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Jurubatiba Restinga: Chemical profiles of the essential oils from leaves, stems, and unripe fruits of *Neomitranthes obscura* (DC.) N. Silveira

Restinga de Jurubatiba: Perfis químicos do óleo essencial de folhas, caules e frutos imaturos da espécie Neomitranthes obscura (DC.) N. Silveira

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Abstract

The Brazilian Restinga ecosystem faces constant anthropogenic threats and environmental stresses that influence the secondary metabolism of plants. Underexplored species from unique ecosystems such as the Restinga may exhibit significant pharmacological and biotechnological potential, as in the case of *Neomitranthes obscura* (DC.) N. Silveira (Myrtaceae), an endemic species of the Atlantic Forest found in coastal sandy plains. This study focused on collecting leaves, stems, and unripe fruits of *N. obscura* in the Restinga de Jurubatiba National Park, Rio de Janeiro, and extracting their essential oils through hydrodistillation. The chemical composition of the different plant parts was analyzed by GC–MS and confirmed using spectral databases. The essential oils obtained from the various organs of *N. obscura* showed yields of 0.06%, 0.09%, and 0.92%, revealing 20, 27, and 27 chemical constituents for unripe fruits, stems, and leaves, respectively. The major components of the unripe fruit oil were sativene (15.15%), β-selinene (46.14%), and selina-3,7(11)-diene (9.48%), while those of the leaves and stems were zonarene (19.75–21.41%), selina-3,7(11)-diene (12.67–15.12%), and β-selinene (11.77–10.87%). Most of these compounds share a selinane-type structural core, indicating the predominance of this terpenoid skeleton in the essential oil composition of the species. This pattern reflects chemotaxonomic characteristics of the Myrtaceae family and points to potential ecological and pharmacological roles, positioning this species as a promising source of bioactive molecules with possible biotechnological and pharmaceutical applications. This study also represents the first description of the chemical composition of the essential oils extracted from the unripe fruits and stems of *N. obscura*, contributing to the chemical and chemotaxonomic knowledge of the species.

Resumo

A Restinga brasileira enfrenta ameaças antrópicas constantes e possui estresses ambientais que influenciam o metabolismo secundário das plantas. Espécies pouco estudadas de ecossistemas únicos como a Restinga podem apresentar potencial farmacológico e biotecnológico, como a Neomitranthes obscura (DC.) N. Silveira (Myrtaceae), uma espécie endêmica da Mata Atlântica encontrada na Restinga. O presente estudo focou em coletar folhas, caules e frutos verdes de N. obscura no Parque Nacional da Restinga de Jurubatiba, Rio de Janeiro, e extrair seus óleos essenciais através de hidrodestilação. A composição química das diversas partes estudadas foi analisada por CG-EM e confirmada utilizando bases espectrais. O óleo essencial obtido das diferentes partes de N. obscura obteve um rendimento de 0,06, 0,09 e 0,92% e revelou 20, 27 e 27 constituintes químicos para frutos imaturos, caules e folhas, respectivamente. Os componentes majoritários dos frutos imaturos foram sativeno (15,15%), β-selineno (46,14%) e selina-3,7(11)-diene (9,48), enquanto os de folhas e caules foram zonareno (19,75 - 21,41%), selina-3,7(11)-dieno (12,67 - 15,12%) e β-selinene (11,77 - 10,87%). A maioria desses compostos compartilham um núcleo estrutural do tipo selinano, indicando a predominância desse esqueleto terpênico na composição do óleo essencial da espécie. Isso reflete características quimiotaxonômicas da família Myrtaceae e aponta para potenciais papéis ecológicos e farmacológicos, posicionando essa espécie como uma fonte promissora de moléculas bioativas com possíveis aplicações biotecnológicas e farmacêuticas. Este estudo representa ainda a primeira descrição da composição química dos óleos essenciais extraídos dos frutos imaturos e dos caules de N. obscura, contribuindo para o conhecimento químico e quimiotaxonômico da espécie.

Introduction

Brazil boasts the most incredible biodiversity worldwide, with more than 15% of the global species diversity (Valli et al., 2018). Within this biodiversity, the Restinga ecosystem is defined by brazilian legislation as a "sandy deposit parallel to the coastline, generally elongated in shape, formed by sedimentation processes, where distinct communities influenced by marine factors occur, characterized by mosaic vegetation cover, found in beaches, sandbanks, dunes, and depressions, presenting, according to the successional stage, herbaceous, shrubby, and arboreal strata, the latter typically more interior" (Brasil, 2012). This ecosystem is sensitive and severely threatened by anthropogenic pressures, notably urban expansion, introduction of exotic species, alteration of the natural substrate, and selective harvesting of plants for ornamental use (Costa; Dias, 2001). Beyond these anthropic threats, Restinga environment presents natural challenges to plant development, including nutrient-poor sandy soils with low water retention capacity, high salinity, elevated temperatures, and intense solar radiation. In flood-prone areas, soil hypoxia can occur due to waterlogging, which further restricts plant growth. These environmental stresses directly influence the production of secondary metabolites, positioning native Restinga species as potential sources of bioactive molecules of interest (ICMBio, 2017).

Despite the ongoing daily loss of biodiversity in Brazil due to deforestation, the country implements various conservation measures, including the establishment of permanent protection areas such as the Parque Nacional da Restinga de Jurubatiba (PNRJ). Created on April 29, 1998, to preserve the unique Restinga ecosystem, regarded as the best-conserved along the coastline of Rio de Janeiro state. This park is the first Brazilian national park composed exclusively of this ecosystem. Covering approximately 14,922 hectares along 44 km of coastline, the PNRJ encompasses the municipalities of Macaé, Carapebus, and Quissamã, with the latter accounting for around 62% of its total area (Figure 1) (Rocha et al., 2023). These regions exhibit complex environmental mosaics, characterized by rich faunal and floral diversity. The distinct vegetation formations in this area hold potential for various applications due to their economic value, their role in the fishery productivity of associated lagoons, tourism promoted by their natural beauty, and the diverse secondary metabolites produced by the plant species thriving in this environment (Gonçalves-Esteves et al., 2001; Santos et al., 2009; Cogliatti-Carvalho et al., 2010).

Among the diversity present in the PNRJ, the genus *Neomitranthes*, belonging to the family Myrtaceae, which includes guava trees and eucalypts, was first described as a botanical genus in 1977. Endemic to Brazil, its species predominantly occur in the Atlantic Forest biome, including Restingas and coastal slopes. They are generally shrubs or small trees with simple, opposite leaves, often with an aromatic scent when crushed (Maia, 1993). The flowers are small, typically white, with numerous stamens, while the fruits are globose berries exhibiting variable coloration, ranging from purple to black when mature, containing succulent pulp (Vieira et al., 2021). Some *Neomitranthes* species are categorized as being at risk of

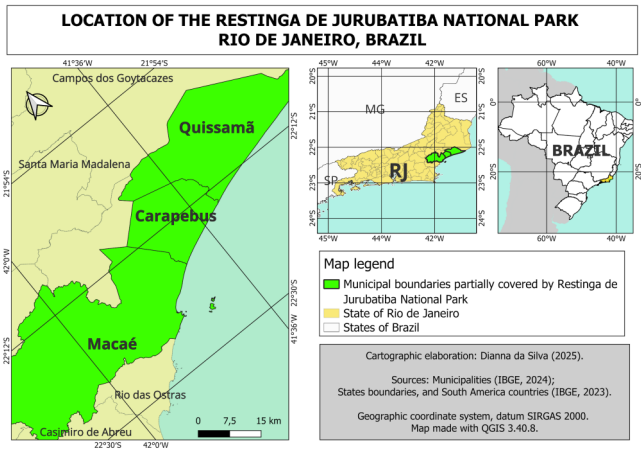


Figure 1. Maps of Restinga de Jurubatiba National Park in different scales.

extinction due to their restricted geographic distribution and habitat degradation. Notably, *Neomitranthes langsdorffii* is classified as Vulnerable (VU) by the International Union for Conservation of Nature (IUCN). Conservation of these species is essential for maintaining Brazilian biodiversity (IUCN, 2025-1).

Among the genus, *Neomitranthes obscura* (DC.) N. Silveira stands out, commonly known as cambuí-doce, araçá-preto, or pitanga-da-Restinga (Figure 2). It manifests as a shrub or small tree with simple, opposite leaves of an oval to elliptical shape, coriaceous texture, and characteristic translucent punctuations typical of the Myrtaceae family. The leaves are aromatic, releasing a distinct odor when macerated (Amaral, 2013; 2014). Axillary inflorescences bear small, closed calyx flowers that open by calyptra, producing globose black berries at maturity, which contain one or two seeds. These fruits, popularly known as "pitanga-de-cachorro" due to their consumption by wild animals such as the maned wolf, are also appreciated by humans. They exhibit high levels of antioxidant compounds, including anthocyanins, flavonoids, and vitamin C. The fruits can be consumed fresh or used in culinary and traditional medicine practices, particularly for treating diarrhea. The species also presents vegetative galls, deformations in leaves and buds induced by insects, that function as nutritive and protective chambers for larvae (Maia, 1993). Endemic to the Atlantic Forest, *N. obscura* preferentially inhabits sandy, well-drained soils, with confirmed distribution from Bahia to Paraná and probable occurrence in Santa Catarina (Flora do Brasil, 2025). Despite its classification as Least Concern (LC) on the Brazilian Flora Red List by the IUCN, it faces threats from deforestation and habitat degradation, emphasizing the importance of protecting its populations in Conservation Units and promoting research focused on its propagation and sustainable use (IUCN, 2025-1).

Given the ecological relevance and traditional uses of *N. obscura*, investigating its volatile metabolites is imprescindível, as essential oils (EOs) produced by different plant organs may exhibit distinct chemical profiles that concentrate compounds of pharmacological or ecological interest. These compositional variations can provide valuable insights into the species' adaptive strategies and biotechnological potential (Zhang et al., 2014). Characterized by their intense and often pleasant aroma, as well as antioxidant and antimicrobial activities, EOs are defined by ISO 9235:1997 as "products obtained from plant parts through steam distillation or by

mechanical processing of citrus fruit pericarps." Their composition is primarily based on terpenes, although phenylpropanoids may also be present. Monoterpenes are the predominant class, accounting for approximately 90% of EO constituents and being widely recognized for their pharmacological properties. Sesquiterpenes, in turn, represent the most structurally diverse group of terpenoids. Studies on the chemical coevolution between plants and insects emphasize their structural variability, reflecting diverse ecological functions and adaptive responses (Vera, 2019).

The essential oil of *N. obscura* can be extracted from various parts of the plant, with leaf and fruit oils being the most frequently studied in the literature, yielding average extractions of approximately 0.2-1.0% for leaves and 0.02-0.03% for fruits (Ramos et al., 2011; Amaral et al., 2013; 2014; Victório et al., 2018; Rangel et al., 2023). Chemical characterization studies reveal that its composition is dominated by hydrocarbon sesquiterpenes, with traces of monoterpenes. The presence of these secondary metabolites is associated with relevant biological activities reported in previous studies, including molluskicidal (LC_{90} = 25.05 μg/ml after 48h) and anticholinesterase activity, suggesting potential biotechnological applications (Rangel et al., 2023; Amaral et al., 2013). Despite these promising results, chemical variability due to environmental, developmental, and organ-specific factors must be considered when evaluating the biosynthetic profile of essential oils. Distinct plant organs often display differences in their enzymatic machinery and ecological functions, leading to unique chemical signatures that reflect their adaptive strategies. Therefore, investigating the composition of essential oils from different plant parts provides valuable insights into their metabolic diversity, ecological roles, and potential biotechnological relevance (Das; Prakash, 2023). The present study aimed to collect various parts of *N. obscura*, extract their essential oils, and determine the chemical profile of EOs from these distinct plant organs.

Methodology

Plant Material Collection

Leaves, stems, and unripe fruits of *Neomitranthes obscura* were collected in winter, at the Restinga de Jurubatiba National Park (22°13'05.7" S, 41°35'17.7" W), located in the municipality of Carapebus, northern coast of Rio de Janeiro state, Brazil, identified by the botanist Dr. Marcelo Guerra Santos. The collection site is characterized by Restinga ecosystems, with sandy soils and typical coastal Atlantic Forest vegetation (22.5 °C temperature, 0.2 mm precipitation, 86% humidity, 11.5 km/h wind). To ensure correct taxonomic identification, a representative voucher specimen was prepared and deposited in the herbarium of the Faculty of Teacher

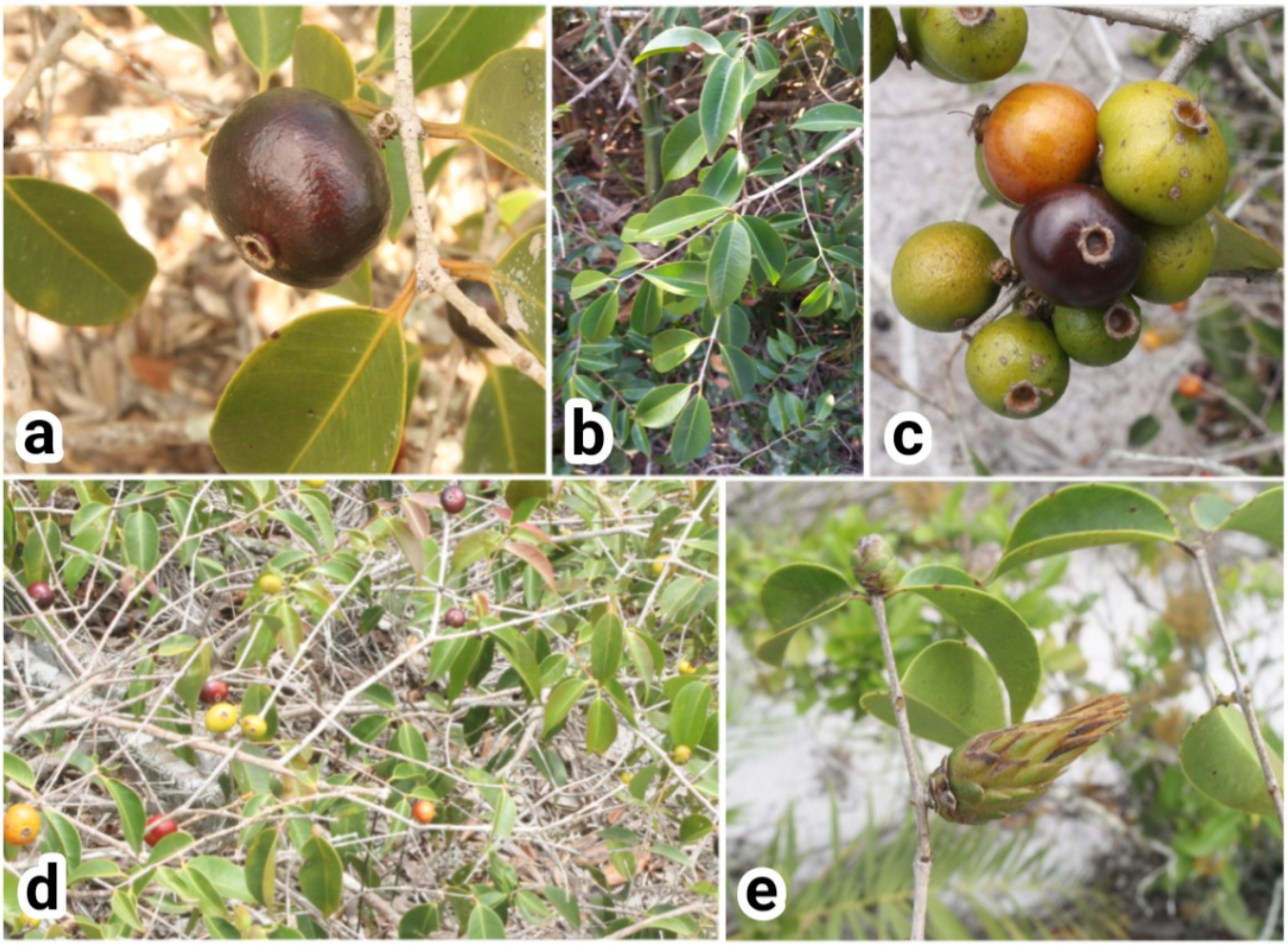


Figure 2. Different parts of *Neomitranthes obscura* at Restinga de Jurubatiba National Park, a - ripe fruit; b - leaves; c - unripe fruits; d - whole plant; e - stems and galls (Source: Marcelo Santos, 2025).

Training (FFP) at the State University of Rio de Janeiro (UERJ), under the registration number RFFP: 15327. Collection was performed under authorization from the competent environmental agencies, with permits obtained from the National System for the Management of Genetic Heritage and Associated Traditional Knowledge (SISGen – process A8941F4) and the Biodiversity Authorization and Information System (SISBio/ICMBio – 13659-21), thus guaranteeing the legal compliance of this work.

Essential Oil Extraction

Essential oil extraction was conducted using hydrodistillation with a modified Clevenger apparatus, a widely employed technique for extracting oils from plant materials. Fresh leaves (555 g) and unripe fruits (220 g) were initially crushed in distilled water to facilitate the release of volatile compounds and subsequently transferred to round-bottom flasks placed on a heating mantle. Stems (300 g) underwent a preliminary grinding step in a hammer mill to increase surface area and optimize oil extraction. The hydrodistillation process was carried out for three consecutive hours, sufficient for complete essential oil extraction, in a single round-bottomed flask for each plant part. The oils were then filtered over anhydrous sodium sulfate to separate them from the hydrolate, weighed, and stored in amber vials. They were kept refrigerated at – 20 °C to preserve their chemical properties and prevent oxidative degradation until further analysis could be conducted.

Chemical Characterization of Essential Oils

Chemical analysis of the essential oils was performed by gas chromatography coupled with mass spectrometry (GC-MS), using a Shimadzu GCMS-QP500 system (Japan). Helium was employed as the carrier gas at a constant flow rate of 1 mL/min. Sample injection was done in split mode at a split ratio of 1:40, with the injector temperature set to 260 °C. The oven temperature program began at 60 °C and increased by 3 °C per minute until it reached 290 °C. Samples were previously diluted in dichloromethane at a concentration of 1 mg/mL (1:100), and injection volumes of 1 µL were applied on an RTX-5MS capillary column (Restek), with an internal diameter of 0.25 mm, a length of 30 m, and a stationary phase film thickness of 0.25 µm. The Mass spectrometry was carried out by electron impact ionization at 70 eV, with a scanning rate of 1 scan per second. Retention indices (RI) were determined using a standard mixture of linear aliphatic hydrocarbons (C7 to C40) under the same chromatographic conditions, allowing interpolation of the retention times of compounds present in the essential oils. Component identification was based on comparison of retention indices and mass spectral fragmentation patterns with bibliographic reference data (Adams, 2017). Additionally, fragmentation spectra were cross-referenced with the National Institute of Standards and Technology database (NIST - Gaithersburg, Maryland, USA), to ensure increased reliability in compound identification. The compound quantification was expressed as a relative percentage, calculated from the peak areas in the GC-MS chromatograms, with the total area set at 100%. It should be noted that no specific detector for absolute quantification, such as GC-FID (flame ionization detector), was employed; therefore, values represent relative estimates of essential oil composition. Analyses were conducted in single runs (no replicates).

Preparation of Chemical Structures

The chemical structures of the major constituents of the essential oils from fresh leaves, unripe fruits, and stems of *N. obscura* were drawn using ChemDraw Pro (version 12.0.2) based on the ChemSpider database.

Chemometric (Statistical) Analysis

To explore the chemical similarity among samples, a Principal Component Analysis (PCA) was performed based on the percentage composition matrix of the essential oils. The analysis was conducted using a correlation matrix and executed in PAST software version 4.03. Two separate analyses were performed: the first compared the leaf oil from this study with literature data, and the second evaluated the variation among plant organs (leaves, stems, and unripe fruits).

Results and Discussion

The essential oil obtained from different parts of *N. obscura* yielded 0.06, 0.09, and 0.92% (w/w) for unripe fruits, stems, and fresh leaves, respectively, displaying a fluid consistency and a light-yellow coloration. In total, 20, 27, and 27 chemical constituents were found, being identified 96.1, 89.6, and 88.8% (Table 1). In the essential oil from unripe fruits, the major compounds were β-selinene (46.14%), sativene (15.14%), and selina-3,7(11)-diene (9.48%). In stems were zonarene (21.41%), selina-3,7(11)-diene (15.12%), and β-selinene (10.87%), evidencing similarities in chemical profiles among the analyzed plant parts. Meanwhile, the fresh leaves, the predominant constituents were zonarene (19.75%), selina-3,7(11)-diene (12.67%), and β-selinene (11.77%). The chemical structures of the major constituents of the essential oils from fresh leaves, unripe fruits, and stems of *N. obscura* are observed in Figure 3. The chromatograms of each essential oil, and the mass spectra (m/z) of unidentified compounds are provided in the Supplementary Material (Figures S1–S3 and Table S1, respectively).

These findings corroborate previous studies that presented similar results. Ramos et al. (2011) were the first to describe the composition of the essential oil from the leaves of *N. obscura*, collected in the Restinga de Jurubatiba National Park in the municipality of Carapebus, the same collection site used in this study, identifying high concentrations of selinene-3,7(11)-diene (10.6%) and β-selinene (7.2%) and, as the major constituent, α-cadinene (16.2%), with a predominance of compounds with a selinane skeleton (Ramos et al., 2011). Subsequently, Victório et al. (2018) collected different specimens of *N. obscura* leaves at different locations in the metropolitan region of the state of Rio de Janeiro: Maricá, Jaconé, Marambaia, and Massambaba, describing δ-cadinene (8.9%), β-caryophyllene (39.7%), α-cadinene (15.0%), and selina-3,7(11)-diene (12.3%), respectively. The author also pointed out that the constituents of the essential oil were mostly cyclic sesquiterpenes, with only traces of monoterpenes (such as α- and β-pinene, limonene, linalool, and *o*-cymene), attributing special relevance to β-caryophyllene, suggested as a defence metabolite against herbivores (Victório et al., 2018).

In 2013, Amaral and colleagues reported the presence of different specimens of *N. obscura* in the Restinga de Jurubatiba

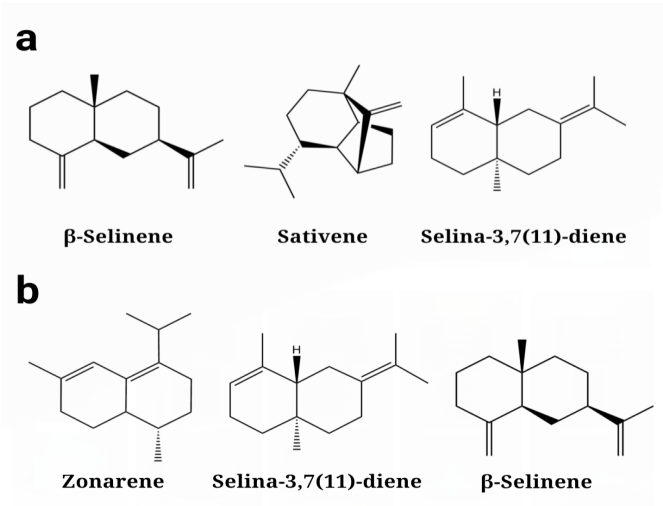


Figure 3. Chemical structures of major compounds from *Neomitranthes obscura* essential oil. (a) fresh leaves and stems; (b) unripe fruits.

National Park, in Carapebus, where they observed individuals with ripe black fruits and others with yellow fruits. This study revealed minor chemical differences in the composition of essential oils of leaves and fruits of the two morphological variants. In the leaves associated with black fruits, the major constituents were germacrene B (21.8%), selina-3,7(11)-diene (14.1%), and trans-dauca-4(11)-diene (11.4%). In the leaves associated with yellow fruits, selina-3,7(11)-diene (18.7%), trans-dauca-4(11)-diene (13.9%), and β-bisabolene (13.4%) stood out. The essential oil of black fruits was predominantly composed of monoterpenes, especially β-pinene (13.5%) and α-pinene (11.0%), while yellow fruits were rich in sesquiterpenes, with caryophyllene oxide (12.6%) being the main constituent. Interestingly, it was observed that the major compounds of one variant were present only in small fractions in the other, suggesting subtle metabolic differences between the morphotypes (Amaral et al., 2013). In subsequent studies, new analyses of the essential oil of *N. obscura* leaves were carried out at the same collection site. Amaral et al. (2014) reported cis-nerolidol (19.3%), trans-nerolidol (17.1%), and β-bisabolene (11.7%) as the major constituents, while Rangel et al. (2023) described for the first time the presence of zonarene (22.4%), in addition to high concentrations of selina-3,7(11)-diene (16.2%) and β-selinene (8.6%) (Amaral et al., 2014; Rangel et al., 2023).

The variability of the composition of secondary metabolites among specimens of *N. obscura* found in the literature may be associated with both genetic and environmental factors that modulate the biosynthesis of these components: edaphoclimatic conditions, such as water availability, light intensity, and soil type, as well as seasonal and ontogenetic factors (Gobbo-Neto and Lopes, 2007). Thus, even in individuals of the same species, fluctuations in chemical composition are expected to occur, reflecting both the metabolic plasticity of the plant and the specific conditions in which each specimen developed.

To evaluate the chemical similarity of the leaf essential oil obtained in this study (Da Silva, 2025) in relation to the profiles previously reported in the literature, Principal Component Analysis (PCA) was employed (Figure 4). The first two principal components (PC1 and PC2) accounted for 53.7% of the total explained variance (PC1 = 32.2% and PC2 = 21.5%), revealing a clear chemical polymorphism within the species. The score plot demonstrated a distinct segregation of the samples into two major groups along Component 1. The essential oil analyzed in this study was positioned within the group exhibiting positive PC1 scores, in proximity to most of the literature data, including Rangel (2013), Amaral (2013), Ramos (2011), and Victório (2018) [Marambaia], thus validating its classification within one of the predominant chemotypes. This cluster was chemically opposed to the negative PC1 group, composed of samples from Victório (2018) [Jaconé, Maricá, Massambaba] and Amaral (2014). Additionally, Component 2 provided a secondary separation, distinguishing subgroups within the main chemotype. The oil obtained in this study clustered specifically with Ramos (2011) in the lower-right quadrant (negative PC2), suggesting a slightly distinct chemical sub profile compared to Rangel (2013) and Amaral (2013), which were positioned in the upper-right quadrant (positive PC2).

Similarly, to compare the chemical profiles of the essential oils obtained from different organs of *N. obscura* (leaves, stems, and unripe fruits), another PCA was performed (Figure 5). This analysis explained the total data variance (100%) through the first two principal components (PC1 = 66.9%; PC2 = 33.1%), revealing a clear organ-specific segregation. The first component, representing the main axis of variation, separated the unripe fruits (negative PC1) from the stems and leaves (positive PC1). This distinction is

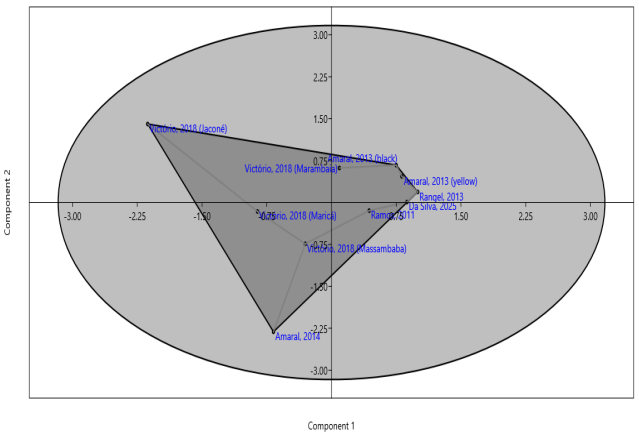


Figure 4. Principal Component Analysis (PCA) of the chemical composition of *N. obscura* leaf essential oil from the present study (Da Silva, 2025) compared with literature data.

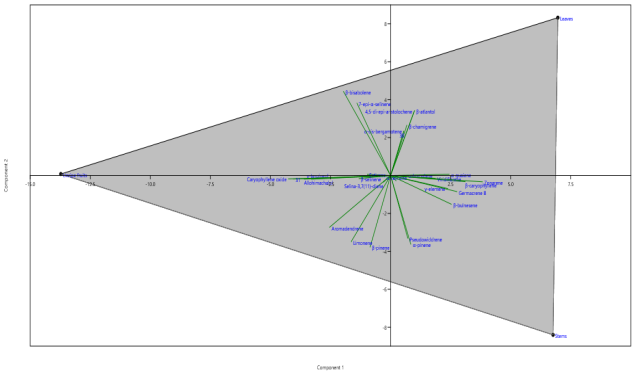


Figure 5. Principal Component Analysis (PCA) of the chemical composition of essential oils extracted from the leaves, stems, and unripe fruits of *N. obscura* in the present study (Da Silva, 2025).

Table 1 – Chemical characterization of essential oils from unripe fruits, fresh leaves, and stems of *Neomitranthes obscura* performed by GC-MS. *AI_{Lit} = Arithmetic Index literature (Adams, 2017); NI = non-identified.

AI_{Lit}	Substances	RELATIVE ABUNDANCE (%)		
		Unripe fruits	Fresh Leaves	Stems
—	NI[1]	1.90	—	—
—	NI[2]	0.45	—	—
—	NI[3]	0.59	—	—
—	NI[4]	0.31	—	—
974	*α*-pinene	—	—	1.25
974	*β*-pinene	0.22	—	1.59
1024	Limonene	0.73	—	1.08
1199	*γ*-terpineol	1.32	—	—
1390	**Sativene**	**15.14**	8.27	5.55
1411	*α-cis*-bergamotene	—	0.40	—
1417	*β*-caryophyllene	—	5.57	6.05
1434	γ-elemene	—	1.19	2.19
1437	*α*-guaiene	—	2.26	1.42
1439	Aromadendrene	2.09	—	0.37
1452	*α*-humulene	—	0.54	0.48
—	NI[5]	0.30	—	—
1471	4,5-di-epi-aristolochene	—	1.76	—
—	NI[6]	—	—	0.48
1476	*β*-chamigrene	—	0.62	—
—	NI[7]	—	0.91	—
—	NI[8]	—	—	0.66
—	NI[9]	—	—	0.74
1489	***β*-selinene**	**46.14**	**11.77**	**10.87**
1496	Viridiflorene	—	0.70	0.60
1498	*α*-selinene	2.04	7.33	7.73
1504	Pseudowiddrene	—	—	0.80
1505	*β*-bulnesene	—	0.87	5.20
1505	*β*-bisabolene	3.69	7.59	—
—	NI[10]	—	—	2.19
1520	7-*epi*-*α*-selinene	0.88	3.16	—
1528	**Zonarene**	—	**19.75**	**21.41**
1545	**Selina-3,7(11)-diene**	**9.48**	**12.67**	**15.12**
1559	Germacrene B	—	2.10	4.84
—	NI[11]	—	—	0.32
1582	Caryophyllene oxide	7.13	—	—
—	NI[12]	—	—	0.73
—	NI[13]	0.19	—	—
—	NI[14]	—	2.74	—
—	NI[15]	—	1.01	—
—	NI[16]	—	1.68	—
—	NI[17]	0.18	—	—
1608	*β*-atlantol	—	1.89	—
—	NI[18]	—	0.49	—
—	NI[19]	—	0.44	—
—	NI[20]	—	0.49	—
—	NI[21]	—	—	0.52
—	NI[22]	—	—	0.92
—	NI[23]	—	—	1.45
1661	Allohimachalol	2.28	—	—
—	NI[24]	—	—	1.76
1681	Occidentalol acetate	—	0.38	—
—	NI[25]	—	0.83	—
1792	8-*α*-acetoxyelemol	4.93	—	—
Total Identified	96.1	88.8	89.6	
Hydrocarbon	0.1	0	3.9	
Oxygenated	0	0	0	
Hydrocarbon	80.8	86.55	85.7	
Oxygenated	14.3	2.27	0	

attributed to the unique chemical profile of the fruits, dominated by β-selinene (46.14%) and sativene (15.14%). In contrast, the leaf and stem oils exhibited high chemical similarity, clustering together in the positive PC1 region, as both were characterized by high levels of zonarene (19.75% and 21.41%, respectively) and selina-3,7(11)-diene (12.67% and 15.12%, respectively). Component 2 (33.1%) was responsible for distinguishing secondary differences between these two vegetative organs: the leaves (positive PC2) were associated with compounds such as β-bisabolene (7.59%), whereas the stems (negative PC2) were characterized by the presence of monoterpenes such as α-pinene (1.25%) and β-pinene (1.59%). The raw data obtained in the PAST software are contained in the supplementary material (Table S2–S3).

Except for sativene, the main compounds share a selinane-type structural nucleus, indicating the predominance of this terpenoid skeleton in the essential oil composition of the species. The recurrence of selinane derivatives is a pattern frequently reported in essential oils of Myrtaceae species, particularly within the genera *Eugenia* and *Myrciaria* (Victório et al., 2018; Stefanello et al., 2011), suggesting a potential chemotaxonomic marker with implications for understanding phylogenetic relationships within the group.

Beyond chemotaxonomic relevance, selinane-type sesquiterpenes have drawn growing attention for their pharmacological potential. In macroalgae of the genus *Laurencia*, for instance, eudesmane sesquiterpenes (structurally related to the selinane skeleton as derivatives of trans-decalin) have shown remarkable cytotoxic and anti-inflammatory effects, comparable to reference drugs (Cikoš et al., 2021). Among the major compounds identified here, β-selinene stands out, having been associated with in vivo anti-inflammatory and analgesic activities in murine models, as well as relevant antioxidant properties (Chandra et al., 2017). Such a profile was also evidenced in the essential oil of *Callicarpa macrophylla*, rich in β-selinene, which exhibited anti-inflammatory, antipyretic, and analgesic effects similar to standard drugs (Chandra et al., 2017). Likewise, essential oils containing selina-3,7(11)-diene as a significant constituent have demonstrated antimicrobial and antioxidant activities. The oil of *Morella pubescens*, in which this compound accounts for about 5% of the composition, showed strong activity against *Enterococcus faecium* (MIC = 250 μg/mL), in addition to high antioxidant capacity in ABTS (scavenging capacity, SC_{50} of 46.4 ± 1.0 μg/mL) and DPPH (SC_{50} of 237.1 ± 1.8 μg/mL) assays, with strong anticholinesterase activity (IC_{50} of 133.5 ± 1.06 μg/mL) (Valarezo et al., 2023). Although it is not possible to attribute such effects solely to these sesquiterpenes, the evidence suggests that they may act synergistically with other constituents, contributing to the overall bioactivity of the oils.

From an ecological viewpoint, the marked variation in secondary metabolite distribution across plant organs is well-documented. For example, in *Myrica gale*, the relative abundance of monoterpene and sesquiterpene hydrocarbons differs significantly between leaves and fruits, indicating organ-specific metabolic partitioning (Ložienė et al., 2023). Zonarene was identified as a major constituent in the essential oils of *N. obscura* fresh leaves and stems but was absent in fruit oil, likely reflecting similar patterns of biosynthetic specialization, since distinct enzymes and regulatory pathways operate in different tissues, leading to differential compound production. Moreover, the ecological function of such compounds helps explain their localization: leaves and stems, being directly exposed to herbivory and abiotic stresses, typically accumulate defensive metabolites, whereas fruits may shift their metabolic investment toward producing attractants for seed dispersers (Yang et al., 2024).

Sativene, in turn, showed a broad distribution, being detected in leaves, unripe fruits, and stems. However, it was a major constituent only in unripe fruits, suggesting an accumulation linked to the developmental stage. Previous studies demonstrated that ripe fruits (yellow and black) of *N. obscura* exhibited decreasing concentrations of sativene, with total absence in black fruits, reinforcing the hypothesis of ontogenetic regulation of this metabolite. Such dynamics may reflect specific functions of sativene in early fruit stages, possibly related to pathogen defense or growth signaling. Indeed, compounds derived from the sativene skeleton have been reported as regulators of plant development. Wang et al. (2024), upon isolating thirteen sativeneid sesquiterpenoids from the endophytic fungus *Bipolaris victoriae* S27, observed that some of these metabolites inhibited, while others stimulated, the growth of *Arabidopsis thaliana*, suggesting that subtle structural modifications within this skeleton can modulate antagonistic effects on plant growth (Wang et al., 2024).

Taken together, these findings indicate that the predominance of selinane- and sativene-type sesquiterpenes in N. obscura reflects chemotaxonomic traits of the Myrtaceae family and corroborates previous reports of bioactive properties associated with these compounds, suggesting that the species may constitute a source of molecules of potential ecological and pharmacological interest.

Conclusion

The findings of the present study demonstrate a clear difference in the chemical composition of the essential oil from Neomitranthes obscura depending on the plant organ analyzed. While the leaves and stems were characterized by the predominance of zonarene, selina-3,7(11)-diene, and β-selinene, the unripe fruits presented a different profile enriched in sativene, β-selinene, and selina-3,7(11)-diene. This study provides the first comprehensive chemical characterization of the essential oils from unripe fruits and stems of N. obscura, revealing organ-specific variation in secondary metabolites and highlighting compounds with potential ecological and pharmacological relevance, while contributing to the chemotaxonomic knowledge of the Myrtaceae family.

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Author Contributions

Conceptualization: DSS, LAP, FPM. Data curation: DSS, ASC, FPM, MGS. Formal analysis: DSS, ASC, FPM. Funding acquisition: FPM, LR. Investigation: DSS, ASC, FPM. Methodology: DSS, FPM. Project administration: DSS, LAP, FPM. Resources: FPM, LR. Software: DSS, FPM. Supervision: LAP, FPM, LR. Validation: FPM, VCRV, MGS, LR. Visualization: MGS, LR. Writing – original draft: DSS, LAP, VCRV. Writing – review and editing: DSS, LAP, VCRV, FPM.

Conflict of Interest

The authors declare there are no conflicts of interest to disclose.

Data Availability

The complete datasets analyzed during the current study are available from the corresponding author upon reasonable request.

Ethical Compliance

National System for the Management of Genetic Heritage and Associated Traditional Knowledge (SISGen – process A8941F4). Biodiversity Authorization and Information System (SISBio/ICMBio – 13659-21)

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Supplementary Material

Table S1. Supplementary Information: GC–MS Mass Spectra of Unidentified Components from the Essential Oils of *Neomitranthes obscura*.

[1]MS *m/z* (Relat. int.): 41; 55; 69; 83; 84 (100).
[2]MS *m/z* (Relat. int.): 83 (100); 85.
[3]MS *m/z* (Relat. int.): 43; 44; 70; 71 (100).
[4]MS *m/z* (Relat. int.): 44; 55; 97 (100).
[5]MS *m/z* (Relat. int.): 44; 105 (100).
[6]MS *m/z* (Relat. int.): 41; 55; 67; 81; 91; 105; 119; 133; 147; 161; 189 (100); 204.
[7]MS *m/z* (Relat. int.): 40; 41; 55; 67; 81; 91; 105; 119; 133 (100); 147; 161; 175; 189; 204.
[8]MS *m/z* (Relat. int.): 41; 55; 67; 81; 91; 105; 119; 133 (100); 147; 161; 175; 189; 204.
[9]MS *m/z* (Relat. int.): 41; 55; 69; 81; 91; 105 (100); 119; 133; 147; 161; 175; 189; 204.
[10]MS *m/z* (Relat. int.): 41; 55; 67; 79; 93; 105; 121 (100); 133; 148; 161; 189; 204.
[11]MS *m/z* (Relat. int.): 41; 55; 67; 79; 93; 108 (100); 119; 133; 147; 161; 189; 204.
[12]MS *m/z* (Relat. int.): 41; 55; 69; 79; 91 (100); 105; 119; 131; 145; 159; 187.
[13]MS *m/z* (Relat. int.): 44; 91; 105 (100).
[14]MS *m/z* (Relat. int.): 40; 41; 55; 69; 79; 91 (100); 105; 119; 131; 145; 159; 173; 187; 202.
[15]MS *m/z* (Relat. int.): 40; 41; 55; 67; 81; 95 (100); 105; 121; 131; 145; 159; 177; 187; 202; 220.
[16]MS *m/z* (Relat. int.): 40; 41; 55; 67; 79; 91; 105; 119; 131; 145; 159; 173; 187; 202 (100); 220.
[17]MS *m/z* (Relat. int.): 44; 187 (100).
[18]MS *m/z* (Relat. int.): 41; 43; 69; 77; 91; 105; 115; 129; 142; 157 (100); 171; 185; 200.
[19]MS *m/z* (Relat. int.): 41; 55; 67; 79; 93 (100); 105; 121; 133; 147; 161; 175; 189; 202.
[20]MS *m/z* (Relat. int.): 41; 55; 69; 79; 91 (100); 105; 119; 131; 145; 159; 173; 187; 202.
[21]MS *m/z* (Relat. int.): 41; 55; 67; 79; 91; 105; 117; 131; 145; 159; 173 187 (100); 202.

Table S2. Raw data of PCA obtained in the PAST software of the chemical composition of *N. obscura* leaf essential oil from the present study (Da Silva, 2025) compared with literature data.

PC	Eigenvalue	% variance
1	199.512	32.227
2	132.815	21.453
3	981.129	15.848
4	75.163	12.141
5	545.424	8.8101
6	240.762	3.889
7	147.735	2.3863
8	131.723	2.1277
9	692.307	1.1183

Table S3. Raw data of PCA obtained in the PAST software of the chemical composition of *N. obscura* leaves, stems, and unripe fruits essential oil from the present study (Da Silva, 2025).

PC	Eigenvalue	% variance
1	172.978	61.778
2	10.7022	38.222

Figure S1. Chromatogram of *N. obscura* unripe fruits essential oil.

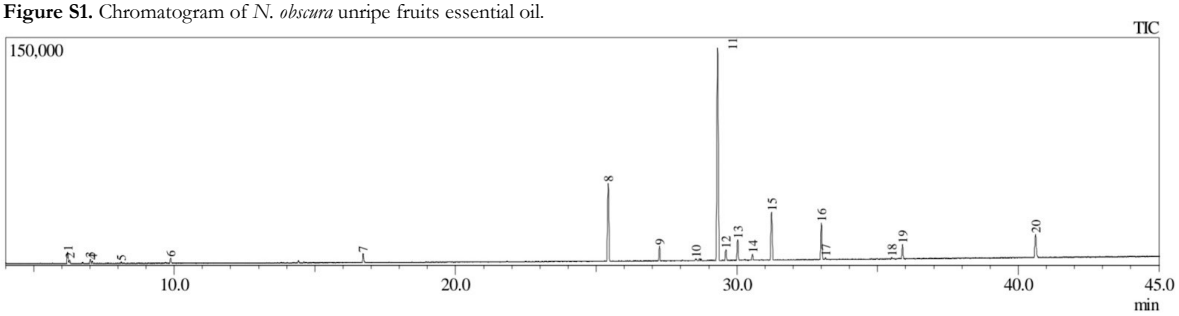


Figure S2. Chromatogram of *N. obscura* stems essential oil.

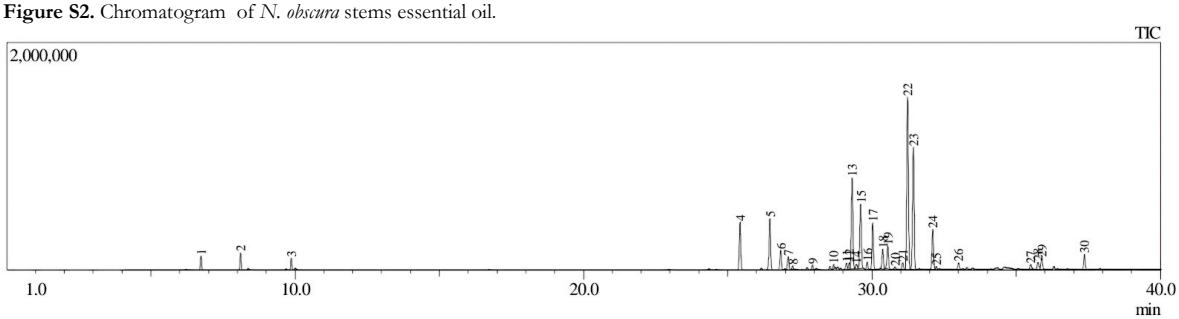


Figure S3. Chromatogram of *N. obscura* leaves essential oil.

