Food Chemistry 525 (2026) 150319

Contents lists available at ScienceDirect

Food Chemistry

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

Metabolomic profile of edible Amazonian Arecaceae fruits by FT-ICR-MS: Insights into chemical, nutritional and antioxidant profiles

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ARTICLE INFO

Keywords:
Amazonian palm fruits
Arecaceae
FT-ICR-MS
Metabolomics
Foodomics
Bioactive compounds

ABSTRACT

Amazonian palm fruits (Arecaceae), including açaí (*Euterpe oleracea*), pupunha (*Bactris gasipaes*), buriti (*Mauritia flexuosa*), bacaba (*Oenocarpus bacaba*), and tucumã (*Astrocaryum aculeatum*) are traditionally consumed for their nutritional and therapeutic properties, yet their comprehensive metabolomic characterization remains limited. Here, an integrative foodomics approach combining untargeted and targeted analyses was applied. Direct infusion FT-ICR-MS enabled the annotation of over 10,000 molecular formulas, revealing extensive chemical diversity. Van Krevelen diagrams and chemometric analyses (HCA, PCA, PLS-DA) highlighted distinct metabolomic signatures across species. Targeted assays showed that açaí and pupunha exhibited the highest total phenolic and flavonoid contents and the strongest antioxidant activities, comparable with Trolox, while tucumã presented the highest folate content (132.64 μg/100 g DW) These findings demonstrate associations between molecular composition and functional properties. This work represents the first FT-ICR-MS-based metabolomic characterization of these fruits, expanding current knowledge and providing a robust framework for their valorization in food and nutraceutical applications.

1. Introduction

The Amazon rainforest is one of the most promising regions for sustainable food systems, offering a vast source of edible fruits and medicinal plants, primarily recognized for their nutritional properties and sustainable agro-extractivism (Amorim et al., 2024; Rodrigues et al., 2023). Among these resources, palm tree fruits (Arecaceae) stand out for their biotechnological potential, with notable examples including açaí (*E. oleracea*), pupunha (*B. gasipaes*), buriti (*M. flexuosa*), bacaba (*O. bacaba*), and tucumã (*A. aculeatum*). These palm trees are considered as keystone source plants and play an important role in the rainforest ecosystem. Beyond their ecological significance, these palms have many applications, such as sources of fiber, oil, construction materials, household utensils, and tools, serving as vital resources for many local communities in the Amazon region. Due to their multifunctional properties and versatility, they hold considerable potential for the sustainable development of high-value-added products (Jaramillo-Vivanco et al., 2022). In addition, these underutilized palm fruits could serve as a valuable nutritional resource for local communities in low-income regions where they are commonly found, and where macro- and micronutrient deficiencies are prevalent. These nutritional deficiencies are associated with a range of adverse health outcomes, such as diminished productivity, mental impairment, and elevated mortality rates (Darnet et al., 2011; Erşan et al., 2020; Jaramillo-Vivanco et al., 2022). However, current knowledge is based on targeted analyses of specific compound classes (Ferreira et al., 2024; Koolen et al., 2013; Nascimento-Silva et al., 2023; Rudke et al., 2019; Silva et al., 2025), and a comprehensive, molecular-level understanding of their metabolomic diversity and its relationship with functional and nutritional properties remains lacking. This limitation may has constrained their full exploitation and commercialization, leaving a gap in accurately assessing their potential for sustainable use.

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https://doi.org/10.1016/j.foodchem.2026.150319
Received 8 January 2026; Received in revised form 3 June 2026; Accepted 4 July 2026
Available online 8 July 2026

These palm tree fruits produce oils rich in saturated and unsaturated fatty acids, vitamin E, and carotenoids, and have been used by local companies in cosmetics manufacturing. Additionally, they are predicted to have compounds that have been reported as potential applications as functional foods or nutraceuticals (Amorim et al., 2024; Neves et al., 2015; Rincón-Cervera et al., 2023). An example is the açaí fruit and buriti oil which are consumed as functional food due to their high nutritional value and beneficial properties (Rodrigues et al., 2024). Ethnopharmacological information shows their use in traditional medicine. Different parts of the tree (roots, seeds, fruits, stems, shells, leaves, kernels) have been used by natives of the Amazon region to treat leishmania, malaria, hepatitis, headaches, gastrointestinal disorders, respiratory infections, skin tissue disorders, metabolic and nutritional issues, and inflammatory disorders (Agostini-Costa, 2018; Coelho-Ferreira, 2009; Nisa et al., 2024; Pedrollo et al., 2016; Ribeiro et al., 2017).

The biological properties of these fruits are primarily attributed to their rich and diverse phytochemical composition, including polyphenols, sterols, carotenoids, alkaloids, and other bioactive compounds (Rodrigues et al., 2023). Among them, polyphenols stand for the largest and most studied group, with over 8000 compounds described. This group includes anthocyanins, flavonoids, phenolic acids, lignans, tannins, and stilbenes, classified according to their chemical structures (Nisa et al., 2024; Quideau et al., 2011). Polyphenols are recognized as potent antioxidants, with regular intake offering protection against various forms of oxidative damage in the human body (Nisa et al., 2024; Santos et al., 2023). In addition to their antioxidant effects, polyphenols support gut health by modulating the human gut microbiota, helping to reduce pro-inflammatory and pathogenic microbial imbalances (Chatterjee et al., 2024; Sánchez-Recillas et al., 2024). Additionally, dietary polyphenols may help prevent neurodegenerative diseases by improving brain and cerebrovascular blood flow and enhancing cognitive performance (Chatterjee et al., 2024). These compounds are also associated with the prevention of several metabolic syndromes such as hyperglycemia, obesity, dyslipidemia, and hypertension (Gasmi et al., 2022), as well as for their anticancer properties (Otun et al., 2024), anti-airway fibrosis (Sahu et al., 2024), antimicrobial (Chen et al., 2024), and anti-inflammatory properties (Arunachalam et al., 2023).

Building on the rich diversity, this study investigates the chemical composition and bioactivity of species from the Arecaceae fruits using advanced analytical techniques. Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR-MS) is renowned for its high-resolution capabilities, allowing an in-depth analysis of complex mixtures and the classification of compounds. This technique offers several advantages, including rapid analysis, high accuracy in assigning elemental formulas, and exceptional sensitivity and dynamic range, enabling swift untargeted metabolic profiling before more focused LC–MS analyses of specific samples (Junot & Fenaille, 2019; Pieczonka, Hemmler, et al., 2021; Pieczonka, Paravicini, et al., 2021; Rychlik et al., 2019; Woodward et al., 2025). Additionally, quantification of phenolic compounds and folate vitamers provides a deeper understanding of their nutritional and therapeutic potential (Garzón et al., 2010).

Despite the recognized nutritional importance of Amazonian palm fruits, a comprehensive molecular-level understanding of their metabolome and its relationship with bioactivity remains limited. This study addresses this gap by introducing a multi-layered foodomics approach that combines untargeted FT-ICR-MS metabolomics with targeted quantitative and functional analyses. To our knowledge, this is the first work to provide an in-depth molecular fingerprint of Arecaceae palm fruits using direct infusion FT-ICR-MS, to characterize folate vitamer distributions across multiple species, and to integrate compositional data with antioxidant activity profiles. Our objectives are to offer a comprehensive characterization of these fruits, enabling deeper insight into their chemical diversity and bioactive potential, while emphasizing the role of Amazonian biodiversity in supporting sustainable development and functional food innovation.

2. Experimental

2.1. Chemicals

Methanol and ethanol (LC-MS grade) were supplied by Fischer Scientific (Schwerte, Germany). Formic acid was supplied by Sigma-Aldrich (St. Louis, MO, USA). Bond Elut™ cartridges (100 mg) were purchased from Agilent (Santa Clara, CA, US). Ultra-pure water (18.2 MΩ) was obtained from a Millipore system (Merck, Darmstadt, Germany). Standard compounds quercetin, catechin, gallic acid, aluminum chloride, and 2,2-diphenyl-1-picrylhydrazyl (DPPH) were purchased from Sigma-Aldrich (Merck, Darmstadt, Germany). Sodium acetate, vanillin, and sulfuric acid were purchased from Neon (Neon, São Paulo, Brazil).

2.2. Plant material and extract preparation

Arecaceae palm fruits were purchased from a local street market in Mâncio Lima, Acre State, Brazil (latitude 07° 36′ 51“ S and longitude: 72° 53’ 45” W). As the fruits were obtained from a local market, detailed information regarding harvest conditions, including exact geographic origin, seasonality, and post-harvest handling were not available. Therefore, the samples analyzed represent fruits as commercially available to consumers rather than controlled agricultural specimens. The fruits were transported to the Federal University of Goiás (UFG) under cooled conditions in a container with ice. Upon arrival, the fruits were stored at 4 °C and processed within 3 h to minimize metabolic degradation. The fruits were selected, discarding imperfect ones, and washed. Due to differences in fruit size, a variable number of individual fruits (1−10) were combined to obtain 4.0 g of sample for extraction, resulting in a composite sample representative of each fruit type. The fruits were cut, and placed in Erlenmeyer flasks, and extracted with 40 mL of ethanol for 30 min in an ultrasonic bath at 25 °C. The extraction was performed in triplicate (technical replicates). The extracts were passed through a filter paper, transferred to caps, and concentrated in a speedvac at 45 °C for 2 h. The extracts were kept at −80 °C until analysis. Access to the selected fruits was registered in the Brazilian National System for the Management of Genetic Heritage and Associated Traditional Knowledge (SisGen, AD49CF).

2.3. Sample preparation

To avoid excessive ion suppression in the ESI source and space charge effects in the ICR cell caused by saccharide ions and adducts (Cl^-, $H_3PO_4^-$; Na^+, K^+), the ethanolic extracts of freeze-dried tropical fruits from the Arecaceae family were prepared using solid-phase extraction. Various phases and elution conditions were tested based on the resulting feature count, mass resolution, and mass accuracy in the FT-ICR-MS spectra. The developed protocol involves dissolving 1 mg of extract in 1 mL of H_2O/formic acid (0.1%). The conditioned Bond Elut™ PPL (styrene-divinylbenzene polymer) cartridge was loaded with the extract, washed with 1.0 mL of H_2O/formic acid (0.1%), and eluted with 1 mL of methanol (MeOH Eluate). A subsequent elution step was performed with 1 mL of ethanol (EtOH Eluate). Methanol and ethanol were selected as sequential elution solvents to fractionate the extracts based on polarity. Methanol effectively elutes polar compounds (e.g., glycosylated phenolics, amino acids), while ethanol elutes moderately polar to non-polar compounds (e.g., aglycones, terpenes, lipids). This approach minimizes ion suppression and maximizes metabolomic coverage.

2.4. FT-ICR-MS measurement

Both resulting eluates (MeOH and EtOH) were subsequently analyzed using a direct infusion approach on a Bruker solariX ion cyclotron resonance Fourier transform mass spectrometer (Bruker Daltonik GmbH, Bremen, Germany), equipped with a 12 T superconducting

magnet (Magnex Scientific Inc., Yarnton, UK) and an APOLLO II ESI source (Bruker Daltonik GmbH) operated in positive ionization mode. Samples were directly infused at a flow rate of 120 μL h^{-1}. Data sets of 4 MW were acquired through the magnitude mode with a detection range of *m/z* 120–1000, and 400 scans were accumulated per sample to obtain spectra with excellent signal-to-noise values. The level of confidence in compound annotation was assigned according to the Metabolomics Standards Initiative (MSI) (Sumner et al., 2007). Given the nature of (DI) FT-ICR-MS analysis and the absence of MS/MS fragmentation or authentic standards, all molecular formula assignments were classified as MSI Level 3 (putatively characterized compound classes), based on accurate mass measurements and elemental composition. The MoNA - MassBank of North America, Natural Products Atlas, and LOTUS databases were used for the putative annotation of compounds. Following acquisition, the data from both fractions were combined during the metabolomic analysis to generate a comprehensive molecular profile for each fruit sample, ensuring broad coverage of the chemical diversity present.

2.5. FT-ICR-MS data processing, visualization, and interpretation

The FT-ICR spectra were processed using Data Analysis 4.2 software, exporting peak lists with a signal-to-noise ratio (S/N) cut-off of 4 and a minimum intensity threshold of 1.4×10^6. Only singly charged ions were included. Initial external instrument calibration was performed using ion clusters of arginine, followed by internal calibration with a list of 4200 compositions commonly found in polyphenol-rich extracts. Space charge effects were corrected through mass difference mapping (Smirnov et al., 2019). Peak lists were processed and curated using an in-house R-based workflow, including Fourier transform–side loop handling and isotopologue filtering (^{13}C, ^{15}N, ^{18}O) applied at a mass tolerance of 2 ppm and an expected isotopic intensity tolerance of 20%. Signals detected in at least two of three replicates were retained. Peak alignment was conducted with a tolerance of ±2 ppm, resulting in a matrix of 11,600 masses. Accurate masses were analyzed for molecular formulae using mass difference network (MDiN) analysis with the in-house NetCalc software (Tziotis et al., 2011). The network calculation was repeated three times, retaining consistent formula assignments, which yielded approximately 10,480 unambiguous molecular formulae annotations within a mass error range of ±1 ppm and an average absolute mass error of ±0.19 ppm. Despite filtering, residual ^{13}C isotopologues persisted and were partly misassigned as sulfur-containing CHNOS species. Inspection of ^{34}S isotopologues indicated that these misassignments accounted for the majority of the already minor sulfur-containing fraction of the chemical space (3%). The analysis was therefore restricted to the CHNONa chemical space to ensure highest confidence in molecular assignments. In addition, constraints were applied to H/C (0.5–2.5), O/C (0–1.2), and DBE (0–1.5). Double bond equivalents (DBE) reached values of up to 25 ($C_{38}H_{30}O_{13}$). $[M + Na]^+$ adducts were converted in silico to the protonated equivalents. The resulting molecular formulas for each extract and sample were visualized in van Krevelen diagrams by plotting their H/C versus O/C ratios. Intensities were scaled to the highest value within the dataset. When combining the MeOH and EtOH extracts, the intensities of overlapping features were averaged.

For a qualitative comparison of similarities and differences between fruits in the van Krevelen representation, molecular features were evaluated on a binary presence/absence basis. A semi-quantitative assessment was obtained using unsupervised hierarchical clustering analysis (HCA; Euclidean distance, complete linkage) and supervised PLS-DA for fruit differentiation. Prior to analysis, signal intensities were zero-filled (random values between noise level − 2σ and noise level − σ) and z-score normalized. Model performance was evaluated using precision, goodness of fit (R^2), and goodness of prediction (Q^2), while variable importance in projection (VIP) scores was used to identify the most influential features.

2.6. Total phenolic

Total phenolic content (TPC) was determined according to the method of Singleton and Rossi (1965) with modifications by Hossain et al. (2011) Gallic acid standard solutions (0.0, 20.0, 40.0, 60.0, 80.0, and 100.0 μg mL^{-1}) were prepared in methanol and used to construct a calibration curve. The results were calculated using the linear regression equation $y = 0.01882 + 0.00809\times$, with a coefficient of determination $R^2 = 0.995$. TPC was expressed as milligrams of gallic acid equivalents per gram of dry extract (mg GAE/g).

2.7. Total flavonoid content

Total flavonoid content (TFC) was measured according to the Woisky and Salatino (1998) method, with modifications by Hossain et al. (2011). Quercetin standard solutions (0.0, 5.0, 10.0, 15.0, 20.0, and 30.0 μg mL^{-1}) were prepared in methanol and used to construct a calibration curve. The results were determined using the linear regression equation $y = -0.02143 + 0.01107\times$, with a coefficient of determination $R^2 = 0.995$. TFC was expressed as milligrams of quercetin equivalents per gram of dry extract (mg QE/g).

2.8. Total condensed tannin content

Total condensed tannin content (TCT), specifically proanthocyanidins, was determined according to Nunes et al. (2016). Catechin standard solutions (0.0, 5.0, 10.0, 15.0, 20.0, 30.0, 40.0, 50.0, 60.0, 70.0, and 80.0 μg mL^{-1}) were prepared in methanol and used to construct a calibration curve. The results were calculated using the linear regression equation $y = 0.00521 + 0.01826\times$, with a coefficient of determination $R^2 = 0.996$. TCT was expressed as milligrams of catechin equivalents per gram of dry extract (mg CE/g).

2.9. DPPH radical scavenging activity

The DPPH radical scavenging method was performed according to Nunes et al. (2016) Samples along with Trolox as a positive control were solubilized in methanol (1 mg mL^{-1}) and diluted to different concentrations ranging from 500 to 3.9 μg mL^{-1}. A 0.1 mL aliquot of each sample extract was added to 2.9 mL of DPPH methanolic solution (60 μg mL^{-1}) and kept at room temperature for 120 min under controlled light conditions. The DPPH scavenging activity was determined using a UV–Vis spectrophotometer (JASCO V-630, Tokyo, Japan) at 515 nm. The IC_{50} value, which is the concentration of the sample required to inhibit 50% of the DPPH free radical, was calculated from the log(inhibitor) versus normalized response in GraphPad Prism 8.0.1.

2.10. Folate determination

The determination of vitamin B_9, also known as folate, and its derivatives was performed following to the method described by Obermaier et al. (2023). The quantification included five folate vitamers: folic acid (PteGlu), tetrahydrofolate (H_4folate), 5-methyltetrahydrofolate (5-CH_3-H_4folate), 5-formyltetrahydrofolate (5-CHO-H_4folate), and 10-formylfolic acid (10-CHO-H_4folate). Twenty milligrams of freeze-dried fruit samples were utilized. The folates were extracted from the sample matrix and enzymatically deconjugated to their corresponding monoglutamate forms. Protein removal was achieved by precipitation with acetonitrile (ACN), followed by centrifugation. The supernatant was further purified using solid phase extraction (SPE) and the final eluate was analyzed by LC–MS/MS on a LCMS-8050 triple quadrupole mass spectrometer coupled to a Shimadzu Nexera X2 UHPLC system (Shimadzu, Kyoto, Japan). All samples were determined in triplicate, with results reported as mean values ± standard deviation. All results are based on dry biomass. Detailed information on chemicals, solution preparation, and method validation is available in (Obermaier et al.,

2023). Statistical differences in total glutamate content among fruit types were assessed using Welch's analysis of variance (ANOVA) to account for potential heterogeneity of variances, followed by Games–Howell post hoc comparisons. Effect sizes were calculated using Hedges' g to quantify the magnitude of pairwise differences.

3. Results and discussion

3.1. The chemical map of Amazonian palm tree fruits

To explain the bioactive effects of tropical plants at the molecular level, a comprehensive understanding of the metabolites present is essential, which highlights the need for alternative methods that do not require sample chromatography separation yet provide comprehensive metabolite coverage and accurate mass measurement for the characterization of bioactive compounds in complex mixtures. FT-ICR-MS enabled an unprecedented molecular-level resolution of the metabolome of Amazonian palm fruits, allowing the annotation of over 10,000 molecular formulas and revealing a level of chemical diversity that has not been previously reported for these matrices. To capture the total metabolite content of the ethanolic extracts without overloading the ICR cell, the MeOH and EtOH eluates from the solid-phase extraction of the ethanolic extracts were analyzed separately. Strong ion suppression and ICR cell overloading by abundant organic acids limited reliable acquisition in negative ionization mode. The analysis was therefore restricted to positive ionization, likely underrepresenting typical acidic compounds such as hydroxybenzoic and hydroxycinnamic acids. An overview of the metabolite diversity in the fruit extracts is presented as a van Krevelen diagram in **Fig. 1**.

In the Van Krevelen representation (H/C-ratio against O/C-ratio), distinct areas indicate various compound classes, reflecting the atomic composition of biochemical precursors (Schmitt-Kopplin et al., 2019). The molecular complexity of the fruits is evident from their diverse chemical profile, which span from oxygenated and saturated carbohydrates (H/C ~ 2; O/C ~ 1) to peptides, CHO- and nitrogen-containing lipids, and highly unsaturated compounds such as terpenes and polyphenols. These fruits exhibit a richness in terpenes and terpenoids like a wide range of polyphenolic compounds, including phenolic acids and flavanols (Dou et al., 2022; Pieczonka et al., 2025). Polyphenols and terpenes were also found in fresh goji berries from two different cultivars using ESI (±) FT-ICR-MS.(Spano et al., 2021) The same compound class was identified in banana cultivars in different stages of maturation by ESI (−) FT-ICR-MS analyses (Oliveira et al., 2020). FT-ICR-MS was also successfully employed to elucidate the chemical composition of fresh berries (blueberry, bilberry, mulberry, and cranberry), and the analyses allowed the identification of more than thirty polyphenol compounds (Xiao et al., 2017). However, structural identification based solely on accurate mass (MS^1) data remains inherently ambiguous. While assignment to compound classes can be inferred from molecular composition of biosynthetic building blocks, overlaps between classes do occur (Schmitt-Kopplin et al., 2019). Unambiguous identification requires tandem mass spectrometric data (MS^2) and diagnostic fragmentation patterns.

The chemical composition observed in this study is consistent with previous LC-MS/MS investigations of these Amazonian Arecaceae fruits. Açaí has been widely reported as a rich source of flavonoids and anthocyanins, including orientin, luteolin, quercetin, and cyanidin derivatives (Heck et al., 2023; Kang et al., 2010). Similarly, buriti contains phenolic acids (e.g., chlorogenic and caffeic acids), flavonoids, and high levels of carotenoids, particularly β-carotene (Koolen et al., 2013; Nascimento-Silva et al., 2023; Rudke et al., 2019). In addition, pupunha and tucumã have been reported as important sources of carotenoids and phenolic compounds, including di-C-glycosyl flavones and phenolic acids (Chisté et al., 2021; Sagrillo et al., 2015).

To the best of our knowledge, no previous studies have applied FT-ICR-MS–based metabolomics to these fruits, which limits direct comparison at the molecular formula level. Nevertheless, the molecular classes inferred in the present study are in agreement with the compound profiles described in LC-MS/MS-based investigations. While LC-MS/MS approaches provide structural elucidation based on fragmentation patterns, the (DI) FT-ICR-MS strategy adopted here enables the assignment of thousands of molecular formulas with ultrahigh mass accuracy. Therefore, the integration of ultrahigh-resolution mass spectrometry with chemometric tools provides a comprehensive overview of the chemical space and highlights the metabolic diversity of these Amazonian palm fruits.

Concerning the oxygenation pattern analysis of molecular formulas, the detected metabolites were systematically classified according to their oxygen atom content (O_n classes) to provide deeper insight into their chemical diversity and potential functional roles. This classification enables the assessment of the oxidation degree, a key molecular descriptor directly associated with polarity, chemical reactivity, and bioactivity. The distribution of compounds across oxygen classes revealed a clear predominance of O_3–O_7 species, particularly in samples exhibiting higher antioxidant activity. These oxygenation levels are typically characteristic of polyphenolic compounds, including flavonoids and phenolic acids, which possess multiple hydroxyl and carbonyl groups that enhance their radical scavenging capacity.

In contrast, lower oxygen classes (O_1–O_2) were mainly associated with less oxidized metabolites such as lipids, fatty acids, and terpenoids, which generally display reduced antioxidant potential. Compounds within the O_3–O_5 range were primarily assigned to phenolic acids, phenylpropanoids, and low-oxygenated flavonoid aglycones, including protocatechuic acid ($C_7H_6O_4$), vanillic acid ($C_8H_8O_4$), gallic acid ($C_7H_6O_5$), and apigenin ($C_{15}H_{10}O_5$), which are widely reported in Arecaceae species (Morais et al., 2022). The O6 class was predominantly associated with flavonoid aglycones such as velutin ($C_{17}H_{14}O_6$), kaempferol ($C_{15}H_{10}O_6$), and catechin ($C_{15}H_{14}O_6$) (Morais et al., 2022), all recognized for their strong free radical inhibition capacity, as well as hexose-type sugars ($C_6H_{12}O_6$).

Highly oxygenated species (upper to O_7) were less abundant but likely correspond to structurally complex polyphenols, including condensed tannins and glycosylated derivatives such as flavonoid heterosides (e.g., rutin, $C_{27}H_{30}O_{16}$) and proanthocyanidins, as well as esterified phenolic acids like chlorogenic acid ($C_{16}H_{18}O_9$) (Morais et al., 2022). These compounds are particularly relevant due to their high density of hydroxyl groups, which enhances their ability to donate electrons and stabilize radical species. Overall, this oxygen-based classification demonstrates that the antioxidant potential of these Arecaceae fruits is strongly governed by the relative abundance of highly oxygenated metabolites, reinforcing that molecular composition and oxidation degree are more informative descriptors of bioactivity than metabolite diversity alone.

A detailed examination of the individual fruits, including both SPE elution solutions, reveals that the ethanol elution step primarily extracts the lipid fraction that remains on the PPL cartridge (Fig. 9**-II**). While this lipid fraction shows significant similarity across all fruits in the Arecaceae family, the initial methanol elution is more diverse (Fig. 9**-I**). For instance, the methanol extract of the açaí fruit is notably rich in lipid compounds, complemented by terpenes (Fig. 9A-I). In contrast, the Pupunha fruit has a particularly pronounced amino compound chemical space (Fig. 9D-I). Besides peptides and their potential reaction products, nitrogen-containing lipids and glycosylated flavones ($C_{21}H_{20}O_{10}$) are prominent. Bacaba, buriti, and tucumã exhibit similar metabolite profiles, but specific characteristic compound classes, such as procyanidins ($C_{30}H_{26}O_{12}$) in tucumã (Fig. 9E-I), flavonoids ($C_{16}H_{16}O_4$) in buriti (Fig. 9C-I), or fatty acid amides ($C_{23}H_{48}NO_4$) in bacaba (Fig. 9B-I)), allow for differentiation among them. Overall, despite the nuanced differences that do exist, it is striking that the fruits of the Arecaceae family exhibit a remarkably similar metabolite profile. On a molecular level, their biological relatedness is evident, even though the fruits differ significantly in their visual appearance (**Fig. S1**). Indeed, of the 6738

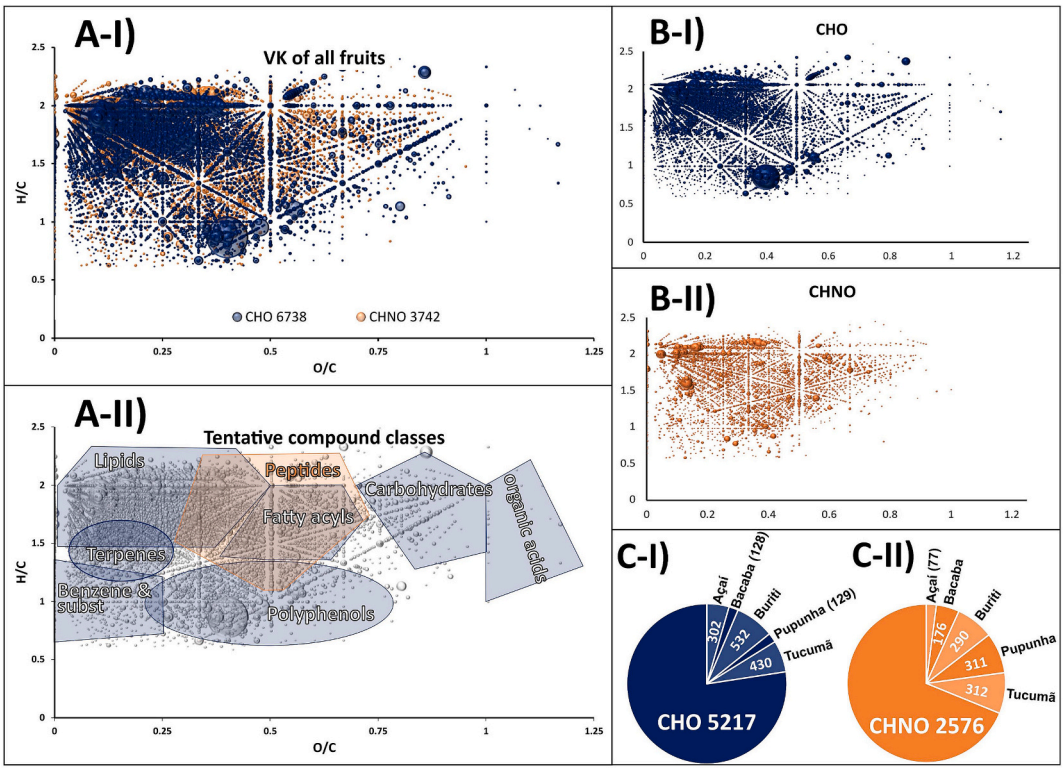


Fig. 1. Van Krevelen diagram of the compound signals resolved in the fruit extracts (**A–I**), divided into the CHO (**B—I**) and CHNO (**B–II**) chemical spaces. Tentative compound class annotations based on molecular compositions are depicted in **A–II**. The similarity in the molecular composition of the palm fruits is reflected in the substantial overlap of annotations, with only a few unique features per fruit (**C**).

Table 1
Total phenolic, flavonoid, condensed tannin content and IC_{50} antioxidant activity compared with Trolox (reference standard).

Sample	Quantification			Antioxidant activity
	Phenolic mg GAE/g	Flavonoids mg QE/g	Tannin mg CE/g	IC_{50} μg mL^{-1}
Tucumã	313.22 ± 2.10^{d}	233.48 ± 0.86^{e}	44.60 ± 0.66^{b}	59.53 ± 1.00^{c}
Buriti	368.54 ± 2.47^{c}	213.69 ± 1.91^{c}	49.96 ± 0.69^{c}	46.02 ± 1.12^{b}
Bacaba	349.98 ± 3.56^{b}	165.54 ± 1.36^{b}	46.97 ± 1.91^{b}	41.35 ± 1.68^{b}
Pupunha	367.94 ± 2.98^{c}	182.28 ± 1.49^{d}	36.23 ± 1.13^{d}	27.62 ± 0.69^{a}
Açaí	407.03 ± 2.84^{a}	253.93 ± 0.89^{a}	58.43 ± 0.92^{a}	25.12 ± 1.46^{a}
Trolox	–	–	–	23.77 ± 0.12^{a}

Values followed by different letters are significantly different at $p \leq 0.05$ by Tukey test mg GAE/g – mg gallic acid equivalent/g dry extract; mg QE/g – mg quercetin equivalent/g dry extract; mg CE/g - mg catechin equivalent/g dry extract.

CHO and 3742 CHNO compounds analyzed, only 1521 CHO (22.5%) and 1166 CHNO (31.5%) compounds are unique to a specific sample (**Fig. 1C**). This information is further supported by Venn diagrams (**Fig. S2**), which illustrate the large proportion of shared metabolites among the five fruit species, along with a smaller fraction of unique features contributing to their differentiation. (See Fig. 1.)

Here, we demonstrate that Amazonian Arecaceae fruits exhibit a complex and diverse metabolome, which can be resolved and differentiated at the molecular level using ultra-high-resolution mass spectrometry. The biological relatedness of the fruits is reflected in their metabolite profiles, which show considerable similarity despite the fruits' significant visual differences. Our comprehensive chemical map, however, allows for the analytical distinction of nuanced differences among the fruits based on characteristic compound classes and unique molecular profiles (Fig. 10). The metabolite map generated through ultrahigh-resolution mass spectrometry provides a detailed molecular characterization of the fruits, laying a solid groundwork for further investigation into the causal molecular mechanisms underlying their bioactivity.

These molecular-level differences provide a basis for understanding the functional properties of the fruits, particularly their antioxidant potential, which is further explored through quantitative assays in the following section.

3.2. Total phenolic, flavonoids, condensed tannins content and antioxidant activity

To further link the molecular composition with functional properties the total phenolic content (TPC), total flavonoids (TFC) and total condensed tannin contents (TCT) were determined in each fruit extract, and the results are presented in Table 1. TPC was evaluated using the Folin-Ciocalteu assay by manipulating the regression equation of the gallic acid calibration curve (**Fig. S3**), and the concentration of phenolic compounds per extract was expressed as mg GAE/g). The TPC assessed in our assays demonstrated that these Arecaceae fruits are potential sources of phenolic compounds. TPC content ranged from 313.22 to 407.03 mg GAE/g. The highest TPC was observed in açaí (407.03 mg GAE/g), followed by buriti (368.54 mg GAE/g) and pupunha (367.94 mg GAE/g), which showed no statistic significant difference. On the other hand, tucumã extract presented the lowest TPC (313.22 mg GAE/g).

The total flavonoid content was quantified based on the complexation reaction between aluminum chloride and the keto group at the C-4 position, along with the hydroxyl groups at C-3 or C-5 of flavones and

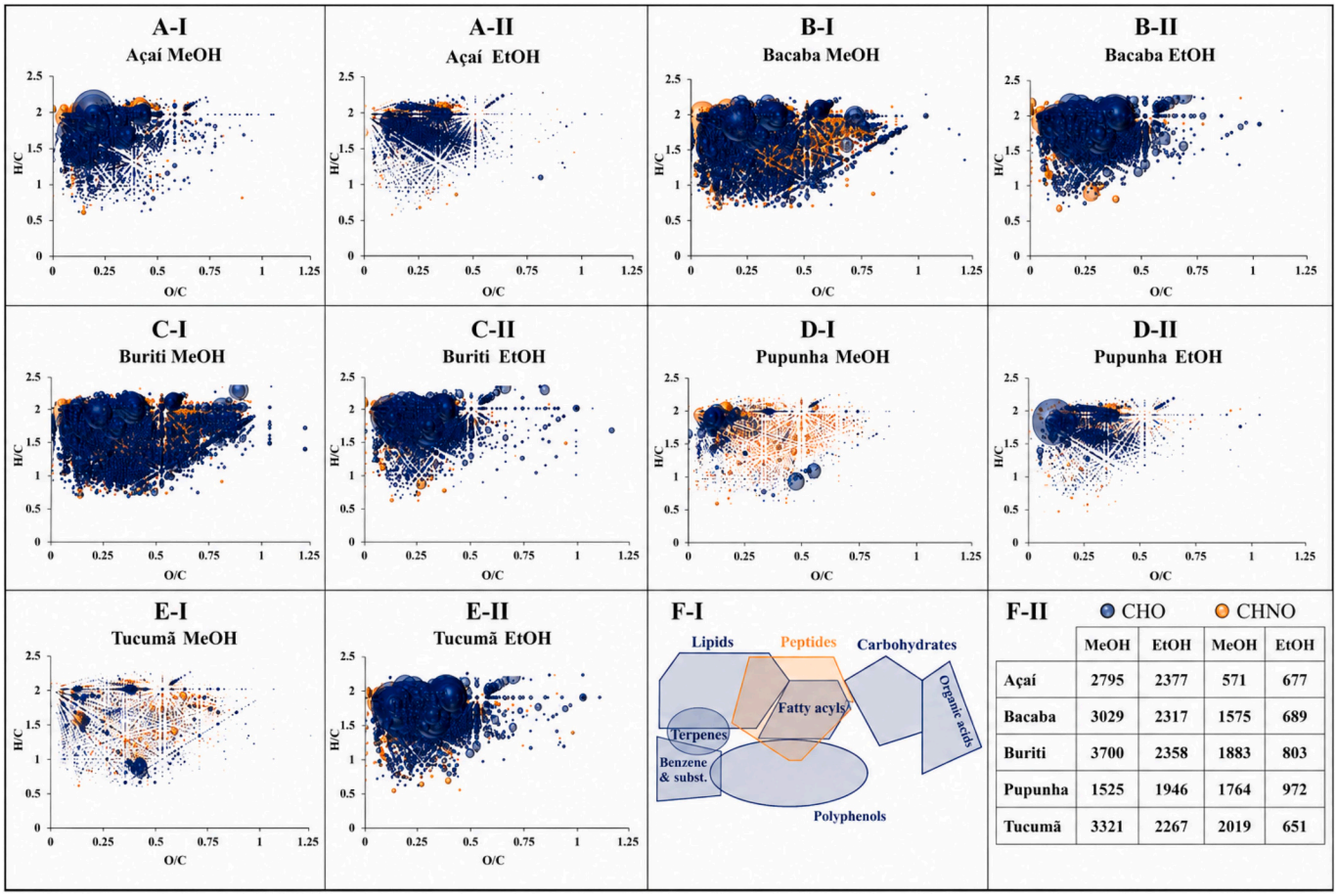


Fig. 4. Pearson correlation coefficients between the variables of the date varieties studied; (2,2- diphenyl-1-picrylhydrazyl) radical scavenging assay (DPPH); total phenolics content (TPC); total flavonoids content (TFC) and total condensed tannins content (TCT) in the Amazonian Arecaeae fruits. Correlation coefficients are indicated within each cell, while color intensity reflects the magnitude and direction of the correlations.

flavonols. Quercetin served as the reference standard since it is a flavonol holding a C-4 carbonyl group and hydroxyl groups at the C-3 and C-5 positions (Belew & Gebre, 2025).The regression equation of the quercetin calibration curve (**Fig. S3**), and the concentration of total flavonoid compounds per extract was expressed as mg QE/g). The TFC of the Arecaceae fruits showed notable variation among the samples, with TFC varied from 165.54 to 253.93 mg EQ/g. The açaí extract presented the highest TFC (253.93 mg EQ/g), followed by tucumã (233.48 mg EQ/g), while bacaba presented the lowest content (165.54 mg GAE/g).

The total condensed tannins (proanthocyanidins) content was determined by interpolating the samples absorbance values against a standard curve constructed from catechin standard solutions (**Fig. S3**), and the results were expressed as catechin equivalents per gram of dry extract (mg CE/g). In general, tannins are found in fruits in the non-polymerized form and have accentuated astringent characteristic and antioxidant potential. The TCT of the Arecaceae fruits showed subtle variation among the samples, with TCT varied from 36.23 to 58.43 mg CE/g. Like in the TPC and TFC assays, açaí exhibited the highest tannin content (58.43 mg CE/g), followed by buriti (49.96 mg CE/g), whereas pupunha presented the lowest content (36.23 mg CE/g).

Consistent with the molecular profiles observed in Section 3.1, açaí extract presented the highest TPC, TFC and TCT content among the Arecaceae fruits. In comparison to previous reports on TPC in açaí fruit, our value is higher than the content found by (Hassimotto et al., 2005) (3.28 ± 0.09 mg GAE/g); to those reported by (Rufino et al., 2010), by (Gordon et al., 2012) and (Kang et al., 2012) (32.68 ± 5.27 mg GAE/g, 34.37 ± 1.54 mg GAE/g DW, 73.00 ± 48 mg GAE/g, respectively); and lower to those reported by (Melo et al., 2016) (490.99 ± 0.08 mg GAE/g). Our finds on TFC content are following those conducted with eight genotypes from two species of açaí from the Brazilian Amazonian (TFC in *E. precatoria* genotypes ranged from164.45 to 325.07 mg QE/100 g; and TFC in *E. oleracea* genotypes ranged from 136.75 to 306.55 mg/100 g) (Lisboa et al., 2022). Açaí fresh seeds, flour and roasted seed power are known for their high content of tannins. In an earlier study, the fresh seed and seed flour exhibited TCT of 43.92 and 45.54 mg CE/100 g, respectively (Alves et al., 2022). Silva et al. (2025) evaluated the TCT in six samples of roasted açaí seeds powder from different places in Brazil. The results showed a lower content of condensed tannins (from 0.24 to 0.82 mg tannic acid/g). In contrast, fresh seeds showed a high TCT content (158 mg EC/g). These results corroborate with our findings and reinforce the potential application of the entire fruit as source of some bioactive compounds.

The DPPH method employs the stable radical 1,1-diphenyl-2-picryl-hydrazyl to assess the capacity of compounds to scavenge free radicals. The results are commonly expressed as IC_{50}, standing for the antioxidant concentration needed to decrease the initial DPPH level by 50%. A lower IC_{50} value indicates a stronger antioxidant activity. The antioxidant power of Arecaceae fruit extracts tested by DPPH ranged from 25.12 to 59.53 μg mL^{-1} (Table 1 and **Fig. S4**). The extracts of açaí and pupunha demonstrated remarkable antioxidant efficacy with IC_{50} values of 25.12 μg mL^{-1} and 27.62 μg mL^{-1}, respectively. Statistically significant variations were not observed for açaí and pupunha extract when compared with Trolox standard, which presented an IC_{50} of 23.77 μg mL^{-1}. The lower IC_{50} values for açaí and pupunha suggest these species have superior capabilities to scavenge DPPH radicals and mitigate oxidative stress compared to the other extracts. Earlier studies have shown that

Arecaceae species can be considered a promising source of antioxidants (Amorim et al., 2024; Cabral et al., 2020; Pacheco-Palencia et al., 2009; Teixeira et al., 2022). These findings highlight the nutritional relevance of these fruits as natural sources of dietary antioxidants, which may contribute to antioxidant capacity, although their biological effects in vivo were not evaluated in this study. From an application perspective, the high phenolic and flavonoid contents indicate their potential use as functional ingredients in food formulations, including natural antioxidant additives and products with potential health-promoting properties, as suggested by their chemical composition.

To evaluate the influence of the TPC, TFC and TCT elements on the antioxidant activity of Arecaceae fruits, we calculated Pearson correlation coefficients (Fig. 4). A strong negative correlation was found between the IC_{50} values of the DPPH test and the phenolic compounds ($r = -0.87$) showing that samples with higher concentrations of phenolics require smaller amounts of extract to inhibit 50% of the radical, which could reflect a higher antioxidant efficiency. In contrast, a moderate positive correlation was found between flavonoids and tannins ($r = 0.65$) and between total phenolics and flavonoids ($r = 0.54$), denoting an expected co-occurrence, considering that flavonoids constitute a subclass of phenolics and share common biosynthetic pathways. These results provide molecular-level evidence linking phenolic composition to antioxidant activity, demonstrating a structure–function relationship that extends beyond conventional bulk quantification approaches. The findings obtained are consistent with previous studies that report a correlation between the phenolic compounds content and antioxidant capacity in different plant matrices (Alahyane et al., 2019; Benmeddour et al., 2013; Ouamnina et al., 2024).

To further strengthen the relationship between metabolomic composition and antioxidant activity, the molecular features detected by FT-ICR-MS were examined considering their structural characteristics associated with redox properties. As observed, the antioxidant potential of Arecaceae fruits is closely correlated with the total phenolic content, particularly total flavonoids, which are known for their strong electron-donating and radical-scavenging capacities. The FT-IC-MS analysis, interpreted through the Van Krevelen diagram (**Fig. 1 A-I**), revealed a predominance of these compounds, as shown by high O/C ratios, indicative of abundant hydroxyl and glycosidic groups, and relatively low H/C ratios, reflecting their aromatic character.

Flavonoids typically exhibited intermediate to high O/C (0.4–0.6) and low H/C (0.67–1.11) ratios, consistent with polycyclic, oxygen-rich structures. In contrast, phenolic acids, such as gallic and vanillic acids, which are widely reported in the Arecaceae family (Morais et al., 2022), are easily recognized by their low molecular weight, aromatic nature, and high oxygenation level (O/C ~ 0.6–0.7), which contribute to their pronounced antioxidant activity. Phenylpropanoids, including cinnamic acid derivatives such as caffeic, *p*-coumaric, rosmarinic, and chlorogenic acids, which are also abundantly found in these palms (Morais et al., 2022; Rincón-Cervera et al., 2023) displayed moderate O/C (0.33–0.56) and H/C (~0.89) ratios, consistent with partially oxygenated side chains derived from phenylalanine. Simple phenols and tannins from Arecaceae family (Hamed et al., 2025) showed high O/C (0.5–0.69) and intermediate H/C (0.86–1.23) ratios, indicating extensive hydroxylation and possible glycosidic conjugation. Conversely, quinones exhibited lower O/C (0.21–0.27) and H/C (0.66–0.86) ratios, denoting highly conjugated, oxidized aromatic structures.

In summary, the antioxidant activity of Arecaceae fruits is primarily associated with oxygen-rich phenolic compounds, including anthocyanins (cyanidin derivatives), flavonoids (e.g., quercetin ($C_{15}H_{10}O_7$), kaempferol ($C_{15}H_{10}O_6$), rutin ($C_{27}H_{30}O_{16}$)), and phenolic acids (e.g., gallic ($C_7H_6O_5$), chlorogenic ($C_{16}H_{18}O_9$), and protocatechuic ($C_7H_6O_4$) acids) (Morais et al., 2022), whose high degree of hydroxylation and conjugated aromatic structures enable efficient hydrogen or electron donation and radical stabilization via resonance. The superior antioxidant performance observed for açaí can be mechanistically attributed to its enrichment in oxygenated aromatic metabolites, particularly anthocyanins such as cyanidin-3-*O*-glycoside and cyanidin-3-*O*-rutinoside, as well as carotenoids like lutein (Morais et al., 2022). These compounds are characterized by highly conjugated structures and multiple hydroxyl functionalities, which enhance their radical scavenging capacity. This interpretation is further supported by their distribution in the van Krevelen diagram, where they occupy regions of high O/C and low H/C ratios, indicative of highly oxidized and structurally functionalized metabolites associated with strong antioxidant activity. Additionally, the presence of conjugated carbonyl-containing compounds, such as quinones and oxidized polyphenols, may further enhance redox cycling and radical scavenging capacity. Altogether, the elemental composition patterns observed in the Van Krevelen diagram, combined with the chemotaxonomic profile of the Arecaceae family, highlight the predominance of polyphenolic compounds, particularly flavonoids, phenolic acids, tannins, and phenylpropanoids, as the main contributors to the strong antioxidant activity exhibited by these species.

Table 2
Vitamer distribution of folates in [μg/100 g] on dry weight and total folate content calculated as PteGlu in [μg/100 g] on dry weight. Different letters (^{a,b,c}) indicate statistically significant differences in the total folate content (Games–Howell; $\alpha = 0.05$).

Sample	vitamer content [μg/100 g dry weight]					Total folate [μg/100 g PteGlu]
	PteGlu	H_4folate	5-CH_3-H_4folate	5-CHO-H_4folate	10-CHO-PteGlu	
Açaí	3.13 ± 0.67	n.d.	17.70 ± 0.81	4.10 ± 0.52	11.99 ± 6.16	35.21 ± 6.45^{a}
Bacaba	n.d.	n.d.	28.24 ± 2.10	1.66 ± 0.19	5.58 ± 0.16	33.89 ± 1.81^{a}
Pupunha	n.d.	n.d.	18.50 ± 1.45	< LOQ	< LOQ	19.25 ± 1.36^{b}
Tucumã	1.45 ± 1.15	1.17 ± 0.22	131.89 ± 15.94	1.33 ± 0.06	2.32 ± 0.33	132.64 ± 16.27^{c}

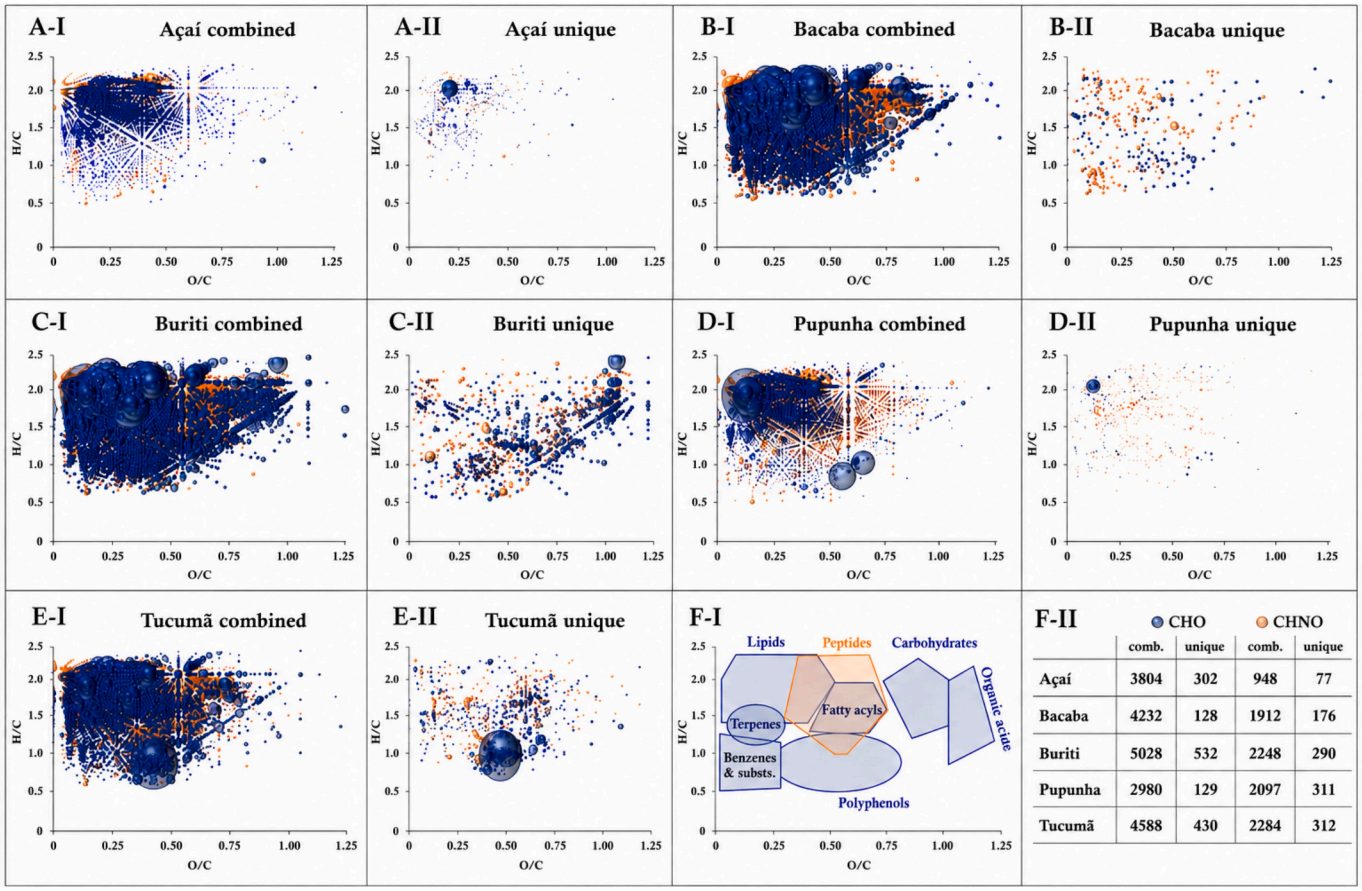
In addition to phenolic compounds, peptides also exhibit potent antioxidant activity through multiple mechanisms, including the neutralization of reactive oxygen species (ROS), stabilization of free radicals via hydrogen atom transfer or electron donation, formation of stable complexes with metal ions, and modulation of the body's endogenous defense systems, which could be related to their structure-activity relationships (Bahut et al., 2020; Zhu et al., 2024). Plant-derived antioxidant peptides represent a class of small molecules, in general composed of 2–20 amino acids, with molecular weights typically below 0.3 kDa (Zhu et al., 2024). As illustrated in the Van Krevelen diagram (**Fig. 1 A-I**), the Arecaceae fruits display a high abundance of peptide-related compounds, characterized by O/C (~0.3–0.7) and H/C (~1.1–2.25) ratios, consistent with nitrogen- and carbon-rich backbones.

Since our protocols for the antioxidant activity tests were designed for phenolic and flavonoid compounds, and peptides were not quantified in this study, their molecular signatures strongly suggest a complementary contribution to the overall antioxidant potential of Arecaceae fruits. Thus, the combined presence of both phenolic and peptide antioxidants underlies the robust free radical–scavenging ability observed in these species.

While phenolic compounds explain the antioxidant properties of these fruits, a comprehensive assessment of their nutritional value also requires the evaluation of essential micronutrients, such as folates, which are investigated in the following section.

3.3. Folate content and vitamer distribution

To complement the functional characterization and provide a



	CHO comb.	CHO unique	CHNO comb.	CHNO unique
Açaí	3804	302	948	77
Bacaba	4232	128	1912	176
Buriti	5028	532	2248	290
Pupunha	2980	129	2097	311
Tucumã	4588	430	2284	312

Fig. 5. HCA dendrograms generated from FT-ICR-MS molecular fingerprints of açaí, bacaba, buriti, pupunha, and tucumã fruits, illustrating sample grouping according to methanolic (A-I) and ethanolic (A-II) eluates.

broader nutritional perspective, the total folate content and vitamer distribution were quantified based on dry weight. Comprehensive analyses of folate vitamers in palm fruits are currently lacking; existing studies, such as those on dates, have been restricted to total folate quantification without characterizing individual vitamer distributions (Aslam et al., 2013). In contrast, this study represents the first comprehensive characterization of folate vitamer distribution in Amazonian Arecaceae fruits, addressing a significant gap in the nutritional profiling of these species. Our stable isotope dilution analysis (SIDA) enables the accurate quantification of the key food-derived vitamers, including PteGlu, H_4folate, 5-CH_3-H_4folate, 5-CHO-H_4folate, and 10-CHO-H_4folate. The total folate contents and their respective vitamer distributions are summarized in Table 2**.** Across the four fruits analyzed, total folate levels ranged from 19.25 ± 1.36 to 132.64 ± 16.27 μg/100 g dry weight. The vitamer 5-CH_3-H_4folate is often described as the main vitamer in fruits (Obermaier et al., 2023; Striegel et al., 2018). The results show that this also applies to the four palm fruits açaí, bacaba, pupunha and tucumã. Considering the water contents of approximately 30.36% (bacaba), 37.17% (açaí), 51.27% (pupunha) (Gualberto et al., 2025), and 52.37% (tucumã) (Oliveira et al., 2020), the total folate concentrations on a fresh weight basis are 23.60 μg/100 g for bacaba, 22.12 μg/100 g for açaí, 9.38 μg/100 g for Pupunha, and 63.17 μg/100 g for tucumã. When evaluated against the average daily folate intake of 376 μg in the Brazilian population (Steluti et al., 2017), tucumã represents a particularly rich source of folate. Its folate content was significantly higher than that of the other analyzed fruits (Welch's ANOVA $p < 0.001$) with Games–Howell post hoc test, $\alpha = 0.05$). This difference was further supported by large effect sizes (Hedges' $g > 6.76$), indicating a pronounced separation between tucumã and the remaining fruit types. Statistical analysis was performed using the statistics package (version 4.5.2) within the Rstudio environment. This highlights tucumã's substantial potential to contribute to daily folate intake, underscores its nutritional relevance, and supports further investigation into its folate bioavailability and dietary contribution. From a nutritional perspective, these results suggest that tucumã can be considered a valuable dietary source of folates, suggesting its potential relevance in strategies aimed at improving micronutrient intake. Furthermore, the characterization of individual vitamers provides relevant information for food processing and nutritional bioavailability studies. Folate plays an essential role in various metabolic pathways. It is especially important in cell proliferation and in on-carbon transfers for the synthesis of DNA (Bailey et al., 2015; Schirch & Strong, 1989). The folate content of tucumã is comparable to that of well-known tropical fruits like mango (55.8–74.5 μg/100 g) and papaya formosa (61.6 μg/100 g) (Striegel et al., 2019). Conversely, the lower folate levels measured in açaí, bacaba, and pupunha are like those found in less folate-rich native Brazilian fruits such as bacupari (9.11 μg/100 g pulp) and canistel (26.38 μg/100 g pulp) (Obermaier et al., 2023).

Although the nutritional and functional potential of these fruits is supported by their chemical composition and antioxidant capacity, it should be noted that no biological or in vivo assays were performed in this study. Therefore, any health-related implications remain indicative and require further experimental validation.

In addition to nutritional profiling, multivariate statistical approaches were applied to further explore the relationships between metabolite composition and fruit differentiation.

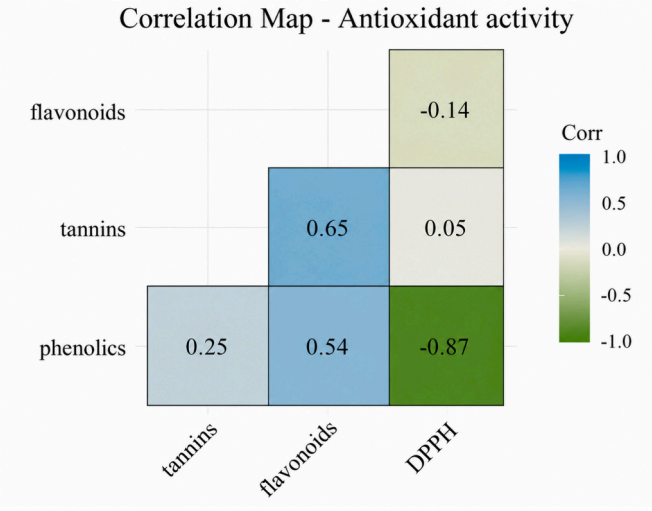


Fig. 6. Partial Least Squares Discriminant Analysis (PLS-DA) of EtOH and MeOH elutions (**A-I** and **A-II**, respectively).

3.4. Chemometric approaches for metabolite discrimination and classification

To further interpret the metabolomic data and identify key features responsible for fruit differentiation, chemometric methods were applied. Both unsupervised and supervised multivariate approaches were used. Principal Component Analysis (PCA) was first employed as an unsupervised exploratory approach, while Hierarchical Cluster Analysis (HCA) and Partial Least Squares Discriminant Analysis (PLS-DA) were used to evaluate sample clustering and identify discriminant metabolites. Statistical validation on the supervised models was performed using repeated stratified cross-validation and permutation testing. Additionally, significant features were identified based on a threshold for the Variable Importance for Projection (VIP) value, allowing us to highlight significant metabolic differences and assess their contribution to fruit differentiation. These chemometric approaches enabled the identification of key molecular discriminants and revealed previously unknow metabolic signatures, highlighting the chemical drivers underlying the differentiation and functional properties of the fruits. PCA was initially performed as an unsupervised exploratory approach to evaluate the intrinsic structure of the dataset. The PCA score plots (**Fig. S5**) revealed grouping tendencies according to fruit species for both eluates, indicating that metabolic differences are already present in the data prior to supervised modeling.

The HCA dendrogram (Fig. 5A-I and **II**) reflects the similarity between the fruit elutions by grouping samples into clusters based on metabolic profiles. All replicates from each fruit are grouped into distinct clusters, confirming consistency within each species. In the MeOH elution, açaí and pupunha clustered together, indicating a certain degree of chemical similarity. Tucumã and bacaba also showed similarity. In the EtOH elution, the fruits are grouped into distinct clusters. Tucumã clustered more closely with buriti, suggesting greater similarity between them. Pupunha formed a distinct cluster, indicating a unique metabolite profile, and highlighting the diversity of its metabolites. To further emphasize metabolic differences between the fruit species, HCA was also performed using only differential metabolites (VIP $>$ 1). The resulting dendograms (**Fig. S6**) showed improved discrimination between fruit species, confirming that the selected variables capture the main sources of metabolic variation.

Partial Least Squares Discriminant Analysis (PLS-DA) was used to identify differential metabolites and develop classification models for the EtOH and MeOH eluates (Fig. 6, **A-I** and **A-II**). Model performance was assessed using repeated stratified cross-validation, which provided estimates of classification accuracy, R^2 and Q^2 for models containing different numbers of components. For both eluates, the supervised models showed high classification performance, with the MeOH model exhibiting slightly superior predictive ability ($Q^2 = 0.91$) compared to the EtOH model ($Q^2 = 0.89$). These metrics, obtained through cross-validation, confirm the strong reliability and robustness of the constructed models.

To further evaluate model robustness and exclude random class separation, permutation testing was also performed (**Fig. S7**). In all cases, the observed model performance was higher than that obtained for permuted models, supporting the statistical significance of the discrimination and indicating that the class separation was not driven by overfitting or random chance.

In PLS-DA, the variable importance in projection (VIP) scores are key indicators, with higher VIP values showing the variables that most significantly influence model discrimination. The most important VIP scores for both models are illustrated in Fig. 7 (**A-I and AII**). VIP score values above 1 are considered significant.

These PLS-DA models constructed from FT-ICR-MS data revealed distinctive metabolic fingerprints among the five Amazonian fruits, reflecting their diverse chemical compositions and antioxidant capacities. The VIP-ranked metabolites (VIP $>$ 1.0) showed clear solvent-dependent extraction patterns: the discriminators in the methanolic elutions were enriched in nitrogen-containing compounds, while ethanolic elutions had a predominance of triterpenoids, and fatty acid

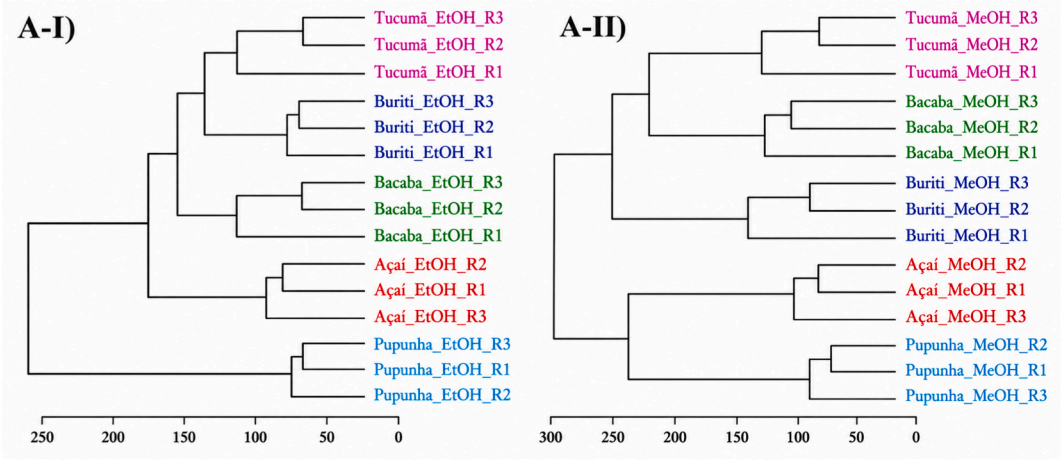
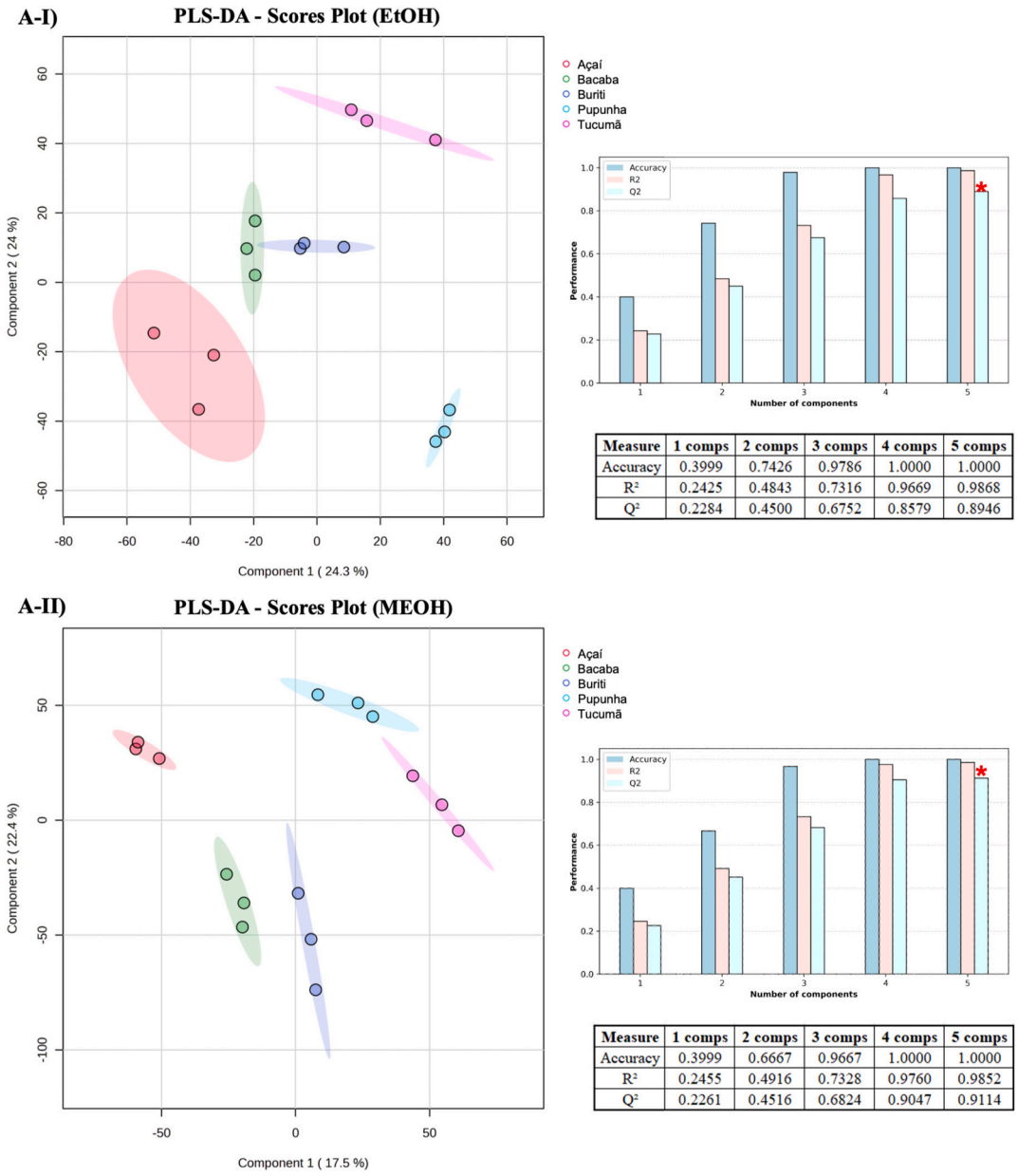


Fig. 7. Variable Importance in Projection (VIP) scores plot showing the most significant ions for differentiating the samples in the EtOH elution (**A-I**) and in the MeOH elution (**A-II**).



Measure	1 comps	2 comps	3 comps	4 comps	5 comps
Accuracy	0.3999	0.7426	0.9786	1.0000	1.0000
R^2	0.2425	0.4843	0.7316	0.9669	0.9868
Q^2	0.2284	0.4500	0.6752	0.8579	0.8946

Measure	1 comps	2 comps	3 comps	4 comps	5 comps
Accuracy	0.3999	0.6667	0.9667	1.0000	1.0000
R^2	0.2455	0.4916	0.7328	0.9760	0.9852
Q^2	0.2261	0.4516	0.6824	0.9047	0.9114

Fig. 8. Schematic representation of the comparative chemical composition and functional characteristics of five Amazonian palm fruits (Arecaceae family), including açaí (*E. oleracea*), pupunha (*B. gasipaes*), tucumã (*A. aculeatum*), buriti (*M. flexuosa*), and bacaba (*O. bacaba*). The diagram integrates key findings from ultra-high-resolution FT-ICR-MS metabolomics, spectrophotometric assays, antioxidant activity, and folate vitamer analysis. Each fruit is characterized by distinct molecular signatures, including phenolic compounds, amino-related metabolites, terpenoids, lipids, and nitrogen-containing species, which are associated with their respective functional and nutritional properties. Compound classes are based on putative annotations derived from accurate mass measurements and should be interpreted accordingly.

derivatives. These findings reinforce the solvent-driven selectivity in extracting distinct chemical classes and support the use of EtOH as a complementary matrix for profiling functional constituents in Arecaceae fruits.

In the methanolic elutions, together, alkaloids and steroidal derivatives accounted for ≈ 75% of the total VIP weight, showing that both classes are key chemical drivers of differentiation among the fruits analyzed. The high-VIP metabolites such as pyridine-derived alkaloid (*m/z* 340.1754 $[C_{17}H_{25}O_6N]^+$); piperidine-derived alkaloids (*m/z* 362.1597 $[C_{19}H_{23}NO_6]^+$); quinone-derived compounds (*m/z* 293.1496) $[C_{15}H_{20}N_2O_4]^+$), and steroids derivatives (*m/z* 355.2245 $[C_{21}H_{32}O_3 + Na]^+$; *m/z* 609.3246 $[C_{30}H_{50}O_{11} + Na]^+$and *m/z* 649.3558 $[C_{33}H_{54}O_{11} + Na]^+$) were the major contributors to the discrimination of açaí and pupunha. These fruits exhibited the highest total phenolic and flavonoid contents (407.03 and 367.94 mg GAE g^{-1}; 253.93 and 182.28 mg QE g^{-1}, respectively) and the strongest antioxidant responses (IC_{50} = 25.12 and 27.62 μg mL^{-1}). The presence of phenolic–nitrogen conjugates suggest the occurrence of amino-phenolic condensation products, which are recognized for synergistic radical-scavenging mechanisms (Carreon-Gonzalez & Alvarez-Idaboy, 2023). Their high VIP values confirm their importance not only as chemotaxonomic markers but also as functional metabolites enhancing the antioxidant profile of these fruits.

The ethanolic extracts were characterized by abundant terpene-derived compounds (*m/z* 529.3500 $[C_{30}H_{50}O_6 + Na]^+$; *m/z* 689.4755 $[C_{42}H_{66}O_6 + Na]^+$ and *m/z* 675.4078 $C_{36}H_{60}O_{10} + Na]^+$, steroidal saponins (*m/z* 681.4184 $[C_{35}H_{62}O_{11} + Na]^+$), and fatty acids (*m/z* 635.5219 $[C_{37}H_{72}O_6 + Na]^+$; *m/z* 637.5377 $[C_{37}H_{74}O_6 + Na]^+$), which dominated the VIP ranking, contrasting with the alkaloid-phenolic

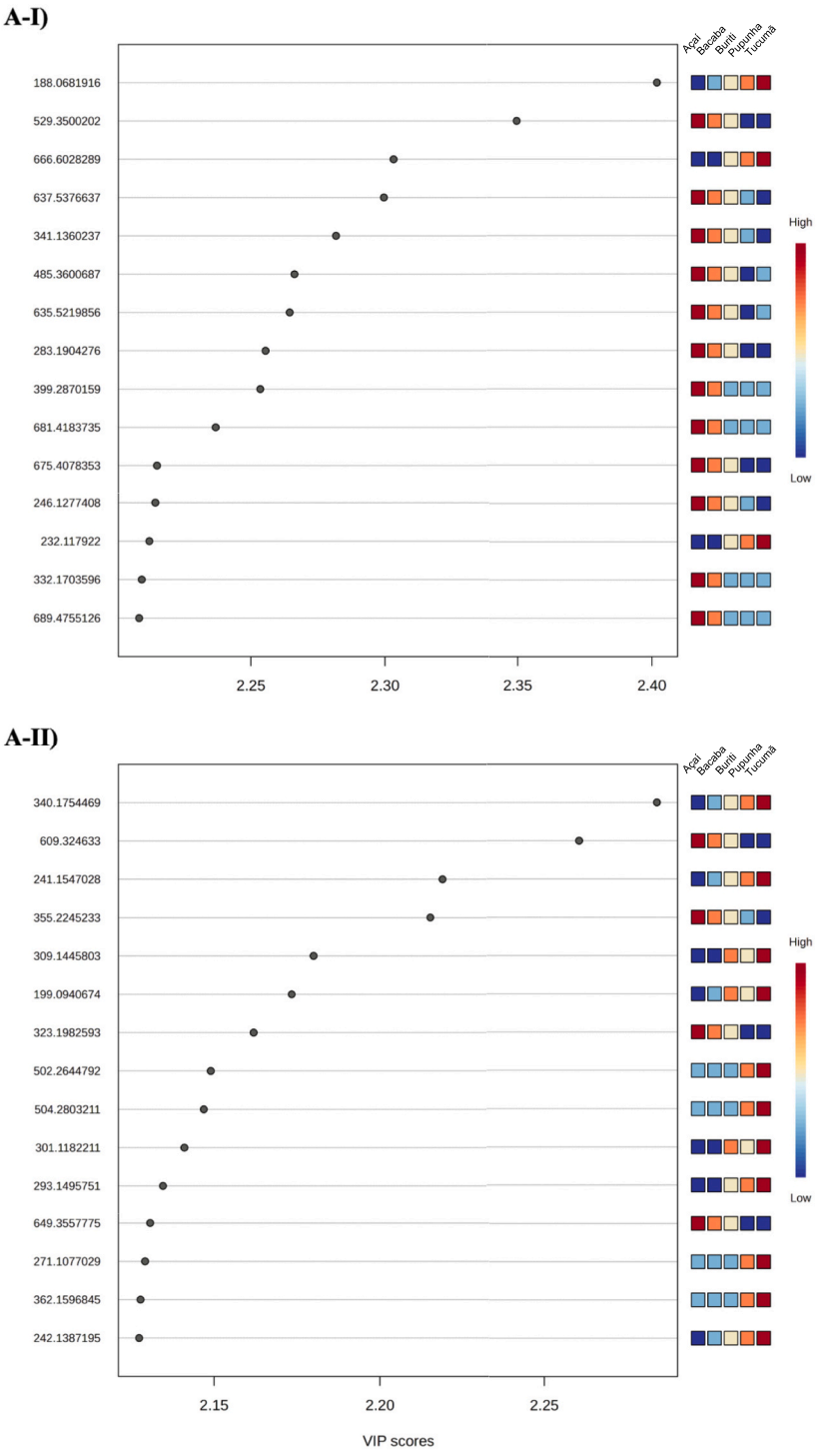


Fig. 9. Van Krevelen diagrams (H/C vs. O/C) of molecular formulas assigned to açaí (A), bacaba (B), buriti (C), pupunha (D), and tucumã (E) fruits. Molecular profiles obtained from methanolic SPE eluates are presented in Panels I, whereas ethanolic SPE eluates are shown in Panels II. Panel F—I summarizes the principal chemical-class regions within the Van Krevelen space, and Panel F-II reports the number of CHO and CHNO formulas detected in MeOH and EtOH molecular datasets. Bubble size reflects the relative abundance of each molecular formula.

enrichment in MeOH extracts. These classes are typical constituents of the Arecaceae family and have been associated with membrane stabilization, anti-inflammatory potential, and modulation of oxidative stress (Câmara et al., 2024; Masyita et al., 2022). Although these fruits displayed higher IC_{50} values in the DPPH assay (46.02–41.35 μg mL^{-1}), the structural complexity of saponins and triterpenes contributes to long-term antioxidant effects, supporting other antioxidants compounds and contributing to a synergetic effect (Sharma et al., 2023).

The predominance of high-VIP phenolic and alkaloid derivatives in açaí and pupunha may explain their superior antioxidant potential and nutritional relevance as dietary sources of radical-scavenging compounds. Conversely, the enrichment of triterpenoids and saponins in buriti and bacaba suggests potential anti-inflammatory and cholesterol-modulating activities, expanding their functional applications beyond

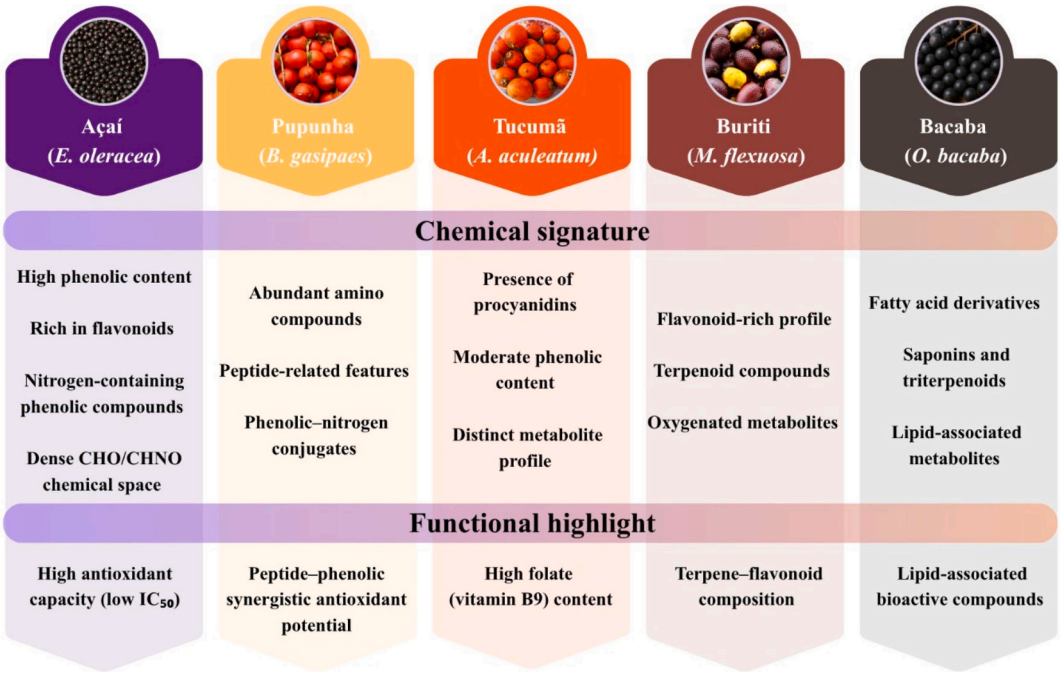


Fig. 10. Van Krevelen diagrams (H/C vs. O/C) of molecular formulas assigned to açaí (A), bacaba (B), buriti (C), pupunha (D), and tucumã (E) fruits. Combined molecular profiles derived from methanolic and ethanolic eluates are shown in Panels I, while fruit-specific molecular signatures are presented in Panels II. Panel F—I summarizes the principal chemical-class regions within the Van Krevelen space, and Panel F-II reports the number of CHO and CHNO formulas detected in the combined and unique molecular datasets. Bubble size reflects the relative abundance of each molecular formula.

antioxidant ability (Câmara et al., 2024; Masyita et al., 2022). These findings suggest that different Arecaceae fruits may serve as sources of distinct functional ingredients, ranging from antioxidant-rich extracts to compounds previously associated with anti-inflammatory and metabolic-related effects in the literature, supporting their targeted use in functional food and nutraceutical formulations. All VIP scores described here were tentatively annotated based on comparisons with earlier studies and database information. The putative annotation is summarized in **Table S1** and **S2**.

It is important to emphasize that compound annotations in this study are based on accurate mass measurements and molecular formula assignment using FT-ICR-MS data. Therefore, these annotations should be considered putative, as structural confirmation would require additional MS/MS experiments and/or comparison with authentic reference standards. Consequently, the classification of compound classes and their associated biological relevance are inferred based on literature reports and should be interpreted with caution.

A schematic overview summarizing the comparative chemical signatures and functional characteristics of the investigated fruits is presented in Fig. 8.

This study advances beyond conventional metabolomic surveys by integrating compositional data with antioxidant activity and molecular-level descriptors such as oxygenation degree. This approach provides a functional interpretation of chemical diversity, allowing the identification of structural features associated with bioactivity. Such integration contributes to the emerging field of food metabolomics by bridging the gap between molecular complexity and biological function, offering a more comprehensive understanding of the health-promoting properties of Amazonian fruits.

Despite the comprehensive molecular coverage achieved by (DI) FT-ICR-MS, some limitations should be considered. Due to the absence of chromatographic separation, MS/MS fragmentation data, and authentic standards, metabolite annotation was restricted to MSI Level 3. As a result, individual compound identities could not be unequivocally confirmed. Nevertheless, the ultrahigh mass resolution and accuracy of FT-ICR-MS, combined with chemometric analyses such as Van Krevelen diagrams and PCA, provide a robust framework for comparative metabolomic profiling and enable the characterization of broad chemical trends across samples. Future studies integrating LC-MS/MS or complementary structural techniques are recommended to achieve higher confidence in compound identification.

4. Conclusions

This study provides an integrative foodomics characterization of Amazonian Arecaceae fruits, combining untargeted (DI) FT-ICR-MS metabolomics with targeted nutritional and functional analyses. By integrating ultra-high-resolution chemical mapping with total phenolic, flavonoid, condensed tannins quantification, antioxidant activity, and chemometric models, we revealed both shared and unique bioactive molecular profiles among these species. Açaí and pupunha exhibited the highest total phenolic and flavonoid contents (407.03 and 367.94 mg GAE g^{-1}; 253.93 and 182.28 mg QE g^{-1}, respectively) and the strongest antioxidant responses (IC_{50} = 25.12 and 27.62 μg mL^{-1}). Quantification of the B_9 vitamer contents revealed that tucumã exhibited the highest concentration at 132.64 μg/100 g dry weight, suggesting its considerable potential to contribute meaningfully to the fulfillment of daily folate intake requirements. The chemometric approaches confirmed metabolic consistency within species and allowed the discrimination between them, identifying significant features with high VIP scores that differentiate their profiles.

The findings support the nutritional and antioxidant potential of these Amazonian palm fruits, especially açaí, tucumã and pupunha, providing molecular evidence for their potential classification as promising sources of functional bioactive compounds. However, while in vitro assays offer valuable insights into their functional properties, further studies are necessary to evaluate their bioavailability, metabolism, and in vivo biological activity of their bioactive constituents to substantiate their applicability in food and nutraceutical contexts. Future research should focus on translating these findings into food product development, including the formulation of functional ingredients and the assessment of their stability in food matrices, as well as

conducting in vivo studies to validate their health benefits. Importantly, this study goes beyond conventional compositional analyses by establishing direct links between molecular-level diversity and functional properties, representing a significant advancement in the foodomics characterization of underexplored tropical fruits. The integration of ultra-high-resolution metabolomics, chemometric modeling, and targeted nutritional analysis provides a robust framework for the bioeconomy and valorization of Amazonian biodiversity and supports the development of novel functional food ingredients, contributing to bridge the knowledge gap on the chemical composition of native Amazonian fruits and reinforcing their importance for sustainable exploitation and health-oriented innovation.

CRediT authorship contribution statement

Gesiane da S. Lima: Writing – review & editing, Writing – original draft, Visualization, Validation, Formal analysis, Data curation, Conceptualization. **Lanaia I.L. Maciel:** Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Conceptualization. **Tamara Lenz:** Writing – review & editing, Writing – original draft, Methodology, Investigation, Data curation. **Hugo G. Machado:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation. **Nerilson M. Lima:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation. **Jorge L.S. Simão:** Writing – review & editing, Writing – original draft, Visualization, Validation, Investigation, Formal analysis, Data curation. **Vanessa G.P. Severino:** Writing – review & editing, Writing – original draft, Methodology, Investigation, Data curation. **Michael Rychlik:** Writing – review & editing, Writing – original draft, Visualization, Resources, Formal analysis, Data curation. **Boniek Gontijo:** Writing – review & editing, Visualization, Validation, Supervision, Resources, Project administration, Methodology, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Stefan A. Pieczonka:** Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Data curation, Conceptualization. **Philippe Schmitt-Kopplin:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Resources, Project administration, Methodology, Funding acquisition, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

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

Acknowledgments

The authors gratefully thank the National Council for Scientific and Technological Development (CNPq, Conselho Nacional de Desenvolvimento Científico e Tecnológico, Brazil) for the financial support (Grant No. 200261/2023-1 and 200260/2023-5).

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.foodchem.2026.150319.

Data availability

Data will be made available on request.

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Update

Food Chemistry

Volume 525, Issue P3, 1 October 2026, Page

DOI: https://doi.org/10.1016/j.foodchem.2026.150767

Food Chemistry 525 (2026) 150767

Contents lists available at ScienceDirect

Food Chemistry

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

Corrigendum

Corrigendum to "Metabolomic profile of edible Amazonian Arecaceae fruits by FT-ICR-MS: Insights into chemical, nutritional and antioxidant profiles" [Food Chem. 525 (2026) 150319]

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The authors regret that, during the production process, the figure files became systematically mismatched with their corresponding figure numbers and captions. As a consequence, the original Figs. 2 and 3 do not appear as Figs. 2 and 3 in the published article. Instead, they were published as Figs. 4 and 5, respectively, together with captions belonging to different figures. Additionally, the original Figs. 2–8 were published under incorrect figure numbers (Figs. 4–10), while the associated captions were also displaced, resulting in incorrect correspondence between figure images, figure numbers, captions, and the corresponding in-text citations throughout the manuscript.

This corrigendum is intended solely to restore the correct correspondence between each figure, its caption, and its citations in the text. These corrections are editorial in nature and do not affect any experimental data, results, discussion, interpretation, or conclusions presented in the article.

For clarity, the correct figure sequence, together with the corresponding captions, is provided below.

A revised manuscript showing all corrected in-text figure citations has been provided separately to facilitate the editorial review and implementation of these corrections.

The authors would like to apologies for any inconvenience caused.

Original Figure (correct)	Published as	Published caption	Correct caption
Fig. 2	Fig. 4	**Fig. 4.** Pearson correlation coefficients between the variables of the date varieties studied; (2,2- diphenyl-1-picrylhydrazyl) radical scavenging assay (DPPH); total phenolics content (TPC); total flavonoids content (TFC) and total condensed tannins content (TCT) in the Amazonian Arecaceae fruits. Correlation coefficients are indicated within each cell, while color intensity reflects the magnitude and direction of the correlations.	**Fig. 2.** Van Krevelen diagrams (H/C vs. O/C) of molecular formulas assigned to açaí (A), bacaba (B), buriti (C), pupunha (D), and tucumã (E) fruits. Molecular profiles obtained from methanolic SPE eluates are presented in Panels I, whereas ethanolic SPE eluates are shown in Panels II. Panel FI summarizes the principal chemical-class regions within the Van Krevelen space, and Panel F-II reports the number of CHO and CHNO formulas detected in MeOH and EtOH molecular datasets. Bubble size reflects the relative abundance of each molecular formula.
Fig. 3	Fig. 5	**Fig. 5.** HCA dendrograms generated from FT-ICR-MS molecular fingerprints of açaí, bacaba, buriti, pupunha, and tucumã fruits, illustrating sample grouping according to methanolic (A-I) and ethanolic (A-II) eluates.	**Fig. 3.** Van Krevelen diagrams (H/C vs. O/C) of molecular formulas assigned to açaí (A), bacaba (B), buriti (C), pupunha (D), and tucumã (E) fruits. Combined molecular profiles derived from methanolic and ethanolic eluates are shown in Panels I, while fruit-specific molecular signatures are presented in Panels II. Panel FI summarizes the principal chemical-class regions within the Van Krevelen space, and Panel F-II reports the number of CHO and CHNO formulas detected in

(*continued on next page*)

DOI of original article: https://doi.org/10.1016/j.foodchem.2026.150319.

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https://doi.org/10.1016/j.foodchem.2026.150767

Available online 31 August 2026

(*continued*)

Original Figure (correct)	Published as	Published caption	Correct caption
			the combined and unique molecular datasets. Bubble size reflects the relative abundance of each molecular formula.
Fig. 4	Fig. 6	**Fig. 6.** Partial Least Squares Discriminant Analysis (PLS-DA) of EtOH and MeOH elutions (A-I and A-II, respectively).	**Fig. 4.** Pearson correlation coefficients between the variables of the date varieties studied; (2,2- diphenyl-1-picrylhydrazyl) radical scavenging assay (DPPH); total phenolics content (TPC); total flavonoids content (TFC) and total condensed tannins content (TCT) in the Amazonian Arecaceae fruits. Correlation coefficients are indicated within each cell, while color intensity reflects the magnitude and direction of the correlations.
Fig. 5	Fig. 7	**Fig. 7.** Variable Importance in Projection (VIP) scores plot showing the most significant ions for differentiating the samples in the EtOH elution (A-I) and in the MeOH elution (A-II).	Fig. 5. HCA dendrograms generated from FT-ICR-MS molecular fingerprints of açaí, bacaba, buriti, pupunha, and tucumã fruits, illustrating sample grouping according to methanolic (A-I) and ethanolic (A-II) eluates.
Fig. 6	Fig. 8	**Fig. 8.** Schematic representation of the comparative chemical composition and functional characteristics of five Amazonian palm fruits (Arecaceae family), including açaí (*E. oleracea*), pupunha (*B. gasipaes*), tucumã (*A. aculeatum*), buriti (*M. flexuosa*), and bacaba (*O. bacaba*). The diagram integrates key findings from ultra-high-resolution FT-ICR-MS metabolomics, spectrophotometric assays, antioxidant activity, and folate vitamer analysis. Each fruit is characterized by distinct molecular signatures, including phenolic compounds, amino-related metabolites, terpenoids, lipids, and nitrogen-containing species, which are associated with their respective functional and nutritional properties. Compound classes are based on putative annotations derived from accurate mass measurements and should be interpreted accordingly.	**Fig. 6.** Partial Least Squares Discriminant Analysis (PLS-DA) of EtOH and MeOH elutions (A-I and A-II, respectively).
Fig. 7	Fig. 9	**Fig. 9.** Van Krevelen diagrams (H/C vs. O/C) of molecular formulas assigned to açaí (A), bacaba (B), buriti (C), pupunha (D), and tucumã (E) fruits. Molecular profiles obtained from methanolic SPE eluates are presented in Panels I, whereas ethanolic SPE eluates are shown in Panels II. Panel F–I summarizes the principal chemical-class regions within the Van Krevelen space, and Panel F-II reports the number of CHO and CHNO formulas detected in MeOH and EtOH molecular datasets. Bubble size reflects the relative abundance of each molecular formula.	**Fig. 7.** Variable Importance in Projection (VIP) scores plot showing the most significant ions for differentiating the samples in the EtOH elution (A-I) and in the MeOH elution (A-II).
Fig. 8	Fig. 10	**Fig. 10.** Van Krevelen diagrams (H/C vs. O/C) of molecular formulas assigned to açaí (A), bacaba (B), buriti (C), pupunha (D), and tucumã (E) fruits. Combined molecular profiles derived from methanolic and ethanolic eluates are shown in Panels I, while fruit-specific molecular signatures are presented in Panels II. Panel F–I summarizes the principal chemical-class regions within the Van Krevelen space, and Panel F-II reports the number of CHO and CHNO formulas detected in the combined and unique molecular datasets. Bubble size reflects the relative abundance of each molecular formula.	**Fig. 8.** Schematic representation of the comparative chemical composition and functional characteristics of five Amazonian palm fruits (Arecaceae family), including açaí (*E. oleracea*), pupunha (*B. gasipaes*), tucumã (*A. aculeatum*), buriti (*M. flexuosa*), and bacaba (*O. bacaba*). The diagram integrates key findings from ultra-high-resolution FT-ICR-MS metabolomics, spectrophotometric assays, antioxidant activity, and folate vitamer analysis. Each fruit is characterized by distinct molecular signatures, including phenolic compounds, amino-related metabolites, terpenoids, lipids, and nitrogen-containing species, which are associated with their respective functional and nutritional properties. Compound classes are based on putative annotations derived from accurate mass measurements and should be interpreted accordingly.