weight fatty acids. This parameter measures the amount of KOH needed to saponify one gram of fat, reflecting the average molecular weight of the triglycerides. Consequently, higher saponification values correspond to lower molecular weights of triglycerides [26]. The iodine index of 89.00 gI/100 g suggests that pequi oil has a substantial amount of unsaturated fatty acids, as this measure indicates the degree of unsaturation in the oil [27].

When evaluating different vegetable oils of Brazilian origin, including pequi oil obtained by mechanical pressing, the following values were reported: acidity index of 5.25 mg KOH/g, peroxide index of 9.60 mEq O_2/kg, saponification index of 184.54 mg KOH/g, and iodine index of 110.02 gI/100 g [25]. Therefore, the oil in this study exhibited lower acidity, peroxide, and iodine indices, while the saponification index was higher.

Acording to Borges [28], pequi oil extracted by cooking had an acidity of 1.67 mg KOH/g, a peroxide index of 0.63 mEq O_2/kg, a saponification index of 200.55 mg KOH/g, and an iodine index of 60.11 gI/100 g. While the oil obtained through hydraulic pressing showed an acidity of 0.17 mg KOH/g, a peroxide index of 1.22 mEq/kg, a saponification index of 209.65 mg KOH/g, and an iodine index of 54.13 gI/100g [29]. Within this context, it is evident that variations in the quality indices of pequi oil reported in the literature are influenced by factors such as the extraction method employed and the geographical origin of the fruit.

Fatty acids profile

According to Tables 2 and 8 unsaturated fatty acids and 7 saturated fatty acids were observed, representing 60.79% and 39.21%, respectively, of the fatty acids profile in pequi oil. Oleic acid (C18:1 cis) was the majority acid (58.27%) followed by palmitic acid (C16:0) (37.21%). The results demonstrate that the oleic acid content in pequi oil observed

in this study is slightly higher than the values reported in the existing literature. Previous studies reported values of 38.80% oleic acid and 37.59% palmitic acid [25]; 42.47% oleic acid and 39.49% palmitic acid [29]; 52.67% oleic acid and 26.50% palmitic acid in pequi oil [30].Vegetable oils with a large amount of oleic acid in their composition are desirable for the food industry, as it gives them a thermal stability that allows them to be used in frying and cooking [31].

It is important to note that the percentage of oleic acid obtained in pequi oil was close to the value quantified in olive oil (55–80%), so it is believed that this oil can offer the same benefits to human health, as these are attributed precisely to oleic acid, such as helping to reduce cholesterol levels and protecting against cardiovascular diseases [32].

The pequi oil has a high content of saturated fatty acids, particularly palmitic acid (C16:0). Although excessive consumption should be avoided in order to prevent cardiovascular disease, moderate consumption is important for maintaining structural biological functions and storing energy [33, 34]. In addition, saturated fatty acids play a role in the food industry. Myristic, palmitic and stearic acids are used as flavoring additives in food products and pose no health risks if their daily intake levels are respected [35, 36].

The fatty acids present in pequi oil play an important role in its sensory quality. The literature shows that fat can be detected and sized by taste [37, 38]. The length of the fatty acid chain is a determining factor for its sensory characteristics [38]. Because they contain carboxylic acid groups that absorb hydrogen ions, long-chain fatty acids retain an acidic character [39]. Short-chain fatty acids are described as having a sour flavor, medium-chain fatty acids as "rough," and long-chain fatty acids with terms such as "rough" and "greasy" [40]. Additionally, long-chain fatty acids are characterized as bitter, sour, and spicy [39]. As shown in Table 2, all the fatty acids found in pequi oil are long chain, which further emphasizes the presence of sensory descriptors that negatively impact pequi oil.

Determining the profile of volatile compounds

Table 3 shows the volatile compounds identified in pequi oil, as well as their retention indices, % area and the sensory descriptors in the literature.

In the pequi oil evaluated in this study, 50 volatile compounds were identified, with 42% being esters, 24% aldehydes, 10% terpenes, 8% alcohols, 8% carboxylic acids, and 8% ketones. The essential oil of pequi exhibited a volatile profile in which 58.3% were esters and 25% were monoterpenes [14]. The variation in the identified compounds, as well as their quantities across studies in literature, is attributed to differences in the regions from which the samples originate, as well as factors such as harvesting practices, handling, and the oil extraction method [52]. Additionally, the material of the fiber used in analysis influences the compounds that are extracted, with PDMS-coated fibers—like the one used in this study—showing a greater affinity for non-polar compounds such as esters and terpenes [53]. The classes of compounds found the aroma of citrus fruits such as pequi and its oil [54].

The presence of esters and organic acids can be explained by lipid metabolism. The enzyme lipoxygenase oxidizes linolenic (18:3) and linoleic (18:2) acids, which are then cleaved by hydroperoxide lyase (HPL) to form esters (Silva et al. 2021). The ester found in the greatest quantity was hexanoic acid, described as sweaty, fermented, and vinegary, as shown in Table 3. The second most abundant ester was octanoic acid, described as oily and greasy (Table 3). Therefore, both are considered to contribute negatively to the aroma of pequi oil.

The ripeness of the fruit from which the oil was extracted influences the compounds formed, since in ripe fruit, branched amino acids undergo deamination and decarboxylation, forming aldehydes, which can subsequently be converted into alcohols and acids. When esterified, these compounds contribute to odorous volatiles. Aldehydes, alcohols, and acids directly contribute to the flavor of ripe fruit, but esters are considered to have the greatest impact on aroma [42].

In pequi oil, the aldehydes present in the greatest quantities were 5-methyl-2-furancarboxaldehyde, followed by furfural were described as toasted, roasted, boiled, caramelized, oxidized, and reminiscent of used oil (Table 3). The aldehyde class compounds identified by GC-MS in these samples are responsible for the oily smell [55]. These compounds are produced via the Maillard reaction [42]. Hexanal found in pequi oil is the main product of linoleic acid oxidation [51].

The terpenes found in pequi oil are formed via the mevalonic acid pathway (3,5-dihydroxy-3-methylvalerianic acid), which undergoes phosphorylation and decarboxylation to produce isopentenyl pyrophosphate (IPP). IPP isomerizes to dimethylallyl pyrophosphate (DMAPP), a highly reactive compound that forms geranyl pyrophosphate (GPP), leading to monoterpene formation [56]. The most abundant terpene was the monoterpene trans-β-ocimene, followed by 2,6-dimethyl-1,3,5,7-octatetraene, E, E-. These compounds have a significant impact on aroma due to their lower molar mass and higher volatility [57].

Carboxylic acids, alcohols, and ketones in pequi oil are formed through autoxidation of unsaturated fatty acids [42]. Studies on induced oxidation of oils have shown that formic and acetic acids are the primary short-chain carboxylic acids formed [58–60]. The most abundant carboxylic acid

Table 3 Volatile profile of pequi oil

Compounds [a]	Area (%) [b]	RI[c]	Sensory descriptors
Aldehydes			
Acetaldehyde	0.36	721	Spicy, sweet, ethe[41]
Pentanal	0.78	757	Woody, bitter, oily [41]
Hexanal	0.95	808	Green, green apple, cut grass, tallow, fatty [41]
Furfural	1.90	832	Toasted, boiled, roasted, caramel [42]
Heptanal	0.16	893	Oily, fatty, woody [41]
2-Furancarboxaldehyde, 5-methyl-	3.64	955	Acid, almond, burnt sugar [43]
Octanal	0.80	1001	Fatty, citrus, green, soap [41]
2-Octenal, (E)-	0.23	1054	Herbaceous, spicy [41]
Nonanal	1.58	1103	Fatty, wax, spicy, citrus, green [41]
Decanal	0.76	1206	Sweet, wax, soap, orange peel, tallow [41]
2-Decena l, (E)-	0.36	1261	Ink, fish, tallow [41]
2-Undecenal	0.11	1370	Cabbage [44]
Alcohols			
Ethanol	0.40	723	Alcohol [41]
2,3-Butanediol	0.02	797	Butter, caramelized, chlorine, creamy, fruity, pungent [43]
2-Furanmethanol	0.22	852	Burnt [43]
Butyrolactone	0.21	902	Acid, sour [39]
Carboxylic Acids			
Formic acid	3.00	725	Pungency [45]
Acetic acid	7.83	741	Fermented, Vinegar [41]
Hexanoic acid	1.28	1032	Spicy, rancid [41]
Hexanoic acid, anhydride	0.17	1295	-
Ketones			
2-Pentanone	0.12	754	Acetone, fishy, fruity, phenolic [43]
3-Penten-2-one, (E)-	1.64	774	Fish, pungency [46]
2-Pentenal, (E)-	0.32	782	Green, bitter almond [41]
2-Propanone, 1-hydroxy-	0.36	747	-
Maltol	0.30	1113	Burnt sugar [47]
Esters			
Hexanoic acid, ethyl ester	34.35	1000	Sweat, fermented, vinegar [48, 49]
Methacrylic acid, ethyl ester	0.19	843	Fruity [49]
Hexanoic acid, methyl ester	0.10	917	Acid, sour [39]
2-Hexenoic acid, ethyl ester	1.53	1043	Fatty [46]
δ-Caprolactone	0.28	1089	Sweet [50]
Hexanoic acid, propyl ester	0.30	1094	Acid, sour [39]
Heptanoic acid, ethyl ester	0.23	1098	Fatty [49]
Octanoic acid, methyl ester	0.11	1124	Oily, greasy[41]
Octanoic acid, ethyl ester	24.36	1206	Oily, greasy [41]
Ethyl (E)−2-octenoate	3.32	1248	Sweet, fruity [51]
Isopentyl hexanoate	0.46	1251	Fruity [49]
Hexanoic acid, 2-methylbutyl ester	0.20	1254	Acid, sour [39]
δ-Octalactone	0.17	1283	Sweet [50]
Propyl octanoate	0.08	1293	-
Hexanoic acid, hexyl ester	0.13	1390	Acid, sour [50]
Decanoic acid, ethyl ester	0.81	1398	Greasy [49]
Ethyl trans-2-decenoate	0.05	1452	Greasy [46]
2,4-Decadienoic acid, ethyl ester, (E, Z)-	0.02	1473	-
δ -Decalactone	0.04	1497	Cheese [46]
δ-Dodecalactone	0.01	1717	Cheese [46]
Terpenes			
1,3,8-p-Menthatriene	0.18	1120	Terbitin [46]
2,6-Dimethyl-1,3,5,7-octatetraene, E, E-	0.69	1128	-
2,4,6-Octatriene, 2,6-dimethyl-, (E, Z) -	0.41	1140	-

Table 3 (continued)

Compounds [a]	Area (%) [b]	RI[c]	Sensory descriptors
,cis-β-Ocimene	0.27	1035	Floral [44]
trans-β-Ocimene	4.21	1046	Citrus, herbaceous, floral [46]

[a] Compound list according to identification by comparing the mass spectral with the NIST library (2005). [b] Relative percentage of peak area of each compound to that standard. [c] RI: Retention indices calculating using n-alkane standards (C8-C40)

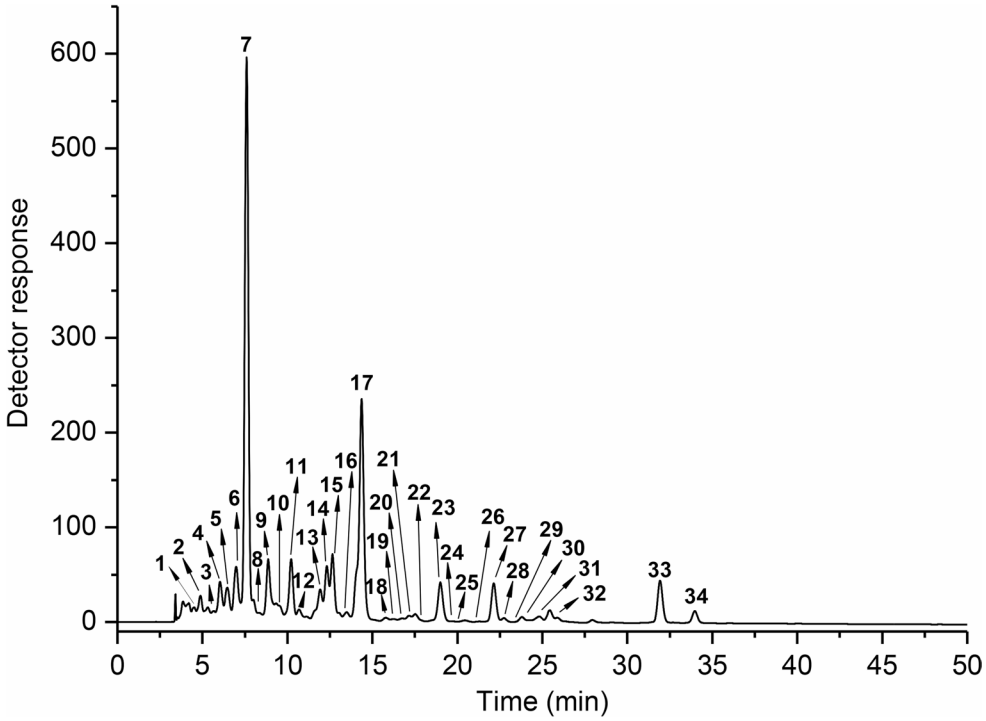


Fig. 1 The chromatogram (processed at 450 nm) of the carotenoids obtained from pequi oil

detected was acetic acid, followed by formic and hexanoic acids. Notably, acetic acid was the second most prevalent compound in this analysis. As shown in Table 3, the acid acetic is described as characteristic of cooked pineapple, medicinal, and undesirable [41]. The formic acid is described as intense, irritating, and sour (Table 3). Overall, the volatile profile of pequi oil comprises compounds produced via plant metabolism as well as those formed during oil oxidation. Consequently, extraction methods and storage conditions are crucial parameters influencing the formation of volatile compounds.

Carotenoid profile

The column allowed the separation of 34 carotenoids, some of which could not be identified by HPLC-DAD-MS/MS (Fig. 1). The MS/MS experiments confirmed the assignment of the protonated molecule ($[M+H]^+$) of all identified peaks through the expected fragments for the polyenoic chain of carotenoids and functional groups (Table 4). Although fragmentation has occurred, the MS/MS allowed the unambiguous assignment of some functional groups due to specific losses of the protonated molecule.

The Peaks 1–13 and 15–16 (Fig. 1) were quantified as all-trans-lutein (48.75 µg/g). Peaks 7, 9, 11, and 17 were named as lutein-like carotenoids because they exhibited some spectroscopic characteristics like lutein [22]. Peaks 14, 17, and 23 were quantified as all-trans-zeaxanthin (12.67 µg/g); peaks 18–20, 27–28, and 31 were quantified as all-trans-β-cryptoxanthin (5.39 µg/g); peaks 21–22, 24–26, 29–30, and 32–34 were quantified as all-trans-β-carotene (20.54 µg/g). Peaks 19–20, 21–22, and 24–26 appeared as distinct peaks because they exhibited most of the different spectroscopic characteristics, although the fragment ions were identical (Table 4). The chromatogram with the peaks obtained is illustrated in the Fig. 1.

Other studies have reported amounts of all-trans-zeaxanthin (15.32%), all-trans-β-cryptoxanthin (18.79%), all-trans-β-carotene (20.27%), and 9-cis-β-carotene (5.00%) in pequi oil [61]. Were previously reported 4.37 µg/g of all-trans-zeaxanthin, 36 µg/g of all-trans-β-cryptoxanthin, and 7.20 µg/g of all-trans-β-carotene [62]. According to the same authors, several factors influence the carotenoid profile of pequi oil, such as fruit ripeness and degradation processes that occur after oil extraction, which are caused by exposure to light.

Table 4 Identification and quantification of carotenoids of pequi oil

Peak	Carotenoid	$[M+H]^+$ (m/z)	Fragmentions (m/z)	Concentration (μg/g)
1	cis-auroxanthin[a]	601	583 $[M+H–18]^+$, 565 $[M+H–18–18]^+$, 221	0.61 ± 0.02
2	Not identified 1[a]	n.d.	n.d.	1.20 ± 0.02
3	Not identified 2[a]	n.d.	n.d.	1.33 ± 0.19
4	all-trans-lutein[a]	n.d.	n.d.	1.81 ± 0.09
5	Not identified 3[a]	569	551 $[M+H–18]^+$, 477 $[M+H–92]^+$	1.71 ± 0.06
6	Neochrome[a]	601	583 $[M+H-18]^+$, 565 $[M+H-18-18]^+$, 547 $[M+H-18-18-18]^+$	2.75 ± 0.08
7	Lutein-like[a]	n.d.	**583 $[M+H-18]^+$** → 565 $[M+H-18-18]^+$, 547 $[M+H-18-18-18]^+$	22.18 ± 0.68
8	Not identified 4[a]	n.d.	n.d.	1.18 ± 0.02
9	cis-lutein like[a]	n.d.	**583 $[M+H-18]^+$** → 565 $[M+H-18-18]^+$, 547 $[M+H-18-18-18]^+$	3.10 ± 0.13
10	all-trans-lutein[a]	n.d.	n.d.	1.30 ± 0.13
11	cis-lutein like[a]	n.d.	**583 $[M+H-18]^+$** → 565 $[M+H-18-18]^+$, 547 $[M+H-18-18-18]^+$	2.96 ± 0.11
12	all-trans-auroxanthin[a]	601	583 $[M+H-18]^+$, 565 $[M+H-18-18]^+$, 547 $[M+H-18-18-18]^+$	0.94 ± 0.10
13	Mutatoxanthin epimer[a]	585	567 $[M+H-18]^+$, 549 $[M+H-18-18]^+$, 493 $[M+H-92]^+$, 221	1.93 ± 0.09
14	cis-zeaxanthin[b]	569	551 $[M+H-18]^+$, 533 $[M+H-18-18]^+$, 477 $[M+H-92]^+$	1.93 ± 0.03
15	Mutatoxanthin epimer[a]	585	567 $[M+H-18]^+$, 549 $[M+H-18-18]^+$, 493 $[M+H-92]^+$, 221	3.24 ± 0.15
16	Not identified 5[a]	569	551 $[M+H-18]^+$, 533 $[M+H-18-18]^+$	0.58 ± 0.05
17	cis-lutein like + all-trans-zeaxanthin[b]	583/569	565 $[M+H-18]^+$, 547 $[M+H-18-18]^+$ 551 $[M+H-18]^+$, 533 $[M+H-18-18]^+$, 477 $[M+H-92]^+$	8.99 ± 0.25
18	5,8-epoxy-β-cryptoxanthin[c]	569	551 $[M+H-18]^+$, 533 $[M+H-18-18]^+$, 221	0.52 ± 0.08
19	cis-β-cryptoxanthin[c]	553	535 $[M+H-18]^+$, 460 $[M-92]^+$	0.43 ± 0.07
20	cis-β-cryptoxanthin[c]	553	535 $[M+H-18]^+$, 460 [M-92]+	0.47 ± 0.07
21	all-trans-phytoene + not identified 6[d]	545	503, 489, 475, 463 n.d.	10.46 ± 0.23
22	cis-phytoene[d]	545	503, 489, 475, 463	0.93 ± 0.19
23	9-cis-zeaxanthin[b]	569	551 $[M+H-18]^+$, 533 $[M+H-18-18]^+$, 495 $[M+H-56-18]^+$, 477 $[M+H-56-18-18]^+$	1.75 ± 0.05
24	cis-phytofluene[d]	543	461 $[M+H-82]^+$, 393, 337	0.76 ± 0.19
25	cis-phytofluene[d]	543	461 $[M+H-82]^+$, 393, 337	0.80 ± 0.20
26	cis-phytofluene[d]	543	461 $[M+H-82]^+$, 393, 337	0.64 ± 0.19
27	all-trans-β-cryptoxanthin + all-trans-phytofluene[c]	553/543	535 $[M+H-18]^+$, 460 $[M-92]^+$ 461 $[M+H-82]^+$, 393, 337	2.87 ± 0.09
28	Not identified 7[c]	n.d.	n.d.	0.45 ± 0.09
29	cis-phytofluene[d]	543	461 $[M+H-82]^+$, 393, 337	0.84 ± 0.18
30	5,8-epoxy-carotene[d]	553	535 $[M+H-18]^+$, 205	0.85 ± 0.17
31	9-cis -β-cryptoxantine[c]	553	535 $[M+H-18]^+$, 461 $[M+H-92]^+$	0.65 ± 0.08
32	13-cis-β-carotene[d]	537	444 $[M-92]^+$	1.38 ± 0.16
33	all-trans-β-carotene[d]	537	444 $[M-92]^+$	2.72 ± 0.14
34	9-cis-β-carotene[d]	537	444 $[M-92]^+$	1.16 ± 0.18
	Total			85.14 ± 1.4

[a] quantified as all-trans-lutein; [b] quantified as all-trans-zeaxanthin; [c] quantified as all-trans- β-cryptoxanthin; [d] quantified as all-trans-β-carotene; n.d.: not detected; Ions fragmented in bold indicate fragmentation *in source*

Carotenoids offer numerous health benefits, including immune enhancement due to their antioxidant and anti-inflammatory activities, and they can serve as immune protectors against diseases such as COVID-19 and other related illnesses [63]. β-carotene has been linked to protection against diseases like Alzheimer's and various cancers [64], and together with β-cryptoxanthin, it has been associated with increased production of retinoic acid [65]. Although zeaxanthin does not have provitamin A activity, it possesses antioxidant properties that are important for maintaining eye health [66]. Lutein, the predominant carotenoid in the pequi oil evaluated, has

demonstrated benefits against ocular, neurological, cardiac, dermatological diseases, microbial infections, and bone degradation [67].

The carotenoid content in vegetable oils is an important sensory quality parameter because it influences color [68]. Lutein is described as yellow-orange [69], like β-carotene [70] and zeaxanthin [71]. Cryptoxanthin imparts a reddish hue [72]. Studies on carotenoid degradation in carrots have shown that as carotenoids degrade, there is an increase in C13-norisoprenoids and a decrease in terpenes and sesquiterpenes responsible for the "fresh" aroma. Additionally, sensory attributes such as "color," "carrot smell," "sweet taste," and "fruity taste" decrease, while attributes like "darkening," "earthy smell," and "earthy taste" become more prominent. Consequently, given the significant carotenoid content in pequi oil, it is believed that their degradation also affects its sensory properties.

Conclusions

In conclusion, the pequi oil extracted through the conventional cooking method meets the quality parameters required for vegetable oils, as indicated by the evaluated indexes. The fatty acid profile showed oleic acid as the major component, followed by palmitic acid. Its long-chain content was related to sensory descriptors such as rough, greasy, sour and spicy. The volatile profile of pequi oil showed 50 volatile compounds, of which 42% were from the ester class, with hexanoic and octanoic acids being the most abundant, described in the literature as sweet, fermented, vinegary, oily and fatty. The carotenoids found in the largest quantity were all-trans-lutein and all-trans-β-carotene and their degradation was also related to negative sensory descriptors. Therefore, it is observed that the application of pequi oil in food matrices directly will not have good sensory acceptance, because the raw material is formed by compounds with negative sensory descriptors, requiring the development of delivery systems for the oil, such as encapsulation.

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Declarations

Competing interests Authors declare that they have no competing interests.

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