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Investigaciones en pecán en Sudamérica

Bioactive Compounds and Physicochemical Characteristics of Pecan Nut Cultivars Grown in Southern Brazil

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Abstract

Pecan nuts are oilseeds, well recognized for their constituent unsaturated fatty acids. Pecan cultivation in the state of Rio Grande do Sul has increased in recent years, warranting greater information on the composition of this oilseed. Therefore, the present study aimed to evaluate the physicochemical characteristics, fatty acid profile, and bioactive compounds of the pecan cultivars grown in the southern region of Rio Grande do Sul. Fruit samples from seven cultivars and a selection of pecan trees were subjected to experiments to evaluate the color, centesimal composition, oil content, acidity, peroxide value, specific extraction coefficient, composition of fatty acids, tocopherols, and phenolic compounds. The resulting data were analyzed statistically using Tukey's test. The 'Elliot' cultivar was revealed to have the greatest lipid content with 77.08%. The 'Shawnee' cultivar exhibited higher oxidation levels, represented by the high acidity and greater peroxide content in the samples. The 'Elliot' cultivar presented the highest gamma-tocopherol index, while the 'Success' cultivar presented the highest delta-tocopherol index. The 'Shawnee', 'Elliot', and 'Mohawk' cultivars exhibited higher amounts of saturated fatty acids, monounsaturated fatty acids, and polyunsaturated fatty acids, respectively. The main phenolic compounds identified and quantified in the pecan nut samples were gallic acid, procyanidin type B, (+)-catechin, methyl gallate, ellagic acid pentose, ellagic acid, and methylated ellagic acid pentose. The fatty acid profile varied with the cultivars, although unsaturated fatty acids remained predominant, indicating better nutritional quality and a greater oxidation potential.

Keywords: pecan nut, fatty acid profile, phenolic compounds, tocopherols, physicochemical properties

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Compuestos bioactivos y características fisicoquímicas de cultivares de nuez pecana cultivados en el sur de Brasil

Resumen

Las nueces pecanas son semillas oleaginosas, muy conocidas por la cantidad de ácidos grasos insaturados en su composición. En los últimos años, el cultivo de nuez pecanera aumentó en el estado de Río Grande del Sur y, con ello, se vio la necesidad de cualificar el conocimiento sobre la composición de este alimento. El objetivo de este estudio fue evaluar las características fisicoquímicas, el perfil de ácidos grasos y los compuestos bioactivos de cultivares de nuez pecana cultivados en el sur de Río Grande del Sur. Para realizar este experimento, se recolectaron muestras de frutos de siete cultivares y una selección de árboles de nuez pecanera, en las que se realizaron análisis de color, composición centesimal, contenido de aceite, acidez, índice de peróxidos, coeficiente de extracción específico, composición de ácidos grasos, tocoferoles y compuestos fenólicos, analizados estadísticamente mediante la prueba de Tukey. Los resultados mostraron que el cultivar 'Elliot' se destacó en la cantidad de lípidos con 77,08 %. El cultivar 'Shawnee' mostró mayores niveles de oxidación, representados por la alta acidez y el contenido de peróxido de la muestra. El cultivar 'Elliot' tuvo el índice de gamma-tocoferol más alto y el cultivar 'Success', el índice de delta-tocoferol más alto. Los cultivares 'Shawnee', 'Elliot' y 'Mohawk' mostraron mayores cantidades de ácidos grasos saturados, ácidos grasos monoinsaturados y ácidos grasos poliinsaturados, respectivamente. Además, los principales compuestos fenólicos identificados y cuantificados en las muestras de nuez pecana fueron ácido gálico, procianidina tipo B, (+)-catequina, galato de metilo, ácido pentosa elágico, ácido elágico y ácido pentosa elágico metilado. Aunque existe variación en el perfil de ácidos grasos entre cultivares, los ácidos grasos insaturados predominaron, lo que indica una mejor calidad nutricional, pero también un mayor potencial de oxidación.

Palabras clave: nuez pecana, perfil de ácidos grasos, compuestos fenólicos, tocoferoles, propiedades fisicoquímicas

Compostos bioativos e características físico-químicas de cultivares de noz-pecã cultivadas no sul do Brasil

Resumo

A noz-pecã é uma oleaginosa, muito conhecida pela quantidade de ácidos graxos insaturados em sua composição. Nos últimos anos o cultivo de noz-pecã vem aumentando no estado do Rio Grande do Sul e com isso percebeu-se a necessidade de qualificar o conhecimento sobre a composição deste alimento. O objetivo deste estudo foi avaliar as características físico-químicas, perfil de ácidos graxos e compostos bioativos de cultivares de noz-pecã cultivadas no sul do Rio Grande do Sul. Para a realização deste experimento, foram coletadas amostras de frutos de sete cultivares de nogueira-pecã onde realizou-se análises de coloração, composição centesimal, teores de óleo, acidez, índice de peróxidos, coeficiente de extração específica, composição de ácidos graxos, tocoferóis e compostos fenólicos, analisados estatisticamente pelo teste de Tukey. Os resultados demonstraram um destaque da cultivar 'Elliot' na quantidade de lipídios com 77,08%. A cultivar 'Shawnee' apresentou maiores níveis de oxidação, representados pelo alto teor de acidez e peróxidos da amostra. A cultivar 'Elliot' foi a que teve maior índice de gama-tocoferol e a cultivar 'Success' que apresentou maior índice de delta-tocoferol. As cultivares 'Shawnee', 'Elliot' e 'Mohawk' apresentaram maiores quantidade de ácido graxo saturado, ácidos graxos monoinsaturados e ácido graxo polinsaturados, respectivamente. Além disso, os principais compostos fenólicos identificados e quantificados nas amostras de nozes pecã foram os ácido gálico, procianidina tipo b, (+)-catequina, galato de metila, ácido elágico pentose, ácido elágico e ácido elágico pentose metilado. Embora haja variação no perfil de ácidos graxos entre cultivares, os ácidos graxos insaturados foram predominantes, indicando melhor qualidade nutricional, mas também maior potencial de oxidação.

Palavras-chave: noz-pecã, perfil de ácidos graxos, compostos fenólicos, tocoferóis, propriedades físico-químicas

1. Introduction

Pecan nut (*Carya illinoinensis*) cultivation in Brazil is primarily concentrated in the southern states, with the state of Rio Grande do Sul accounting for the largest cultivation area. In the 2022/2023 season, global pecan nut production reached 154,266 tons, with Mexico and the United States leading worldwide production. During the same period, Brazil ranked fourth globally, with a record production of 1,400 tons (International Nut and Dried Fruit Council, 2023).

The Brazilian Ministry of Agriculture and Livestock (MAPA) has registered 42 pecan cultivars currently grown in the country (Ministério da Agricultura, Pecuária e Abastecimento, n.d.). Among these, 17 cultivars are cultivated in Rio Grande do Sul, with 'Barton', 'Melhorada', 'Imperial', 'Importada', 'Jackson', and 'Shawnee' being the predominant varieties in the region (Crosa et al. 2020). The continuous increase in production and the growing popularity of pecans are attributed to their status as a preferred natural food. This preference is largely due to the health benefits associated with pecan consumption.

Pecans are rich in phenolic compounds, monounsaturated and polyunsaturated fatty acids, phytosterols, tocopherols, and micronutrients that contribute to reducing the risk of various diseases (Fronza et al., 2018; Siebeneichler et al., 2023). The primary phytochemicals found in pecans include ellagic acid, gallic acid, and catechin (Jia et al., 2023; Villasante et al., 2019). These compounds are naturally produced by plants to defend against fungal and bacterial pathogens. When consumed by humans, they contribute to the control of oxidative stress due to their antioxidant properties (Bottari et al., 2017; McKay et al., 2018).

Daily consumption of pecans has been shown to lower blood insulin levels, owing to the presence of polyunsaturated fats and phytochemicals, thereby offering protection against the development of diabetes mellitus and cardiovascular diseases (McKay et al., 2018). However, the high content of polyunsaturated fatty acids in pecans also makes them susceptible to oxidation over time, leading to undesirable odors and flavors (Ferrari et al., 1998).

Understanding the nutritional composition of pecan nuts is important for improving cultivation and breeding practices, particularly among family farmers in the region. It also contributes to the development of new strategies for kernel utilization and commercialization, adding value to local agriculture (Martins et al., 2017).

The quality of pecan nuts is influenced by several factors related to orchard and postharvest management. Among these, cultivar selection has a direct impact on the nutritional composition of the nuts. Due to their high oil content, particularly in unsaturated fatty acids, lipid oxidation is a significant concern during storage (Siebeneichler et al., 2023).

This study aimed to evaluate the physicochemical composition, determine the fatty acid profile, and identify the main bioactive compounds present in pecan cultivars grown in southern Brazil.

2. Materials and Methods

2.1 Sample Collection and Preparation

Pecan nuts used in this study were obtained from a commercial orchard located in the municipality of Canguçu, in the state of Rio Grande do Sul, Brazil. The orchard was established in 2009, with a high planting density of 9 × 7 m between trees. Ten kilograms of each cultivar were harvested in April 2021 at the optimal harvest point. Samples included the cultivars 'Barton', 'Desirable', 'Elliot', 'Farley', 'Mohawk', 'Shawnee', 'Success', and a local selection designated as 'Seleção P' (nursery origin).

The harvested nuts were dried in a forced-air oven at 40 °C until a moisture content below 8% was achieved. Moisture was monitored using a rapid moisture tester (Grain Moisturemeter, Central Brasil). The dried nuts were stored in Styrofoam boxes and transported to the Instituto Tecnológico em Alimentos para a Saúde (ITT Nutrifor) for nutritional and quality analyses. For each cultivar, one kilogram of nuts was selected. The shells were removed and discarded, and the kernels (~500 g per cultivar) were ground in a food processor for 1 min, then stored at –20 ºC until analysis.

2.2 Physicochemical Analysis

2.2.1 Color

Color was measured using the CIE-L*ab** system with a colorimeter (Minolta Chromometer Model CR 300). The L* value represents lightness (L* = 0 indicates black; L* = 100 indicates white), while a* and b* represent the chromatic coordinates. The hue angle (°Hue) was calculated as: °Hue = $\tan^{-1}$(b*/a*). Color parameters were determined in 10 whole kernels per cultivar.

2.2.2 Proximate Composition

Moisture, ash, protein, lipids, and carbohydrate (by difference) contents were determined following AOAC methods (Association of Official Analytical Chemists [AOAC], 2012). Results are expressed as percentages.

2.3 Chemical Properties of Pecan Oil

2.3.1 Oil Extraction

Oil was extracted using the Bligh and Dyer method, involving cold extraction with chloroform, methanol, and water to form a two-phase system (AOAC, 2012).

2.3.2 Acidity

Oil acidity was measured by dissolving the sample in an ethyl ether:ethanol (2:1, v/v) solution (1:10 w/v oil:solvent ratio), adding three drops of 1% phenolphthalein, and titrating with 0.1 N KOH, according to AOCS methodology (American Oil Chemists' Society [AOCS], 2012). Results are expressed as mg KOH/g oil.

2.3.3 Peroxide Value

A 5 g oil sample was mixed with 30 mL of acetic acid:chloroform (3:2, v/v), followed by 0.5 mL saturated potassium iodide. The mixture was stored in the dark for 1 minute, then 30 mL of distilled water and 0.5 mL of 1% starch solution were added. The sample was titrated with 0.1 N sodium thiosulfate until color disappearance. Results are expressed in meq O_2/kg sample (AOCS, 2012).

2.3.4 Specific Extinction Coefficient at 232 nm and 270 nm

Clean, filtered oil (100 mg) was dissolved in isooctane in a 10 mL volumetric flask. Absorbance at 232 nm and 270 nm was measured using a spectrophotometer. Specific extinction coefficients were calculated according to AOCS guidelines (AOCS, 2012).

2.3.5 Fatty Acid Composition

The fatty acid composition of each pecan oil sample was determined using gas chromatography-mass spectrometry (GCMS). The method described by COI (International Olive Council, 2015) was adopted for this determination. The transesterification reaction was achieved by mixing 0.1 g of the sample, 2 mL of hexane, and 0.2 mL of methanolic potassium hydroxide (2 M) under vigorous stirring for 30 s. The upper layer containing

methyl esters was collected and injected into the gas chromatography equipment. A Shimadzu QP2010 Ultra GC-MS equipped with AOC-20i autoinjector and NIST 2011 mass spectral library was the equipment used. The injected sample volume was 1 µL. The injector temperature was 200 °C, and split mode was used. Helium was used as the carrier gas at a flow rate of 1.78 mL min^{-1} and linear velocity as the flow control mode. SP 2380 (60 m × 0.25 mm, 0.20 µm) was the capillary column. The temperature gradient was as follows: at 78 °C for 6.5 min, increased at a rate of 60 °C min^{-1} to 180 °C for 13.44 min, followed by an increase at a rate of 35 °C min^{-1} to 280 °C, which was maintained for 5.5 min. The ion source temperature as well as the interface temperature was set to 200 °C. The mass scan range was from 35 to 500 m/z, and 0.3 scans s^{-1} were performed. Fatty acid methyl esters were identified through comparison with the retention times of the reference standards, and the results were expressed as the relative percentage of fatty acids.

2.3.6 Tocopherols

In a 5 mL volumetric flask, 150 mg of oil was added, and the volume was made up using HPLC-grade isopropanol. The mixture was shaken gently and then transferred to microcentrifuge tubes for centrifugation at 8600 g for 6 min. The resulting supernatant was filtered through a 0.22 µm nylon membrane (AllCrom, St. Louis, MO, USA) and then injected into liquid chromatography equipment for the determination of the tocopherol content. Shimadzu liquid chromatograph equipped with a fluorescence detector system and a CLC-ODS reversed-phase column (3.9 cm × 150 mm × 4 µm) was the equipment. The analyses were performed under the following chromatographic conditions: injection volume, 10 µL; flow rate, 1 mL min^{-1}; excitation wavelength, 290 nm; emission wavelength, 330 nm. The initial mobile phase comprised acetonitrile:methanol:isopropanol 50:40:10 (v/v/v) for 10 min, changed linearly to acetonitrile:methanol:isopropanol (30:65:5, v/v/v) from 10 min to 12 min, and then returning linearly to the initial mobile phase until 15 min. The identification and the quantification of tocopherols were performed using the external calibration curves α, γ, and δ-tocopherol. The result data were expressed as mg 100 g^{-1}.

2.4 Phenolic Compounds

2.4.1 Extraction

Defatted samples (5 g) were extracted with 50 mL of 80% methanol in an ultrasonic bath for 30 min, followed by centrifugation at 5000 rpm for 10 min. The supernatant was used for analysis.

2.4.2 Identification and Quantification of Individual Phenolic Compounds

The phenolic compounds in the samples were identified using Shimadzu UHPLC (Kyoto, Japan) equipped with quaternary pumps (LC-30AD), an online degasser (DGU-20A3R), an automatic injector (SIL-30AC) programmed for 20 µL injection, and a DAD detector (Shimadzu, SPD-M20A) connected in series to a mass spectrometer with an electrospray ionization (ESI) source and a quadrupole-time-of-flight (QTOF) analyzer (Impact HD, Bruker Daltonics, Bremen, Germany). The separation of the phenolic compounds was performed on a Shimpack XR-ODS III column (50 mm × 2.1 mm × 1.6 µm) using acidified water (0.1% formic acid) and acidified methanol (0.1% formic acid) at a flow rate of 0.3 mL/min at 30 ºC. The elution gradient was as follows: 0–90% B, 0–5 min; 90% B, 5–7 min; 5% B, 7–10 min; maintained for 5 min for pressure stabilization. The injection volume was 5 µL. The mass spectra acquisition conditions were as follows: scanning range from 100 to 1500 m/z; negative ionization mode; capillary voltage, 3000 V; drying gas temperature and flow, 310 °C and 8 L min^{-1}, respectively; nebulizer gas pressure, 30 psi; MS2, automatic mode with fragmentation energy ranging from 35 to 50 eV. The separated phenolic acids were identified by comparing the UV-vis spectral profiles, the accurate mass values, and the fragmentation characteristics using the information available for the analytical standards and that in online databases (FooDB, Metlin). Quantification was performed using the available analytical standards.

2.5 Statistical Analysis

Results were expressed as mean ± standard deviation. Statistical differences among cultivars were analyzed by one-way ANOVA, followed by Tukey's post hoc test ($p < 0.05$), when applicable.

3. Results

3.1 Physicochemical Properties

The colorimetric profiles of the different pecan cultivars are presented in Table 1. Regarding lightness (L*), the darkest cultivar was 'Barton' (L* = 46.9), while the lightest was 'Shawnee' (L* = 52.2). The a* value, which represents the red-green axis, was highest for the 'Seleção P' and 'Mohawk' cultivars (a* = 9.0), whereas the 'Desirable' cultivar exhibited the lowest a* value (a* = 6.9). The b* value, which corresponds to the yellow-blue axis, was highest for 'Shawnee' (b* = 18.6) and lowest for 'Barton' (b* = 13.8).

Chroma (C*), which indicates color intensity or saturation, was highest in 'Seleção P' (C* = 20.2) and lowest in 'Barton' (C* = 15.3). Higher chroma values suggest more vivid and saturated colors, whereas lower values indicate duller, more grayish tones.

The hue angle (ºHue), which defines the dominant color perception, ranged from 60.0° in 'Mohawk'–indicating a more reddish hue– to 67.1° in 'Shawnee', reflecting a more yellowish hue.

Table 1. Color parameters (L*, a*, b*, Chroma, and Hue angle) of seven pecan cultivars and one selected genotype (*'Seleção P'*) grown in the municipality of Canguçu, Rio Grande do Sul, Brazil

Cultivar	L*	a*	b*	Chroma	ºHue	Color palette
Barton	46.9 ± 2.5 ^{d}	6.7 ± 0.6^{d}	13.8 ± 1.1^{d}	15.3 ± 1.2 ^{b}	64.0 ± 1.7^{abc}	
Desirable	48.3 ± 2.9^{bcd}	6.9 ± 0.8^{d}	14.6 ± 3.2^{bcd}	16.2 ± 3.1^{b}	64.4 ± 4.1^{abc}	
Elliot	51.3 ± 1.5 ^{ab}	8.1 ± 0.5^{abc}	18.3 ± 1.1^{ab}	20.0 ± 0.9^{a}	65.9 ± 2.3^{ab}	
Farley	47.4 ± 1.2 ^{cd}	7.7 ± 0.7 ^{cd}	14.3 ± 1.8^{cd}	16.2 ± 1.9^{b}	61.7 ± 1.1^{bc}	
Mohawk	49.4 ± 1.8 ^{abcd}	9.0 ± 0.3^{a}	15.7 ± 1.8^{abcd}	18.1 ± 1.6^{ab}	60.0 ± 2.4^{c}	
Seleção P	50.9 ± 2.5 ^{abc}	9.0 ± 0.9 ^{ab}	18.1 ± 3.4^{abc}	20.2 ± 3.4^{a}	63.3 ± 3.2^{abc}	
Shawnee	52.2 ± 2.3 ^{a}	7.8 ± 0.7 ^{bcd}	18.6 ± 2.0^{a}	20.1 ± 1.9^{a}	67.1 ± 2.4^{a}	
Success	48.1 ± 0.8^{bcd}	8.2 ± 0.3^{abc}	15.0 ± 0.8^{abcd}	17.1 ± 0.7^{ab}	61.4 ± 1.3^{bc}	

Values are expressed as mean ± standard deviation (n = 3). Means followed by the same letter in the same column do not differ significantly according to Tukey's test ($P < 0.05$).

Table 2 presents the proximate composition of the different pecan cultivars. The highest moisture content was observed in the 'Success' cultivar (8.33%), whereas 'Barton' exhibited the lowest moisture content (2.95%), a value lower than that previously reported in the literature, which ranged from 3% to 6% (Tan et al., 2025). Moisture content is a critical factor for kernel preservation, as higher moisture levels can promote fungal growth.

The highest protein content was also recorded for the 'Success' cultivar (9.61%), followed by 'Seleção P' (8.95%). Regarding lipid content, the 'Elliot' cultivar exhibited the highest value, averaging 77.08 g/100 g.

Ash content ranged from 1.52% in the 'Desirable' cultivar –the lowest value observed– to 1.75% in the 'Farley' cultivar. Carbohydrate content varied considerably among the cultivars, with 'Barton' presenting the highest value (31.77 g/100 g) and 'Success' the lowest (12.66 g/100 g).

Table 2. Proximate composition of seven pecan cultivars and one selected genotype ('Seleção P') grown in the municipality of Canguçu, Rio Grande do Sul, Brazil

Cultivar	Moisture content (%)	Protein * (%)	Lipids * (%)	Ash * (%)	Carbohydrates* (%)
Barton	2.95±0.06^{g}	6.87±0.07^{d}	59.70±0.5^{e}	1.66±0.04^{c}	31.77±0.7^{a}
Desirable	3.34±0.04^{e}	8.08±0.10^{c}	73.16±0.3^{c}	1.52±0.03^{d}	17.24±0.4^{c}
Elliot	3.15±0.04^{f}	6.12±0.09^{f}	77.08±0.4^{a}	1.61±0.02^{c}	15.18±0.6^{d}
Farley	5.50±0.01^{b}	6.75±0.03^{d}	74.65±0.8^{c}	1.75±0.01^{a}	16.86±0.8^{c}
Mohawk	4.02±0.04^{d}	6.17±0.01^{e}	74.23±0.7^{c}	1.63±0.01^{c}	17.98±0.7^{c}
Seleção P	5.62±0.03^{b}	8.95±0.13^{b}	76.21±0.6^{b}	1.72±0.04^{b}	13.12±0.7^{e}
Shawnee	4.13±0.02^{c}	6.95±0.07^{d}	69.49±0.5^{d}	1.72±0.03^{b}	21.84±0.5^{b}
Success	8.33±0.01^{a}	9.61±0.09^{a}	76.00±0.1^{b}	1.72±0.05^{b}	12.66±0.3^{e}

Values are expressed as mean ± standard deviation (n = 3). Means followed by the same letter in the same column do not differ significantly according to Tukey's test (P < 0.05). * Results on a dry basis.

3.2 Chemical Properties of Pecan Oil

The acidity of the evaluated samples ranged from 0.46 mg KOH/g in the 'Seleção P' cultivar to 0.62 mg KOH/g in 'Mohawk'. The peroxide values varied between 3.96 meq O_2/kg in the Success cultivar and 9.96 meq O_2/kg in 'Shawnee'. The specific extinction coefficient at 232 nm (K_{232}) reflects the degree of oxidation of polyunsaturated fatty acids, whereas the coefficient at 270 nm (K_{270}) indicates the formation of secondary oxidation products, such as aldehydes and ketones (29,30). In this study, no significant differences were observed in K_{232} and K_{270} values among the cultivars, with all values remaining below 0.03.

Table 3. Acidity, peroxide value, and specific extinction coefficients (K_{232} and K_{270}) of seven cultivars and one selected genotype ('Seleção P') grown in the municipality of Canguçu, Rio Grande do Sul, Brazil

Cultivate	Acidity (mg KOH/g)	Peroxide index (meq O_2/kg)	K_{232}	K_{270}
Barton	0.50 ± 0.00^{ab}	5.90^{c}	0.01 ± 0.01^{NS}	0.01 ± 0.01^{NS}
Desirable	0.56 ± 0.04^{ab}	8.17^{b}	0.01 ± 0.00	0.01 ± 0.00
Elliot	0.57 ± 0.01^{ab}	5.93^{c}	0.01 ± 0.00	0.00 ± 0.00
Farley	0.54 ± 0.03^{ab}	7.97^{b}	0.01 ± 0.00	0.01 ± 0.00
Mohawk	0.62 ± 0.02^{a}	9.89^{a}	0.02 ± 0.00	0.01 ± 0.01
Seleção P	0.46 ± 0.02^{b}	9.90^{a}	0.01 ± 0.00	0.01 ± 0.00
Shawnee	0.58 ± 0.01^{ab}	9.96^{a}	0.02 ± 0.01	0.02 ± 0.00
Success	0.52 ± 0.07^{ab}	3.96^{d}	0.02 ± 0.02	0.02 ± 0.02

Results presented are mean ± standard deviation values (n = 3). Equal letters in the column indicate no significant difference based on Tukey's test (P < 0.05).

Table 4 presents the tocopherol contents in pecan oil samples from the different cultivars evaluated. Alpha-tocopherol was not detected in any of the oil samples. Delta-tocopherol content ranged from 3.20 mg/100 g in the 'Mohawk' cultivar to 3.37 mg/100 g in 'Success'. Gamma-tocopherol levels varied from 18.19 mg/100 g ('Mohawk') to 31.83 mg/100 g ('Elliot').

Table 4. Tocopherol contents (mg/100 g) in pecan oils from seven cultivars and one selected genotype ('Seleção P') grown in the municipality of Canguçu, Rio Grande do Sul, Brazil

Cultivar	Alfa	Delta	Gama (γ)
Barton	ND	3.33 ± 0.02 ^{ab}	24.95 ± 1.60 ^{b}
Desirable	ND	3.26 ± 0.02 ^{ab}	20.66 ± 1.63 ^{bc}
Elliot	ND	3.26 ± 0.04 ^{ab}	31.83 ± 1.19 ^{a}
Farley	ND	3.23 ± 0.08 ^{b}	25.05 ± 1.80 ^{b}
Mohawk	ND	3.20 ± 0.00 ^{b}	18.19 ± 0.16 ^{c}
Seleção P	ND	3.27 ± 0.03 ^{ab}	21.15 ± 1.20 ^{bc}
Shawnee	ND	3.30 ± 0.02 ^{ab}	21.71 ± 2.75 ^{bc}
Success	ND	3.37 ± 0.00 ^{a}	25.95 ± 0.28 ^{ab}

Results presented as mean ± standard deviation (n = 3). Equal letters in the column do not differ from each other by Tukey test (P < 0.05). ND = Not detected

Table 5 presents the fatty acid profiles of pecan oil samples from the different cultivars. Overall, monounsaturated fatty acids (MUFAs) were predominant, followed by polyunsaturated fatty acids (PUFAs). The 'Mohawk' cultivar exhibited the highest MUFA content (53.53%), followed by 'Barton'. Among the MUFAs, oleic acid (omega-9) was the most abundant fatty acid in both 'Mohawk' and 'Barton', with values of 53.21% and 52.78%, respectively. The highest levels of polyunsaturated fatty acids, specifically linoleic acid (omega-6) and alpha-linolenic acid (omega-3), were found in the 'Elliot' cultivar, at 33.94% and 2.39%, respectively. Regarding saturated fatty acids (SFAs), 'Barton' and 'Mohawk' showed the lowest contents (13.77% and 13.73%, respectively), whereas 'Seleção P' presented the highest SFAs content at 14.99%.

Table 5. Fatty acid profiles (%) of seven pecan cultivars and one selected genotype ('Seleção P') grown in the municipality of Canguçu, Rio Grande do Sul, Brazil

		Barton	Desirable	Elliot	Farley	Mohawk	Seleção P	Shawnee	Success
Saturated		13.77±0.25^{c}	14.54±0.07 ^{b}	14.33±0.12^{bc}	14.51±0.10^{b}	13.73 ±0.11^{c}	14.99±0.50 ^{ab}	15.50±0.07^{a}	14.64±0.31^{b}
Monounsaturated (MUFAs)		53.13±0.21^{a}	51.887±0.21^{b}	49.33±0.26^{d}	52.04 ±0.03^{b}	53.53±0.02^{a}	52.20±0.13^{b}	50.43±0.26^{c}	50.51±0.15^{c}
Polyunsaturated (PUFAs)		33.09±0.04^{de}	33.58±0.13^{cd}	36.34 ±0.14^{a}	33.43±0.12^{cde}	32.73± .08^{e}	32.80±0.368	34.07±0.33^{c}	34.84±0.46^{b}
Myristic acid	C14:0	0.043±0.00 ^{b}	0.050±0.01^{ab}	0.043±0.01^{b}	0.045±0.00^{ab}	0.00±0^{c}	0.048±0.00^{ab}	0.054±0.00^{a}	0.044±0.00^{ab}
Palmitic acid	C16:0	8.96±0.09 ^{de}	9.36±0.05^{abc}	8.80±0.08^{e}	8.86±0.05^{de}	9.27±0.06^{bc}	9.11±0.21^{cd}	9.59±0.03^{a}	9.41±0.13^{ab}
Stearic acid	C18:0	4.57±0.16 ^{cd}	4.91±0.02^{bc}	5.26±0.03^{ab}	5.36±0.05^{a}	4.27±0.04^{d}	5.59±0.28^{a}	5.61±0.04	4.98±0.18^{b}
Oleic acid	C18:1	52.78±0.22^{a}	51.58±0.21^{b}	48.96±0.27^{d}	51.70±0.01^{b}	53.21±0.03^{a}	51.91±0.14^{b}	50.08±0.26^{c}	50.22±0.15^{c}
Linoleic acid	C18:2	31.06±0.08^{d}	31.45±0.14^{cd}	33.94±0.06^{a}	31.46±0.13^{cd}	30.85±0.10^{d}	30.91±0.47^{d}	31.90±0.32^{bc}	32.64±0.43^{b}
Linolenic acid	C18:3	2.03±0.04^{cd}	2.12±0.00^{bc}	2.39±0.08^{a}	1.97±0.01^{de}	1.88±0.01^{e}	1.89±0.10	2.16±0.02^{bc}	2.20±0.04^{b}
Arachidic acid	C20:0	0.18±0.01^{c}	0.20±0.00^{b}	0.21±0.00^{b}	0.23±0.00^{a}	0.18±0.00^{c}	0.23±0.01^{a}	0.24±0.00^{a}	0.19±0.01^{bc}
Eicosanoic acid	C20:1	0.34±0.01^{ab}	0.29±0.00^{e}	0.36±0.00^{a}	0.34±0.01^{bc}	0.31±0.01	0.29±0.01^{e}	0.34±0.00^{b}	0.29±0.01^{de}

Results presented as mean ± standard deviation (n = 3). Equal letters in the column do not differ from each other by Tukey test (P < 0.05). ND = Not detected

3.3 Phenolic Compounds

Seven phenolic compounds common to all varieties were identified by LC/MS: gallic acid, procyanidin type B, (+)-catechin, methyl gallate, ellagic acid pentose, ellagic acid, and methylated ellagic acid pentose (Table 6).

Table 6. Qualitative profiles of individual phenolic compounds detected in seven pecan cultivars and one selected genotype ('Seleção P') grown in the municipality of Canguçu, Rio Grande do Sul, Brazil

RT (min)	Identification	Molecular Formula (M-H)	Experimental mass	Theoretical mass	Fragment ion (intensity)	eV	Error (ppm)	mSigma
1.95	Gallic acid	$C_7H_5O_5$	169.0138	169.0138	-		2.8	7
2.74	Procyanidin type B	$C_{30}H_{25}O_{12}$	577.1351	577.1346	289.0717 (100); 125.0247 (86.3); 407.0766 (63.2); 425.0851 (3.9)	37.3	0	41.5
3.05	(+)-Catechin	$C_{15}H_{13}O_6$	289.0716	289.0718	109.0296 (100); 125.0243 (67.9); 245.0812 (37.8); 205.0516 (30); 179.0330 (19.2)	-	5.2	39.2
3.14	Methyl gallate	$C_8H_7O_5$	183.0303	183.0312	183.0276	19.2	4.9	53.2
4.32	Ellagic acid pentose	$C_{19}H_{13}O_{12}$	433.0409	433.0412	300.99 (100); 299.99 (69.8)	31.7	0.7	32
4.50	Ellagic acid	$C_{14}H_5O_8$	300.9998	300.999	300.99	25.1	-2.7	30.2
4.57	Methyl ellagic acid pentose	$C_{20}H_{15}O_{12}$	447.0569	447.0564	315.0152 (100); 299.9896 (24.9)	32.4	-1.2	112.3

The contents of phenolic compounds in samples from the eight pecan cultivars are presented in Table 7. Ellagic acid was the most abundant phenolic compound across all cultivars, ranging from 0.59 mg/100 g in 'Barton' to 2.22 mg/100 g in 'Seleção P'. Regarding ellagic acid pentose, the 'Success' cultivar exhibited the highest content (0.64 mg/100 g), whereas the lowest concentration was observed in 'Barton' (0.27 mg/100 g).

Table 7. Contents of individual phenolic compounds (mg/100 g) in seven pecan cultivars and one selected genotype ('Seleção P') grown in the municipality of Canguçu, Rio Grande do Sul, Brazil

Cultivar	Ellagic acid	Ellagic acid pentose	Methyl ellagic acid pentose	Gallic acid	Catechin	Methyl gallate	Procyanidin type B
Barton	0.59±0.03 d	0.27±0.01 c	0.16±0.00	0.17±0.01b	0.06±0.00 f	0.18±0.01 d	ND
Desirable	1.02±0.04 c	0.35±0.01 bc	0.17±0.00	0.20±0.00ab	0.09±0.01 f	0.20±0.01 cd	ND
Elliot	1.27±0.09 c	0.48±0.04 ab	0.28±0.02	0.22±0.01ab	0.64±0.02 a	0.18±0.00 d	0.92±0.23 a
Farley	2.11±0.15 a	0.63±0.07 a	0.25±0.03	0.21±0.02ab	0.31±0.02 cd	0.26±0.02 bc	0.04±0.04 bc
Mohawk	1.81±0.07 b	0.54±0.06 a	0.29±0.07	0.20±0.04ab	0.25±0.03 de	0.25±0.02 bc	ND
Seleção P	2.22±0.10 a	0.62±0.11 a	0.28±0.01	0.23±0.01ab	0.33±0.02 c	0.29±0.00 ab	0.11±0.06 bc
Shawnee	1.73±0.10 b	0.62±0.06 a	0.16±0.00	0.20±0.00 ab	0.55±0.04 b	0.33±0.01 a	0.27±0.05 b
Success	2.19±0.08 a	0.64±0.08 a	0.22±0.03	0.22±0.04 a	0.19±0.04 e	0.30±0.04 ab	ND

Results presented as mean ± standard deviation (n = 3). Equal letters in the column do not differ from each other by Tukey test ($P < 0.05$). ND = Not detected

4. Discussion

4.1 Physicochemical Properties

The physicochemical and visual characterization of different pecan cultivars can guide management, breeding, processing, and marketing strategies (Siebeneichler et al., 2024). In the present study, we evaluated eight cultivars that exhibited distinct characteristics in terms of color, moisture content, and lipid, protein, and carbohydrate composition. Among the visual attributes, color is a key factor for commercial acceptance, with lighter-colored samples generally being preferred by consumers. The 'Barton' cultivar showed the lowest L*, b*, and C*

values, indicating a darker and less saturated coloration, which may negatively affect its acceptance in the fresh market. On the other hand, 'Shawnee', with higher brightness and yellow intensity (b*), stood out positively in this regard, making it potentially more attractive for direct consumption or for processing purposes where visual uniformity is important. Similar L* values (46.6) were reported for 'Barton' cultivars produced in Cachoeira do Sul, RS, Brazil (Siebeneichler et al., 2024). Although darkening is often associated with oxidation reactions (Ribeiro, Ribeiro et al., 2020), naturally occurring compounds may also play an important role in the color variation observed among cultivars. Flavonoids, particularly flavan-3,4-diols such as leucodelphinidin and leucocyanidin, are unstable in the presence of oxygen and tend to polymerize under acidic and high-temperature conditions, forming reddish pigments such as anthocyanidins and phlobaphenes (Prabhakar et al., 2022). These polymerized compounds may accumulate in the nut tissues, resulting in darker tones even before prolonged storage.

Another compositional factor that affects preservation and sensory characteristics, such as crunchy texture, is the moisture content (Siebeneichler et al., 2023). In the present study, the 'Barton' cultivar exhibited the lowest moisture content at 2.95%, while 'Success' reached 8.33% (Table 2). The ideal moisture content should be up to 4%. When moisture levels slightly exceed this limit, nut quality can still be preserved, but only with complementary methods such as reducing the partial pressure of oxygen (pO_2) (Thewes et al., 2021) or using refrigeration (Ribeiro et al., 2022). These strategies help delay oxidative and microbiological processes, thereby contributing to product stability even under non-ideal humidity conditions. Interestingly, 'Barton', in addition to having the lowest moisture content, also showed the darkest coloration and the lowest b* value. A previous study demonstrated that rapid moisture loss during drying can reduce lightness (L*) and intensify kernel darkening, especially when associated with the oxidation of phenolic compounds (Tan et al., 2025). Therefore, it is possible that more intense drying in 'Barton', combined with its phenolic composition, contributes to its darker tone, since oxidation indicators were low, such as the peroxide value (5.90 meq O_2/kg) and the specific extinction coefficients K_{232} and K_{270} (both at 0.01) (Table 3).

Marked differences in macronutrient content were observed among the evaluated cultivars (Table 2). The 'Success' cultivar stood out for its high lipid (76%) and protein (9.61%) contents. The 'Elliot' and 'Seleção P' cultivars also showed promise as potential sources for oil extraction. In contrast, the 'Barton' cultivar had the highest carbohydrate content (31.77%), which may sensorially contribute to a sweeter taste. In a sensory study involving fourteen cultivars, 'Barton' was among the consumers' favorites (Du et al., 2022). These characteristics can be considered in both the development of diets with specific nutritional profiles and in the processing of roasted products, where higher carbohydrate and protein contents may enhance the formation of volatile compounds responsible for aroma and flavor through the Maillard reaction. Additionally, nuts with higher lipid content tend to exhibit a more buttery flavor (Siebeneichler et al., 2023).

However, it is important to note that the proximate composition can vary depending on the edaphoclimatic conditions of the cultivation region. In the city of Anta Gorda, in southern Brazil, for example, the 'Success' cultivar showed a lipid content of 58.94% (Ribeiro, Klein et al., 2020), a value lower than that observed in the present study (76%) (Table 2). On the other hand, the 'Desirable' cultivar grown in China reached a higher value, with approximately 80% lipids (Jia et al., 2019). These data highlight the influence of the growing environment on the nutritional profile of pecan nuts.

The ash content, which represents the mineral fraction of foods, showed values ranging from 1.52% ('Desirable') to 1.75% ('Farley'). These results are consistent with the values generally reported for pecan nuts, which range from 1.53% to 1.86% (Ferrari et al., 2022). The higher ash content in the 'Farley' cultivar may indicate a greater concentration of essential minerals such as potassium, magnesium, iron, and calcium (Curiel-Maciel et al., 2021; Siebeneichler et al., 2023). However, further studies are needed to individually characterize the minerals present in each cultivar, allowing for a more accurate assessment of their nutritional potential.

4.2 Chemical Properties of Oil

Oil represents the main fraction of pecan nuts; therefore, evaluating its chemical properties is essential to determine its stability and nutritional quality. The acidity determination was carried out according to the official AOCS method for edible oils, as there is no specific methodology available for the kernel. Acidity results from the hydrolysis of triacylglycerols and may indicate oil degradation due to the presence of free fatty acids (Curiel-Maciel et al., 2021). In this study, the 'Mohawk' cultivar exhibited acidity levels exceeding the maximum limit established by Brazilian legislation (Agência Nacional de Vigilância Sanitária [ANVISA], 2021) for oils, which is 0.6 mg KOH/g (ANVISA, 2021) (Table 3). This result, combined with the peroxide value of 9.89 meq O_2/kg (very close to the regulatory limit), the high content of unsaturated fatty acids, and the lowest γ-tocopherol content among the evaluated cultivars, suggests lower oxidative stability. Considering these factors, the oil from the 'Mohawk' cultivar may be more suitable for immediate consumption during the harvest season, rather than for long-term storage or supply during the off-season.

Peroxide values, which indicate the degree of oxidation of triglyceride degradation products, varied among the cultivars, ranging from 3.96 meq O_2/kg in the 'Success' cultivar to 9.96 meq O_2/kg in 'Shawnee'. Although some cultivars presented values close to the limit established by Brazilian legislation (10 meq O_2/kg), the specific extinction coefficients K_{232} and K_{270}, used to assess the oxidation of PUFAs and the formation of secondary compounds such as aldehydes and ketones (Bouali et al., 2022; Rivera-Rangel et al., 2018), were below 0.03. These low values indicate minimal lipid oxidation, reinforcing the initial quality of the extracted oils.

Gamma-tocopherol was the predominant tocopherol isomer, present at levels approximately seven times higher than delta-tocopherol. This predominance of gamma-tocopherol in pecan oil corroborates findings reported by Bouali et al. (2022), Siebeneichler et al. (2024), Ferrari et al. (2022). Tocopherols (vitamin E) exhibit antioxidant properties and play a critical role in stabilizing free radicals. Beyond their health benefits, tocopherols inhibit lipid peroxidation, thereby reducing oxidative degradation in oils and fats present in foods, which helps preserve essential dietary fats (Alvarez-Parrilla et al., 2018). Natural vitamin E comprises several tocopherol isomers, including alpha-, beta-, delta-, and gamma-tocopherol, that differ in methyl group substitution on the chromanol ring and possess a side chain.

The fatty acid profiles in this study partially align with previous research, such as that by Ribeiro, Klein et al. (2020), which reported MUFAs as the predominant type, albeit at higher levels (~69%). Here, PUFA contents were higher than those reported by Ribeiro, Klein et al. (2020). In pecans cultivated in Mexico, PUFAs predominated at 68.65%, followed by MUFAs at 23.92% and saturated fatty acids (SFAs) at 6.05%. In Turkish cultivars, oleic acid (C18:1) predominated with an average of 67.51%, followed by linoleic acid (C18:2) at 22.81% and linolenic acid (C18:3) at 0.77% (Yılmaz et al., 2021). Fernandes et al. (2017) evaluated pecan, almond, and hazelnut oils extracted by pressing and reported lower PUFA contents [palmitic acid (6.4%-7.6%), stearic acid (2.2%-2.8%), oleic acid (omega-9) (49.6%-62.1%), linoleic acid (omega-6) (27.2%-37.7%), and linolenic acid (omega-3) (1.4%-1.9%)] than those found in this study [palmitic acid (8.8%-9.59%), stearic acid (4.27%-5.59%), oleic acid (omega-9) (48.9%-53.2%), linoleic acid (omega-6) (30.8%-33.9%), and linolenic acid (omega-3) (1.8%-2.39%)].

In addition to the influence of edaphoclimatic and genetic characteristics, a recent study compared different extraction methods and found that they directly affect the physicochemical properties and fatty acid composition of pecan oil (Cui et al., 2025). It is worth noting that, in the present study, oil was extracted using the Bligh-Dyer method. This method employs polar solvents, which can promote hydrolysis reactions and may result in higher measured acidity.

Overall, among the evaluated cultivars, 'Elliot' exhibited a remarkable quality profile, evidenced by the combination of intense yellow coloration (high b* value), low peroxide index, high content of PUFAs, and elevated concentration of the antioxidant γ-tocopherol. This composition is particularly relevant, as PUFAs, while beneficial to health, are highly susceptible to oxidation. The simultaneous presence of natural antioxidants, such as γ-tocopherol, catechin, procyanidin type B, and ellagic acid pentose, may act synergistically to protect against lipid oxidation, thereby preserving oil quality and extending its shelf life.

4.3 Phenolic Compounds

In addition to lipophilic antioxidants, pecan nuts are an important source of phenolic compounds, particularly flavonoids and tannins, which contribute to their bioactive properties. These compounds exhibit a range of biological activities, including antioxidant, anti-inflammatory, antimutagenic, and anticancer effects (Bodoira & Maestri, 2020). They also directly influence flavor and even color (Prabhakar et al., 2022), imparting bitter and astringent notes to the nuts (Siebeneichler et al., 2023).

In this study, seven main phenolic compounds were identified: ellagic acid, gallic acid, catechin, ellagic acid pentose, methyl ellagic acid pentose, methyl gallate, and procyanidin type B (Table 7). The results are consistent with previous studies conducted in the United States (Texas) and Tunisia, which also reported the presence of ellagic acid, gallic acid, catechin, and epicatechin in pecan samples (Bouali et al., 2020; Villarreal-Lozoya et al., 2007). Phenolic composition varied significantly among the evaluated cultivars, with 'Seleção P' standing out for its high contents of ellagic acid (2.22 mg/100 g), ellagic acid pentose (0.62 mg/100 g), catechin (0.33 mg/100 g), and methyl gallate (0.29 mg/100 g), surpassing most commercial cultivars. The 'Farley' cultivar also stood out for its high ellagic acid content (2.11 mg/100 g) and for containing procyanidin type B (0.04 mg/100 g), a compound with well-recognized antioxidant activity (Yang et al., 2021). On the other hand, the 'Barton' and 'Desirable' cultivars showed the lowest catechin levels (0.06 and 0.09 mg/100 g, respectively), and procyanidin type B was not detected, which may indicate a lower antioxidant potential in these samples.

Previous studies have indicated that the shells contain the highest levels of phenolic compounds, and this composition can influence the kernel content (Xu et al., 2020). Furthermore, the synthesis of phenolic compounds is dynamic throughout fruit development. During the early stages of maturation, such as the watery phase, there is greater expression of genes involved in phenolic biosynthesis, resulting in high concentrations of compounds like catechin, epicatechin, ellagic acid, and gallic acid (Jia et al., 2018). However, in the later stages, this synthesis decreases, and the fruit predominantly accumulates lipids (Siebeneichler et al., 2023).

5. Conclusions

Pecans cultivated in Rio Grande do Sul exhibit a favorable nutritional profile, characterized by a predominance of monounsaturated and polyunsaturated fatty acids along with significant levels of bioactive phenolic compounds. Among the cultivars studied, 'Elliot' stood out with the highest lipid and gamma-tocopherol contents, while 'Success' showed superior protein and delta-tocopherol levels. The 'Barton' cultivar was distinguished by its darker coloration, elevated carbohydrate content, and greater ellagic acid concentration. Notably, 'Mohawk' exceeded the permissible acidity limit for oilseed products, signaling potential quality concerns. The 'Shawnee', 'Elliot', and 'Mohawk' cultivars were predominant in saturated, monounsaturated, and polyunsaturated fatty acids, respectively. The 'Seleção P' cultivar exhibited a high oil content, along with the lowest levels of acidity and saturated fatty acids, indicating its potential to produce superior quality oil. Catechin was the most variable phenolic compound among all cultivars, highlighting its importance for antioxidant capacity and potential health benefits. Overall, the results of this study provide information to guide the selection of pecan cultivars with superior nutritional and functional properties. The observed variability among cultivars reflects a significant source

of genetic diversity adapted to the edaphoclimatic conditions of the region, which can be harnessed to develop cultivars that meet specific demands related to quality, stability, and nutritional profile. These insights support quality control strategies and contribute to strengthening the local production chain, ultimately enhancing the competitiveness and promotion of pecans as a functional food in both domestic and international markets.

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Transparency of Data

Available data: The entire data set that supports the results of this study was published in the article itself.

Author Contribution Statement

	TDS	SCF	VZ	CDF	IRC	RLC	ADVL	CRM	TJS	ARGD	JFH
Conceptualization	■							■	■	■	■
Funding acquisition										■	■
Investigation	■					■			■		
Methodology		■			■	■	■				
Project administration									■	■	■
Supervision									■	■	■
Writing – original draft	■										
Writing – review and editing			■	■	■			■	■	■	■

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