Unveiling Sesquiterpene Emissions in Dominant Trees of a Brazilian Atlantic Forest Remnant

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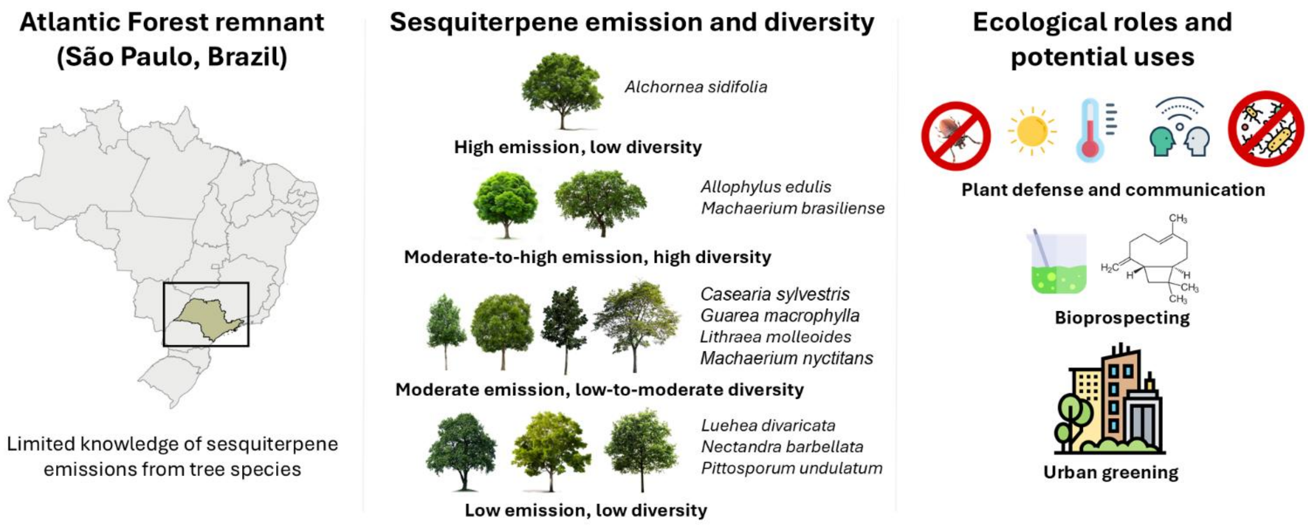

Abstract

Despite the ecological richness and biodiversity of the Atlantic Forest, research on biogenic volatile organic compound (BVOC) emissions from its tree species remains limited. This study characterizes sesquiterpene (SQT) emissions from ten dominant tree species in an Atlantic Forest remnant near São Paulo, Brazil. Emissions and chemical profiles varied significantly, with total SQT emissions ranging from undetectable levels in *Luehea divaricata* to 295.14 ng gdw^{-1} h^{-1} in *Alchornea sidifolia*. Hierarchical clustering revealed four distinct groups: (1) high emission with low chemical diversity (*A. sidifolia*), (2) moderate-to-high emission with high diversity (*Machaerium brasiliense* and *Allophylus edulis*), (3) moderate emission with low (*Guarea macrophylla*) to moderate diversity (*Machaerium nyctitans*, *Lithraea molleoides* and *Casearia sylvestris*), and (4) low emission and diversity (*Nectandra barbellata, Pittosporum undulatum,* and *L. divaricata*). A total of 26 distinct SQTs were identified, including nine oxygenated sesquiterpenes (OSQTs). Most species predominantly emitted α-copaene, β-caryophyllene, or α-cubebene, compounds that may play important defensive and ecological roles, such as antimicrobial activity and herbivore deterrence. Species with high β-caryophyllene emissions, particularly *Allophylus edulis* (48.15 ng gdw^{-1} h^{-1}) and *Lithraea molleoides* (32.54 ng gdw^{-1} h^{-1}), or those with high OSQT diversity, such as *A. sidifolia* (six OSQTs) and *M. nyctitans* (seven OSQTs), show potential for bioprospecting applications. In contrast, species with low total SQT emissions, such as *N. barbellata* (6.75 ng gdw^{-1} h^{-1}), *P. undulatum* (6.18 ng gdw^{-1} h^{-1}), and *L. divaricata* (no detectable emissions), may be better suited for urban greening efforts from a SQT-emission perspective.

Keywords: Biogenic volatile organic compounds (BVOCs)**;** Natural Products; Secondary metabolism; Plant-atmosphere interactions; Tropical trees; Bioprospecting.

Highlights

- Sesquiterpene (SQT) emissions profiled for 10 dominant Atlantic Forest tree species.
- Hierarchical clustering grouped species into four emission-based classes.
- α-Copaene, β-caryophyllene, and α-cubebene were key compounds across species.
- β-Caryophyllene and oxygenated SQT-rich species may have bioprospecting potential.
- Low SQT-emitting species may be candidates for urban greening to reduce pollution.

1. Introduction

Biogenic volatile organic compounds (BVOCs) are small, lipophilic molecules (100–500 Da) produced by living organisms and released into the atmosphere (Chen et al., 2025). Terrestrial vegetation is the primary global source of BVOCs, accounting for up to 90% of total emissions (Yang et al., 2025a). These compounds originate from key secondary metabolic pathways, including the shikimate, methylerythritol phosphate, mevalonic acid, and lipoxygenase pathways (Wang et al., 2024). BVOCs encompass a wide range of chemical groups, such as isoprene (ISO), monoterpenes (MTs), sesquiterpenes (SQTs), green leaf volatiles (GLVs), benzenoids, and phenylpropanoids, each with distinct biosynthetic origins and ecological roles (Bao et al., 2023).

BVOCs primarily serve two key roles: acting as chemical signals and influencing atmospheric chemistry. They mediate interactions between plants and other organisms (Masui et al., 2021), provide defense against herbivores and pathogens (Hirose &Satake, 2024) attract pollinators (Satake et al., 2025), and enhance plants resilience to environmental stressors (Moura et al., 2022). Beyond their biological functions, BVOCs also play a key role in atmospheric processes, acting as precursors of ozone (O_3) and secondary organic aerosols (SOAs), which impact air quality and Earth's radiative balance (Huang et al., 2024; Mahilang et al., 2021).

The SQT concentration and composition of plant emissions depend on multiple factors, including species identity and its developmental stage, temperature, light availability, and other environmental stressors, all of which can strongly influence both the quantity and chemical diversity of BVOCs (Fitzky et al., 2019; Loreto & Schnitzler, 2010; Sindelarova et al., 2014; Vermeuel et al., 2023; Yáñez-Serrano et al., 2020). Despite extensive research on BVOC emissions in various ecosystems, a significant knowledge gap remains regarding the emission profiles of tropical forests in the southern hemisphere, particularly within the highly biodiverse Atlantic Forest (Mata Atlântica) (de Araújo et al., 2025).

A recent study in the Atlantic Forest (Anselmo-Moreira et al., 2025) provided the first assessment of BVOC emissions in this biome, focusing on an urban forest fragment within the Metropolitan Area of São Paulo (MASP). The study found that eight native species primarily emit SQTs, in contrast to other biomes where ISO and MTs typically dominate BVOC emissions (Aydin et al., 2014; Bai et al., 2015;

Chen et al., 2025; Wang et al., 2022). These findings highlight the unique emission profiles of species in the Atlantic Forest remnants and the potential ecological roles in this biome.

SQTs (C_{15}), composed of three ISO units (C_5H_{10}) (Mai et al., 2021), are highly reactive compounds that significantly influence atmospheric chemistry, particularly in SOA formation, and are usually associated with plant defense mechanisms against oxidative damage (Bison et al., 2018). Unlike ISO and MTs, which are more volatile and widely emitted across different biomes, SQTs have lower vapor pressure and higher reactivity, leading to lower ambient concentrations and making them less studied (Barreira et al., 2021; Duhl et al., 2008; Yee et al., 2018).

SQT emissions may vary across plant species, as different species exhibit distinct SQT chemotypes, reflecting variations in biosynthetic pathways and ecological adaptations (Kesselmeier & Staudt, 1999; Smit et al., 2019). These chemotypes can be classified based on the predominant SQT compounds produced, such as caryophyllene-type, farnesene-type, and cadinene-type emitters, which may be linked to specific plant traits, defensive strategies, and environmental interactions (Elbali et al., 2018).

Beyond their atmospheric and plant physiology roles, SQTs have notable medicinal and industrial potential, including applications in fragrances and personal care products, as well as health benefits such as anticancer, anti-inflammatory, cardioprotective, and neuroprotective effects (Durairaj et al., 2019; Zhang et al., 2023). Given their importance in atmospheric processes, plant physiology, and human applications, identifying species with high SQT emissions and characterizing their specific SQT profiles can advance ecological research, support bioprospecting, and inform urban greening strategies for air pollution mitigation.

Therefore, further investigation into SQT profiles across other Atlantic Forest remnants is essential. One particularly valuable site is the Morro Grande Forest Reserve (RMG), a large, well-preserved fragment near São Paulo, hosting a diverse native tree species (de Araújo et al., 2025). This site provides an ideal location for such studies. However, the emission patterns of its dominant trees remain largely unexamined.

In this context, this study aims to investigate the SQT emission profiles of dominant native tree species in the well-preserved urban fragment of Atlantic Forest in the MASP. By identifying the main emitting species and analyzing their emission patterns in terms of quantity and chemical diversity, this research contributes to a better understanding of BVOC emissions in southern subtropical forests. These findings may also support ecological studies, aid in the discovery of valuable plant-derived compounds, and inform sustainable urban greening efforts.

2. Materials and methods

2.1 Site description

Morro Grande Forest Reserve (RMG) (Figure 1) is one of the largest and well-preserved remnants of the Atlantic Forest within MASP. It consists of a successional mosaic of mature forests and forests in intermediate to advanced stages of succession. Studies on its fauna and flora have become more prominent only since the year 2000. This reserve is located in the municipality of Cotia, São Paulo, Brazil (23º39'–23º48'S, 47º01'–46º55'W), approximately 34 km from São Paulo (Catharino et al., 2006; Metzger et al., 2006).

RMG is situated at an altitude of 860–1,075 m and has a temperate climate (Cfb), according to the Köppen classification, characterized by mild summers and relatively wet winters. The average temperature of the coldest and warmest months is below 18°C and 22°C, respectively. The reserve is predominantly composed of ombrophilous forests, with contributions from semideciduous seasonal forests and mixed forests (Barretto & Catharino, 2015).

Due to the presence of a major reservoir that supplies water to MASP, the reserve is managed by the Basic Sanitation Company of the State of São Paulo (Sabesp). Additionally, access to the area is restricted, with entry permitted only via unpaved roads.

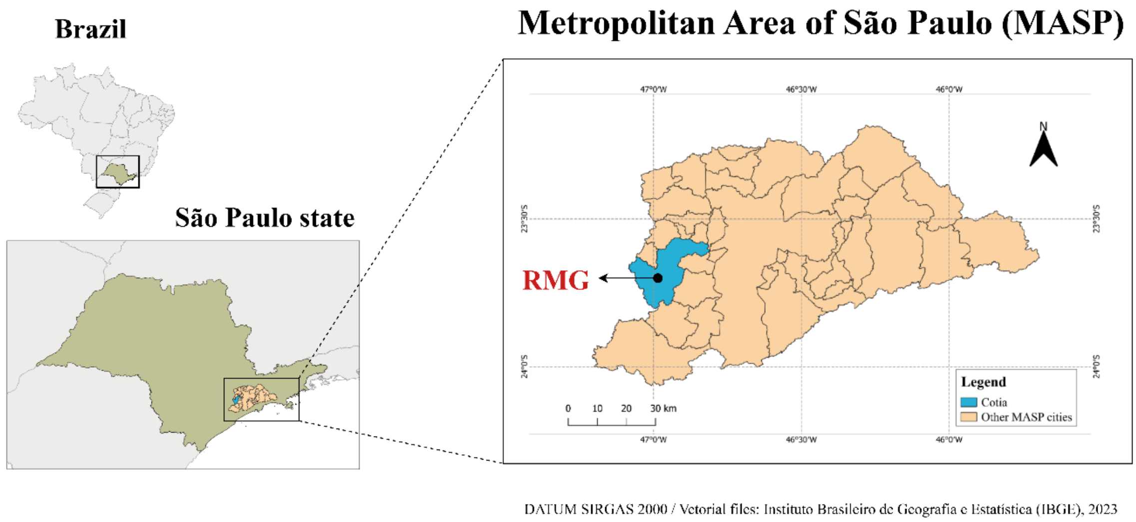

Figure 1. Location of the Morro Grande Forest Reserve (RMG), an Atlantic Forest remnant in Cotia, within the Metropolitan Area of São Paulo (MASP).

2.2 Selection of plant species

For species selection, a vegetation survey was conducted in two plots of 20 m × 50 m (Onaindia et al., 2004). All individuals with a diameter at breast height (DBH) of 9.55 cm (perimeter of 30 cm) or greater were sampled. Plant material in the vegetative and/or reproductive phase was collected, and species identification was carried out through specialized bibliographic consultation, comparison with herbarium specimens, and consultation with experts. Taxonomic classification followed the Angiosperm Phylogeny Group IV system (Byng et al., 2016), while species nomenclature adhered to the Flora e Funga do Brasil database (https://floradobrasil.jbrj.gov.br/consulta/). A total of 41 species, distributed across 21 families, were sampled. The species with the highest number of individuals and easiest access for sampling were selected, including: *Allophylus edulis* (Sapindaceae), *Alchornea sidifolia* (Euphorbiaceae), *Casearia sylvestris* (Salicaceae), *Guarea macrophylla* (Meliaceae), *Lithraea molleoides* (Anacardiaceae), *Luehea divaricata* (Malvaceae), *Machaerium brasiliense* (Fabaceae), *Machaerium nyctitans* (Fabaceae), *Nectandra barbellata* (Lauraceae), and *Pittosporum undulatum* (Pittosporaceae). All selected species are native to the Atlantic Forest, except for *P. undulatum*. Although this species is not native, it was included due to its high abundance in the sampled area.

Detailed information on the vegetation survey and the collected species is provided in Tables S1 and S2, respectively.

2.3 BVOC sampling

Sampling was conducted during the dry season of 2019 (from 09 to 12 July). For each species, three individuals (n = 3) were selected, except for *Nectandra barbellata* (n = 2) and *Machaerium nyctitans* (n = 2). For each individual, branches with fully sun-exposed leaves were cut and immediately submerged in buckets of water. A transverse cut was then made in the submerged portion of the branch to restore hydraulic connectivity. After an acclimation period of 15–20 minutes, the branches were subjected to a dynamic enclosure sampling system. For this purpose, branches were enclosed in an inert Teflon bag (Isebrands et al., 1999). Throughout the sampling period, filtered air was continuously introduced into the system at a flow rate of 1,800 mL min^{-1}. BVOCs emitted by the branches were trapped in tubes containing 100 mg of Tenax TA (Supelco, 60/80 mesh), which were incorporated into the system and connected to a suction pump operating at 200 mL min^{-1}. The sampling period lasted 60–90 minutes. Plant material was collected during the daytime, between 7:00 a.m. and 10:00 a.m. Further details on the BVOC sampling system can be found in Anselmo-Moreira et al. (2025). After BVOC collection, the enclosed leaves were collected, dried at 60°C for 48 hours, and weighed to determine dry mass.

2.4 BVOC analysis

The volatiles trapped in Tenax TA tubes were analyzed using gas chromatography-mass spectrometry (GC-MS) (Agilent 7890B; Agilent 5977A). To this end, the BVOCs were desorbed with a thermal desorption unit (PerkinElmer ATD400 Automatic Thermal Desorption System; PerkinElmer, Waltham, MA, USA) at 250°C for 10 minutes, followed by cryo-focusing at -30°C, and injection into an HP-5 capillary column (Hewlett-Packard; 50 m × 0.2 mm i.d. × 0.5 µm film thickness) using helium as the carrier gas. The oven temperature program was set as follows: an initial temperature of 46°C with a 5-minute hold, followed by an increase to 210°C at a rate of 5°C min^{-1}, with a 20-minute hold, and finally a ramp to 250°C at a rate of 10°C min^{-1}, with a 5-minute hold at the final temperature. SQT were annotated by comparing the experimental e mass spectra with the Wiley/NIST chemical library and commercially available standards analyzed under the same conditions. Quantification was performed using an external standard curve of β-caryophyllene (Sigma-Aldrich; 20–140 ng, $r^2 > 0.99$) and the results were expressed as ng gdw^{-1} h^{-1}.

2.5 Statistical analysis

Statistical analyses were performed in RStudio (version 4.3.1). Boxplots illustrating SQT emission variation across species and donut charts showing the five most abundant emitted SQT per species were created using the ggplot2 package. Hierarchical cluster analysis (HCA) was performed to classify tree species based on SQT emission profiles. Species dissimilarities were calculated using a Euclidean distance matrix, and clustering was conducted applying the Ward.D2 method to optimize grouping. The classification was visualized using heatmaps generated with the heatmap and ComplexHeatmap packages. Additionally, an UpSet plot was created using the ggtext, ggplot2, and ComplexUpset packages to explore shared and unique SQTs among species.

3. Results

The composition of SQT emissions from ten dominant native species in RMG is summarized in Table 1. In total, 26 distinct SQTs were identified across the surveyed species, including 9 oxygenated sesquiterpenes (OSQTs): 4-epi-cubedol, 6-epi-shyobunol, 7-epi-*cis*-sesquisabinene hydrate, α-acorenol, cedran-diol (8S,14)-, cubedol, geranyl isovalerate, isocalamendiol, and limonen-6-ol pivalate. Ranking the species from highest to lowest total SQT emissions, the order was: *Alchornea sidifolia* (295.14 ng gdw^{-1} h^{-1}), *Machaerium brasiliense* (212.94 ng gdw^{-1} h^{-1}), *Allophylus edulis* (164.12 ng gdw^{-1} h^{-1}), *Lithraea molleoides* (96.07 ng gdw^{-1} h^{-1}), *Casearia sylvestris* (56.69 ng gdw^{-1} h^{-1}), *Machaerium nyctitans* (56.61 ng gdw^{-1} h^{-1}), *Guarea macrophylla* (40.53 ng gdw^{-1} h^{-1}), *Nectandra barbellata* (6.75 ng gdw^{-1} h^{-1}), *Pittosporum undulatum* (6.18 ng gdw^{-1} h^{-1}), with *Luehea divaricata* exhibiting no detectable emissions. When considering individual compound emissions, the values also varied widely, ranging from 0.08 ng gdw^{-1} h^{-1} for cubedol emitted by *Lithraea molleoides*, to 159.19 ng gdw^{-1} h^{-1} for α-copaene emitted by *Alchornea sidifolia*.

In addition to SQT concentration, the diversity of the sesquiterpene *bouquet* also varied among species (Table 1, Figure S1). *Allophylus edulis* released the widest range of SQTs, emitting 18 distinct compounds, followed by *Machaerium brasiliense* (14 compounds), *and Lithraea molleoides* (13 compounds). Interestingly, despite this diversity, no single SQT was present in all species (Figure S2). However, several compounds were commonly shared among emitting species. 6-epi-shyobunol was detected in eight species (80% of all species). α-Copaene, α-acorenol**,** cubedol, and 4-epi-cubedol were found in seven species (70% of all species). Geranyl isovalerate, β-guaiene, and *trans*-calamenene were identified in six species (60% of all species). Conversely, some compounds were species-specific. γ-Muurolene, α-muurolene and β-cubebene were unique to *Allophylus edulis*; humulene and β-vatirenene were exclusive to *Lithraea molleoides*, α-guaiene was found only in *Nectandra barbellata*, and isocalamendiol was detected only in *Machaerium brasiliense* (Table 1, Figure S1).

When evaluating only OSQTs, both the number of compounds emitted and their contribution to total emissions also varied widely. Some species, such as *Guarea macrophylla* and *Nectandra barbellata*, emitted only three OSQTs, while others, such as *Machaerium nyctitans* and *Lithraea molleoides*, emitted eight. Similarly, the proportion of OSQTs in the total emissions differed considerably (Figure S3), ranging from just 6.91% in *Casearia sylvestris* to 69.86% in *Machaerium nyctitans*.

Across all species, α-copaene (288.69 ng gdw^{-1} h^{-1}) is the most abundantly emitted compound, followed by α-cubebene (95.78 ng gdw^{-1} h^{-1}) and β-caryophyllene (90.61 ng gdw^{-1} h^{-1}) (Table 1). While these values indicate overall abundance, species-level rankings provide a more detailed perspective. α-Copaene not only leads total emissions but also ranks among the top five SQT in six of ten species. In contrast, α-cubebene and β-caryophyllene, despite their high total emissions, appear in the top five for only two and four species, respectively. Notably, some compounds with lower total emissions are more frequently ranked among the top five within individual species. For example, *trans*-calamenene (26.36 ng gdw^{-1} h^{-1}) appears in the top five for five species, while β-copaene (43.57 ng gdw^{-1} h^{-1}) appears for four species (Figure 2).

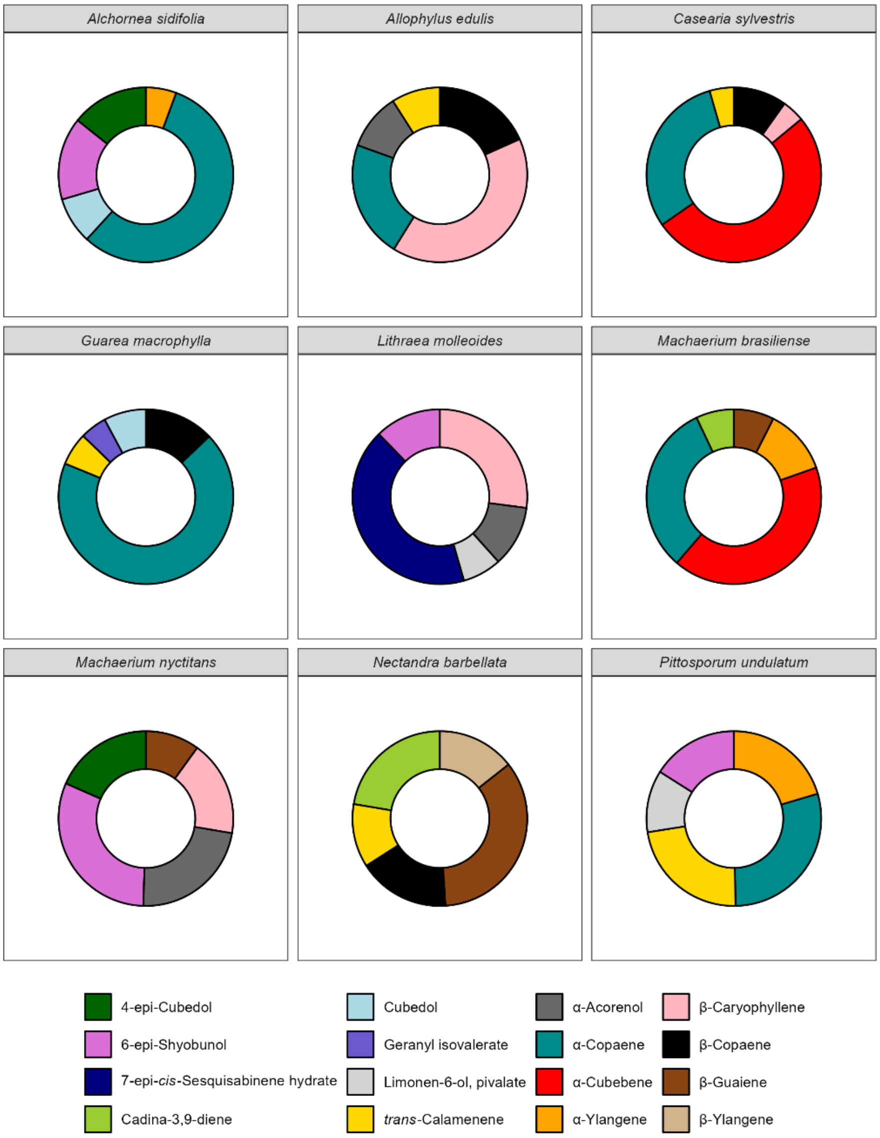

Figure 2. Composition of the five most prominent sesquiterpenes (SQTs) emitted by dominant tree species from Morro Grande Forest Reserve (RMG), São Paulo, Brazil.

In fact, of the 26 detected SQTs, 16 rank in the top five for at least one species. Therefore, this dual approach, examining both total emissions and species-level rankings, reinforces that species vary not only in the amount of SQT they emit but also in the composition of their emissions. To further explore these patterns, we performed a hierarchical clustering analysis (HCA) along with a heatmap to classify species based on both the identity and abundance of their emitted compounds (Figure 3).

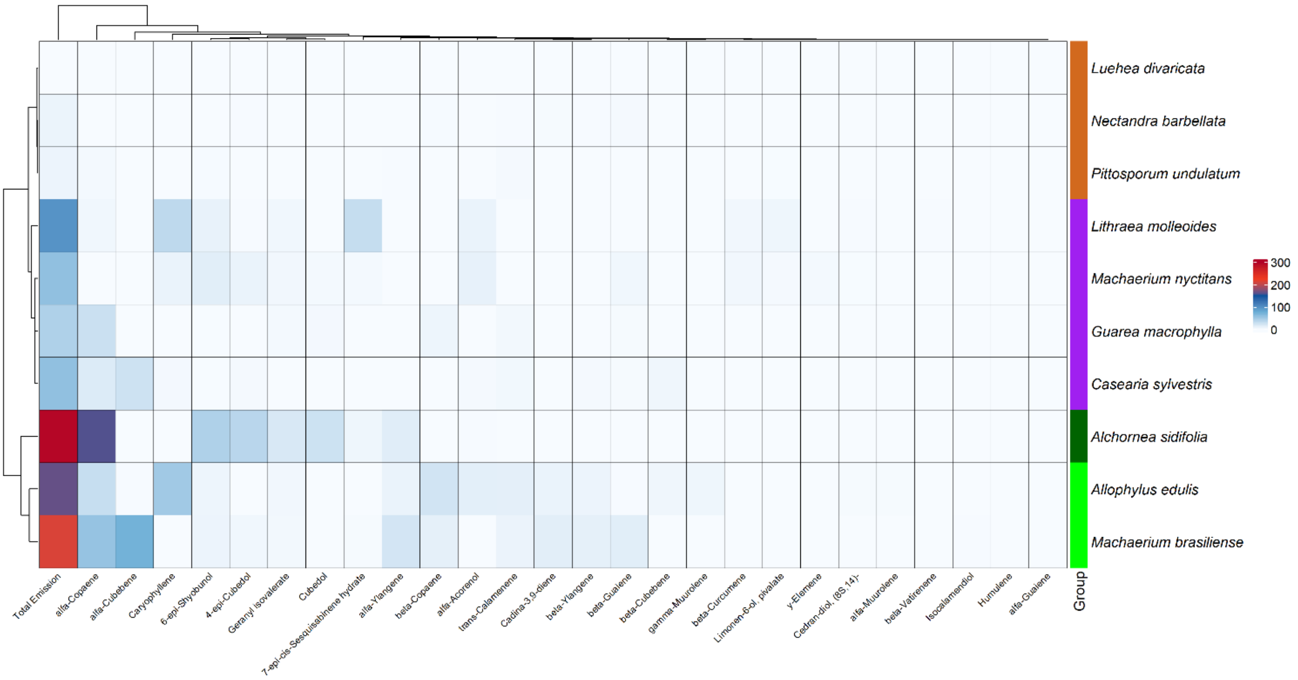

Figure 3. Heatmap analysis combined with hierarchical clustering analysis (HCA) of sesquiterpene (SQT) emission profiles from dominant tree species in Morro Grande Forest Reserve (RMG), São Paulo, Brazil.

This analysis identified four primary groups. Group 1 consists solely of *Alchornea sidifolia*, which is grouped separately due to its notably high total SQT emissions, particularly α-copaene (159.19 ng gdw^{-1} h^{-1}). Its emission profile is characterized by substantial resource investment into fewer compounds, resulting in relatively low SQT diversity (eight distinct SQTs). This focused chemical strategy likely reflects an allocation trade-off, where significant investment in α-copaene synthesis limits the production of other SQTs. Among other compounds emitted by *A. sidifolia*, five occur at moderate levels: 6-epi-shyobunol (40.36 ng gdw^{-1} h^{-1}), 4-epi-cubedol (35.14 ng gdw^{-1} h^{-1}), cubedol (24.30 ng gdw^{-1} h^{-1}), geranyl isovalerate (17.59 ng gdw^{-1} h^{-1}), and α-ylangene (12.97 ng gdw^{-1} h^{-1}). Two additional SQTs, 7-epi-*cis*-sesquisabinene hydrate (5.10 ng gdw^{-1} h^{-1}) and α-acorenol (0.49 ng gdw^{-1} h^{-1}), are present in lower abundance.

Group 2 includes *Machaerium brasiliense* and *Allophylus edulis*, both exhibiting moderate-to-high SQT emissions and the highest compound diversity. In *M. brasiliense*, α-cubebene (71.14 ng gdw^{-1} h^{-1}), α-copaene (53.95 ng gdw^{-1} h^{-1}), and α-ylangene (20.68 ng gdw^{-1} h^{-1}) are the dominant compounds. *A.*

edulis produces the highest β-caryophyllene emissions (48.15 ng gdw^{-1} h^{-1}) among all species, followed by α-copaene (27.92 ng gdw^{-1} h^{-1}) and β-copaene (21.92 ng gdw^{-1} h^{-1}).

Group 3 includes *Lithraea molleoides*, *Casearia sylvestris*, *Machaerium nyctitans*, and *Guarea macrophylla*, all exhibiting moderate total SQT emissions. *L. molleoides*, *C. sylvestris*, and *M. nyctitans* release a similar number of SQT (13, 12, and 12, respectively), while *G. macrophylla* showed a low diversity of SQT emission (seven compounds). Additionally, *C. sylvestris* and *G. macrophylla* show comparable moderate emissions of α-copaene (15.44 and 25.78 ng gdw^{-1} h^{-1}, respectively), which is less prominent in the other species within this group. Finally, group 4 comprises species with low emissions and low SQT diversity. *Nectandra barbellata* (10 compounds) and *Pittosporum undulatum* (8 compounds) emit only trace amounts of SQTs, while emissions from *Luehea divaricata* were below detection limits.

4. Discussion

The present study provides an initial characterization of SQT emissions from dominant tree species in RMG, an Atlantic Forest peri-urban remnant, highlighting high variations in concentrations and chemical profiles. In general, we observed that most species were α-copaene, β-caryophyllene, or α-cubebene-type emitters.

SQTs are synthesized via the mevalonic acid (MVA) pathway in the cytosol, where farnesyl diphosphate (FPP) serves as a universal precursor. Terpene synthases (TPSs) catalyze the conversion of FPP into diverse SQTs through cyclization and rearrangement reactions (Chen et al., 2009; Mischko et al., 2018) which can be further modified with oxygen functional groups to form OSQTs. Therefore, the observed heterogeneity likely results from species-specific differences in TPS activity, which may be influenced by genetic, physiological, and environmental factors, including both biotic and abiotic conditions (Chen et al., 2011; Li et al., 2023; Yu et al., 2015; Zheng et al., 2025).

Building upon this chemical diversity, the hierarchical clustering analysis grouped the species into four distinct clusters based on their SQT emission patterns: Group 1 – high emission, low diversity; Group 2 – moderate-to-high emission, high diversity; Group 3 – moderate emission, moderate diversity (except for *Guarea macrophylla*, which exhibits low chemical diversity); and Group 4 – low emission and diversity. *Alchornea sidifolia* stands apart in Group 1, with α-copaene as the major emitted compound.

This α-copaene-type emission pattern suggests a specialized SQT biosynthesis strategy, potentially favoring a few highly abundant volatiles that may serve key ecological functions. Interestingly, α-copaene has been reported to act as both an insect repellent (Magnani et al., 2025) and as an attractant (Kendra et al., 2017), depending on the ecological context.

In the second group, although both species exhibit similar emissions and high chemical diversity, *Machaerium brasiliense* and *Allophylus edulis* show a notable distinction in their dominant SQT profiles: *M. brasiliense* is primarily an α-cubebene-type emitter, whereas *A. edulis* is characterized by a β-caryophyllene-type profile. Despite their comparable total emissions, this difference in dominant compounds suggests that each species may prioritize distinct chemical strategies for signaling and defense, possibly in response to specific ecological pressures or stress conditions that shape their volatile profiles. β-Caryophyllene is well-documented for its broad-spectrum role in plant responses to biotic stress (Yang et al., 2025b), acting both as a direct deterrent against herbivores and as an indirect defense by attracting predators or parasitoids of herbivorous insects (Peterson et al., 2016). Additionally, the emission of this SQT has been associated with resistance to microbial pathogens in neighboring plants (Frank et al., 2021). Interestingly, although research on α-cubebene's ecological functions is more limited, studies suggest it also has antimicrobial properties (Akçura, 2023).

Like *A. edulis*, *Lithraea molleoides* is also a β-caryophyllene-type emitter but is instead classified into Group 3. This separation suggests that, beyond the dominant sesquiterpene type, the total emission quantity may also influence species grouping. In the case of *L. molleoides*, its moderate overall sesquiterpene emissions align more closely with those of species in the third cluster, including *Casearia sylvestris* (an α-cubebene-type emitter), *Guarea macrophylla* (α-copaene-type), and *Machaerium nyctitans*, whose emissions were predominantly composed of OSQTs.

The absence or near-absence of detectable SQT emissions in Group 4, composed of *Nectandra barbellata*, *Pittosporum undulatum*, and *Luehea divaricata*, suggests that these species may employ alternative defensive strategies. One possibility is the emission of other BVOC classes, such as MTs or green leaf volatiles (GLVs). Alternatively, they may allocate carbon resources to other secondary metabolites, such as flavonoids and tannins, which are known to provide an effective defense against herbivores and pathogens (Barbehenn & Peter Constabel, 2011; Iqbal & Poór, 2024). In fact, according to the Angiosperm Phylogeny Cluster (APG), species in Lauraceae commonly synthesize flavones, 5-*O*-methyl flavonols, acetogenins (polyketides), and tryptamine-derived alkaloids; Pittosporaceae typically produce specialized metabolites such as furanocoumarins, hydroxycoumarins, non-hydrolysable tannins, and abundant fatty acids (e.g., oleic, linoleic, and longer-chain C20–C22 fatty acids); while members of Malvaceae are recognized for their synthesis of cyclopropenoid fatty acids, terpenoid-based quinones, and gums (Stevens, 2001).

Additionally, these species may rely on enzymatic and non-enzymatic antioxidant defenses to mitigate oxidative stress, including enzymes such as superoxide dismutase (SOD), catalase (CAT), and ascorbate peroxidase (APX) (Shafi et al., 2015), as well as elevated glutathione (GSH) levels (Hasanuzzaman et al., 2017). Another interesting finding regarding Group 4 is that *Pittosporum undulatum*, the only non-native species in this study, exhibited some of the lowest SQT emissions. This contrasts with the observation that invasive plants often display greater chemical diversity than native species (McCormick et al., 2023). However, they also emphasize that BVOC emission patterns from non-native species and their ecological effects remain unclear and require further study.

High SQT diversity was also observed by Anselmo-Moreira et al. (2025), which examined the BVOC emission profile of dominant trees in another Atlantic Forest remnant within MASP. Notably, the total number of detected SQT was similar between the two studies (24 and 26, respectively), with comparable species-level emissions ranging from 6.18 to 295.14 ng gdw^{-1} h^{-1} in the present study and from 2 to 332 ng gdw^{-1} h^{-1} in the other study. Remarkably, despite entirely different species compositions, 19 SQT were common to both. These findings highlight the need for further research comparing different Atlantic Forest remnants, ideally using standardized methods with emissions collected during the same period and from the same species, when possible, to better understand BVOC emission patterns and drivers across ecosystems.

A noteworthy finding of our study is that except for *Luehea divaricata*, deciduous species (i.e., those that shed leaves seasonally) emitted higher levels of SQT compared to evergreen species (which retain leaves year-round and replace them gradually) (Table S2). In general, deciduous trees are higher isoprene emitters and lower MT emitters, whereas evergreen trees are low isoprene emitters and can be either low or high MT emitters (Fitzky et al., 2019). However, more research with additional species is needed to investigate SQT emissions, particularly in South American species, to determine whether this trend persists (Bao et al., 2023). For instance, in other regions, as in northern China, BVOC emissions did not show a consistent relationship with leaf habit (deciduous vs. evergreen), indicating that additional factors beyond leaf habit influence emission patterns (Zhang et al., 2024).

Beyond their ecological and physiological roles, the presence and diversity of certain SQTs in these species may also hold potential for medicinal and industrial applications. For instance, β-caryophyllene has been associated with various beneficial effects, including anti-inflammatory, anticancer, antimicrobial, antioxidant, and analgesic properties (Fidyt et al., 2016). This makes caryophyllene-rich species such as *Allophylus edulis* and *Lithraea molleoides* promising candidates for bioprospecting. While *A. edulis* is already being investigated in this context (Santos et al., 2021; Trevizan et al., 2016), *L. molleoides* remains relatively unexplored. OSQTs have also been reported to exhibit cytotoxic and antibacterial activities (De Almeida et al., 2016) and are valued for their aromatic properties, making them useful in the flavor and fragrance industries (Ly et al., 2017; Umezawa et al., 2020). These combined attributes highlight species such as *Alchornea sidifolia*, *L. molleoides*, and *Machaerium nyctitans* as valuable targets for further research and potential commercial applications.

From the perspective of urban greening initiatives aimed at improving air quality and reducing pollution, species with low or negligible SQT emissions may help limit the formation of secondary pollutants like ozone (Wang et al., 2021). In this context, Group 4 species are particularly relevant. However, their suitability for urban environments requires further investigation, including assessments of emissions from other BVOC classes, seasonal variations in BVOC release, and the broader ecological trade-offs associated with their use in urban ecosystems. For instance, Anselmo-Moreira et al. (2025) reported that SQT-emitting species in a tropical forest exhibited higher emissions during the wet season, highlighting the importance of seasonal patterns in BVOC dynamics. A comprehensive understanding of these factors will be essential for optimizing species selection in urban greening strategies that balance air quality benefits with ecological functionality.

5. Conclusion

Our characterization of SQT emissions from dominant trees in RMG reveals substantial variation in both concentration and chemical composition. Hierarchical clustering analysis grouped the species into four distinct categories based on emission patterns: Group 1, characterized by high emission and low diversity; Group 2, with moderate-to-high emission and high diversity; Group 3, showing moderate emission and low-to-moderate diversity; and Group 4, defined by low SQT emissions and diversity. Additionally, certain SQTs, such as α-copaene, β-caryophyllene, and α-cubebene, emerged as key compounds, each potentially serving distinct ecological functions, including defense mechanisms against herbivory and microbial infection. These findings indicate that species may adopt different volatile emission strategies, likely shaped by their ecological interactions, stress responses, and environmental conditions. We also observed that deciduous species generally emitted more SQTs than evergreen species, though this trend requires further validation across broader geographic regions and a wider range of taxa.

The distinct chemical profiles not only highlight ecological adaptations but also have potential implications for economic and urban applications. Species-rich in β-caryophyllene, such as *Allophylus edulis* and *Lithraea molleoides*, could be promising subjects for further investigation into pharmaceutical applications. Similarly, *Machaerium nyctitans* and *Alchornea sidifolia* may be explored for potential uses in the flavor and fragrance industries, particularly due to the high diversity of OSQTs they emit. Conversely, low-emitting species like *Luehea divaricata* may be better suited for urban greening programs. Nevertheless, understanding the full suite of volatile emissions, beyond SQTs, is crucial before implementing these species in urban afforestation programs.

While this study has provided valuable findings into SQT emission patterns among the selected species, several avenues for future research remain. First, our analysis focused exclusively on SQT emissions; however, a comprehensive understanding of emission profiles should include other BVOC classes to evaluate the broader ecological roles and environmental interactions of these species. Additionally, future studies should incorporate multi-seasonal sampling to capture seasonal variability. Comparative studies across a broader taxonomic range and different geographic locations could also enhance the generalizability of our findings. Lastly, assessing the impact of emitted BVOCs on secondary atmospheric pollutant formation, particularly ozone and particulate matter in urban settings, would provide critical information for urban planning and pollution mitigation strategies. Such comprehensive analyses are essential for advancing BVOCs research in South America and understanding its ecological, economic, and urban applications.

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Declaration of interests

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

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Table 1. Sesquiterpene (SQT) emissions (ng gdw^{-1} h^{-1}) from dominant native species in the Morro Grande Forest Reserve (RMG), São Paulo, Brazil.

	Species										
Compounds	*Alchornea sidifolia*	*Allophylus edulis*	*Casearia sylvestris*	*Guarea macrophylla*	*Lithraea molleoides*	*Luehea divaricata*	*Machaerium brasiliense*	*Machaerium nyctitans*	*Nectandra barbellata*	*Pittosporum undulatum*	Total compound emission across all species
4-epi-Cubedol*	35.14 ± 55.05	0.13 ± 0.22	1.53 ± 0.44	-	0.78 ± 1.35	-	4.04 ± 7.00	7.54 ± 10.67	0.64 ± 0.65	-	49.80 ± 75.38
6-epi-Shyobunol*	40.36 ± 57.06	5.73 ± 8.41	0.33 ± 0.28	0.44 ± 0.76	8.32 ± 14.42	-	6.18 ± 7.44	12.75 ± 18.03	-	0.89 ± 0.71	75.00 ± 107.11
7-epi-*cis*-Sesquisabinene hydrate*	5.10 ± 8.83	-	-	-	28.54 ± 49.43	-	1.25 ± 2.17	2.20 ± 3.11	-	-	37.09 ± 63.54
Cadina-3,9-diene	-	7.54 ± 13.06	-	-	-	-	11.96 ± 20.72	-	1.17 ± 1.65	-	20.67 ± 35.43
Cedran-diol, (8S,14)-*	-	0.93 ± 1.61	-	-	0.57 ± 0.99	-	-	0.43 ± 0.60	-	0.25 ± 0.44	2.18 ± 3.64
Cubedol*	24.30 ± 30.51	-	0.28 ± 0.48	2.41 ± 2.91	0.08 ± 0.13	-	0.24 ± 0.42	2.03 ± 2.87	0.27 ± 0.38	-	29.61 ± 37.70
Geranyl isovalerate*	17.59 ± 18.45	3.47 ± 6.01	-	2.25 ± 1.96	4.15 ± 7.06	-	2.78 ± 4.81	3.41 ± 4.83	-	-	33.65 ± 43.12
Humulene	-	-	-	-	0.16 ± 0.28	-	-	-	-	-	0.16 ± 0.28
Isocalamendiol*	-	-	-	-	-	-	0.49 ± 2.76	-	-	-	0.49 ± 2.76
Limonen-6-ol, pivalate*	-	-	-	-	4.87 ± 8.44	-	-	1.85 ± 2.52	-	0.40 ± 0.69	7.12 ± 11.65
trans-Calamenene	-	11.05 ± 16.23	3.18 ± 1.02	2.91 ± 1.29	-	-	7.12 ± 12.33	-	0.61 ± 0.87	1.49 ± 0.77	26.36 ± 32.51
α-Acorenol*	0.49 ± 0.84	11.50 ± 19.92	1.78 ± 1.54	-	7.63 ± 13.22	-	-	9.34 ± 13.21	0.22 ± 0.31	0.15 ± 0.25	31.11 ± 49.29
α-Copaene	159.19 ± 198.94	27.92 ± 37.61	15.44 ± 13.02	25.78 ± 24.69	4.18 ± 7.25	-	53.95 ± 93.44	-	-	2.23 ± 0.76	288.69 ± 375.71
α-Cubebene	-	0.57 ± 0.99	24.07 ± 23.72	-	-	-	71.14 ± 123.22	-	-	-	95.78 ± 147.93
α-Guaiene	-	-	-	-	-	-	-	-	0.13 ± 0.18	-	0.13 ± 0.18
α-Muurolene	-	1.25 ± 2.17	-	-	-	-	-	-	-	-	1.25 ± 2.17
α-Ylangene	12.97 ± 22.46	7.21 ± 11.18	-	-	-	-	20.68 ± 35.81	-	-	0.71 ± 1.22	41.57 ± 70.67
β-Caryophyllene	-	48.15 ± 74.00	2.40 ± 2.09	-	32.54 ± 28.84	-	-	7.25 ± 10.25	0.27 ± 0.39	-	90.61 ± 115.57
β-Copaene	-	21.92 ± 33.31	4.74 ± 4.56	5.81 ± 5.06	-	-	10.22 ± 17.70	-	0.88 ± 1.25	-	43.57 ± 61.88
β-Cubebene	-	4.72 ± 8.17	-	-	-	-	-	-	-	-	9.46 ± 12.73

β-Curcumene	-	-	-	-	3.58 ± 6.20	-	-	3.69 ± 5.22	-	-	7.27 ± 11.42
β-Guaiene	-	0.57 ± 0.98	1.40 ± 1.29	0.93 ± 1.62	-	-	12.70 ± 22.00	4.09 ± 5.78	1.81 ± 2.55	-	21.50 ± 34.22
β-Vatirenene	-	-	-	-	0.67 ± 1.17	-	-	-	-	-	0.67 ± 1.17
β-Ylangene	-	6.20 ± 10.73	1.53 ± 1.36	-	-	-	10.19 ± 17.65	-	0.75 ± 1.06	-	18.67 ± 30.80
γ-Elemene	-	0.09 ± 0.16	0.03 ± 0.02	-	-	-	-	2.03 ± 2.87	-	0.06 ± 0.03	2.21 ± 3.08
γ-Muurolene	-	5.17 ± 8.95	-	-	-	-	-	-	-	-	5.17 ± 8.95
Total emission per species	295.14 ± 392.14	164.12 ± 253.71	56.69 ± 45.94	40.53 ± 38.29	96.07 ± 138.78	-	212.94 ± 367.47	56.61 ± 79.96	6.75 ± 9.29	6.18 ± 4.87	

*Represents oxygenated sesquiterpenes (OSQT).