Research Article

Chemical Diversity in *Lippia alba* (Mill.) N. E. Brown Germplasm

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The aim of this study was to perform chemical characterization of *Lippia alba* accessions from the Active Germplasm Bank of the Federal University of Sergipe. A randomized block experimental design with two replications was applied. The analysis of the chemical composition of the essential oils was conducted using a gas chromatograph coupled to a mass spectrometer. The chemical composition of the essential oils allowed the accessions to be allocated to the following six groups: group 1: linalool, 1,8-cineole, and caryophyllene oxide; group 2: linalool, geranial, neral, 1,8-cineol, and caryophyllene oxide; group 3: limonene, carvone, and sabinene; group 4: carvone, limonene, g-muurolene, and myrcene; group 5: neral, geranial, and caryophyllene oxide; and group 6: geranial, neral, o-cymene, limonene, and caryophyllene oxide.

1. Introduction

The Verbenaceae family consists of approximately 175 genera and 2,800 species distributed in tropical and subtropical regions worldwide and in temperate regions of the southern hemisphere. In addition, a few species are found in temperate regions of the northern hemisphere [1]. The genus *Lippia* includes several plant species of medicinal interest and comprises approximately 200 shrub species with a pantropical distribution and approximately 150 species distributed across ruprestrial grasslands and tropical savannas (cerrados) in Brazil [2]. The species *Lippia alba* (Mill.) N.E. Brown, also known as *Lippia geminata* HBK and *Lantana alba* (Mill), is a shrub with a height of approximately 3 meters [3]. In traditional Brazilian medicine, this species is popularly known as lemon balm [4].

This species is considered by some authors [5] to be promising for use in the pharmaceutical, aromatic, and perfume industries and may also be suitable for the agricultural chemical industry because of its proven antifungal, insecticidal, and repellent properties. The essential oil obtained from *L. alba* has been recognized as a potential source of several commercially important terpenoid compounds [6].

The chemical composition of essential oils consists of a mixture of many organic compounds in various concentrations, ranging from very low quantities (traces) to major compounds. Therefore, the variability of chemical types is a cause for concern from the standpoint of the use of essential oils as herbal medicines because some compounds may be unsuitable for achieving a desired result. This problem regarding medicinal plants is common in Brazil [7].

Essential oils are primarily produced by the plant leaves and are formed through the secondary metabolism of plants. The typical compounds of this type include mono- and sesquiterpenes. Both the oil composition and plant yield,
including biomass, are directly influenced by environmental factors, which represent a challenge for producers in establishing productive and stable genotypes and maintaining the chemical uniformity demanded by the industry [5].

The rich pharmacological potential of *L. alba* is related to the wide chemical variability of its essential oils. This variability allows the classification of this species into chemotypes, which can be defined according to the major chemical components of the essential oils [8]. The essential oils of some chemotypes identified from *L. alba* differ in their chemical composition, with citral, carvone, and linalool representing the major components identified [9]. The limonene-carvone chemotype is characterized by the presence of limonene and carvone and the absence of neral and geranial (citral). Limonene is used as a solvent in cleaning products, foodstuffs, and the cosmetics industry. Carvone is used as a carminative and in cosmetic products and has bactericidal and fungicidal properties [10].

The degree of variability in the active ingredient found in a medicinal species should be very low so that the drugs produced from that species are safe and effective [8]. Therefore, the identification and correct classification of chemotypes, which exhibit distinct active ingredients in medicinal plants, are of great importance for maintaining quality, planning cultivation, and obtaining phytochemicals that do not impair users’ health [11].

Thus, the aim of this study was to perform chemical characterization of accessions of *L. alba* (Mill.) NE Br. from the Active Germplasm Bank (AGB) of the Federal University of Sergipe.

2. Materials and Methods

2.1. Plant Materials. The experiment was conducted at the “Campus Rural da UFS” experimental farm, located in the municipality of São Cristóvão, state of Sergipe, at a latitude of 11° 00’ S and longitude of 37° 12’ W. Plants of 48 accessions of *L. alba* from the AGB at UFS were evaluated (Table 1).

A randomized block experimental design with two replications was employed. Each plot consisted of three plants. Spacing of 1.5 meters was maintained both between individual plants and between rows. The fertilization applied in the field was 5 kg of cattle manure per pit. Culture practices such as weeding and hydration were performed whenever necessary.

2.2. Distillation and Analysis of Essential Oils. The plants were cut at a height of 30 cm from the soil, and the leaves were dried in an incubator with forced airflow at a temperature of 40°C for five days [12]. After drying, the leaves were weighed on an electronic scale, and essential oils were extracted using the hydrodistillation method in a Clevenger apparatus. For hydrodistillation, 75 g of dry leaves and 2.0 L of distilled water were used per flask, and the distillation period was 120 minutes after the initiation of water vapor condensation in the Clevenger apparatus. After extraction, the essential oils were collected and stored in a freezer in amber glass vials.

Chemical analysis of the essential oil was performed at the Laboratory of Chromatography of the Department of Chemistry at the Federal University of Sergipe.

Qualitative analysis of the chemical composition of the essential oil was performed in a gas chromatograph coupled to a mass spectrometer (GC-MS, model QP 5050A, Shimadzu) equipped with an AOC-20i autosampler (Shimadzu) and a fused-silica capillary column (5% phenyl, 95% dimethylpolysiloxane, 30 m x 0.25 mm i.d., and film thickness of 0.25 μm, J&W Scientific) using helium as the carrier gas at a flow rate of 1.2 mL min⁻¹. The temperature ramp was 50°C for 2 min, followed by an increase of 4°C.min⁻¹ until reaching 200°C, then an increase of 15°C until reaching 300°C, after which a constant temperature was maintained for 15 min. The injector temperature was maintained at 250°C, and that of the detector (or interface) was maintained at 280°C. A volume of 0.5 μL was injected using ethyl acetate. The partition rate of the injected volume was 1:100, and the column pressure was 64.20 kPa. The MS conditions included an ion capture detector operated through electron impact and an impact energy of 70 eV, a scan rate of 1,000, a scan interval of 0.50 fragment/s, and a fragment mass range between 40 Da and 500 Da.

Quantitative analysis of the chemical constituents was performed by flame ionization gas chromatography (FID), using a Shimadzu GC-17A (Shimadzu Corporation, Kyoto, Japan) instrument, under the following operational conditions: capillary ZB-5MS column (5% phenyl-arylene-95%-dimethylpolysiloxane) fused-silica capillary column (30 m x 0.25 mm i.d. x 0.25 μm film thickness) from Phenomenex (Torrance, CA, USA), under the same conditions as reported for the GC-MS. Quantification of each constituent was estimated by area normalization (%). Compound concentrations were calculated from the GC peak areas and they were arranged in order of GC elution.

The essential oil components were identified by comparing their mass spectra with the available spectra in the equipment database (NIST05 and WILEY8). Additionally, the measured retention indices were compared with those in the literature [13]. The relative retention indices (RRI) were determined using the van den Dool and Kratz [14] equation and a homologous series of *n*-alkanes (C₈–C₁₈) injected under the chromatography conditions described above.

2.3. Statistical Analysis. The data were subjected to variance analysis, and the means were compared using the Scott-Knott test (*p* ≤ 0.05). The chemical composition data were analyzed through two multivariate analysis methods: principal component analysis (PCA) and arrangement analysis (cluster) based on the similarity and distribution of the compounds, using Statistica software, version 7.0.

3. Results and Discussion

Among the compounds present in the essential oils from 48 accessions, 33 were identified and are listed according to their order of elution (Table 2).
Table 1: Identification and origin of *L. alba* accessions from the Active Germplasm Bank at the Federal University of Sergipe.

| Accession | Municipality/state         | Origin                  | UFS herbarium code |
|-----------|---------------------------|-------------------------|--------------------|
| LA-01     | ABC-Distrito Federal      | University of Brasília  | 14784              |
| LA-02     | Araguaína-Tocantins       | University of Brasília  | 14785              |
| LA-03     | Atibaia-São Paulo         | University of Brasília  | 13466              |
| LA-04     | Botucatu-São Paulo        | University of Brasília  | 13501              |
| LA-08     | Brasilia-Distrito Federal | University of Brasília  | 13475              |
| LA-09     | Brasilia-Distrito Federal | University of Brasília  | 14786              |
| LA-10     | Brasilia-Distrito Federal | University of Brasília  | 13495              |
| LA-13     | Fortaleza-Ceará           | Federal University of Ceará | 13488          |
| LA-15     | Florianópolis-Santa Catarina | University of Brasília | 13486        |
| LA-17     | Brasilia-Distrito Federal | University of Brasília  | 13494              |
| LA-19     | Brasilia-Distrito Federal | University of Brasília  | 13491              |
| LA-22     | Lavras-Minas Gerais       | University of Brasília  | 13476              |
| LA-24     | Luziânia-Goiás            | University of Brasília  | 13477              |
| LA-27     | Piracicaba-São Paulo      | University of Brasília  | 13443              |
| LA-28     | Brasilia-Distrito Federal | University of Brasília  | 13487              |
| LA-29     | Planaltina de Goiás-Goiás| University of Brasília  | 13485              |
| LA-30     | Posse-Goiás               | University of Brasília  | 13454              |
| LA-32     | Rio de Janeiro-Rio de Janeiro | University of Brasília | 13480         |
| LA-36     | Brasilia-Distrito Federal | University of Brasília  | 13472              |
| LA-37     | Brasilia-Distrito Federal | University of Brasília  | 13455              |
| LA-39     | Brasilia-Distrito Federal | University of Brasília  | 13497              |
| LA-40     | Brasilia-Distrito Federal | University of Brasília  | 13456              |
| LA-41     | Curitiba-Paraná           | University of Brasília  | 13484              |
| LA-42     | Brasilia-Distrito Federal | University of Brasília  | 13444              |
| LA-43     | Brasilia-Distrito Federal | University of Brasília  | 13490              |
| LA-44     | Brasilia-Distrito Federal | University of Brasília  | 14788              |
| LA-45     | Vigosa-Minas Gerais       | University of Brasília  | 13498              |
| LA-49     | Aracaju-Sergipe           | Federal University of Sergipe | 13471       |
| LA-52     | Rio Real-Bahia            | Federal University of Sergipe | 13481     |
| LA-53     | Telha-Sergipe             | Federal University of Sergipe | 13446     |
| LA-54     | Rio Real-Bahia            | Federal University of Sergipe | 13478     |
| LA-55     | Rio Real-Bahia            | Federal University of Sergipe | 13468     |
| LA-56     | Rio Real-Bahia            | Federal University of Sergipe | 13465     |
| LA-57     | Rio Real-Bahia            | Federal University of Sergipe | 13469     |
| LA-58     | Rio Real-Bahia            | Federal University of Sergipe | 13482     |
| LA-59     | Rio Real-Bahia            | Federal University of Sergipe | 13500     |
| LA-60     | Rio Real-Bahia            | Federal University of Sergipe | 13499     |
| LA-61     | Rio Real-Bahia            | Federal University of Sergipe | 13479     |
| LA-62     | Rio Real-Bahia            | Federal University of Sergipe | 13451     |
| LA-63     | Santana do São Francisco-Sergipe | Federal University of Sergipe | 13445    |
| LA-67     | Santana do São Francisco-Sergipe | Federal University of Sergipe | 13464    |
| LA-68     | Santana do São Francisco-Sergipe | Federal University of Sergipe | 14789    |
| LA-69     | Gararu-Sergipe            | Federal University of Sergipe | 13467    |
| LA-70     | Cristinópolis-Sergipe     | Federal University of Sergipe | 13473    |
| LA-71     | Paripiranga-Sergipe       | Federal University of Sergipe | 13447    |
| LA-72     | Traipu-Alagoas            | Federal University of Sergipe | 13496    |
### Table 2: Chemical composition of the essential oil of *L. alba* accessions from the Active Germplasm Bank at the Federal University of Sergipe.

| Compound                  | RRI  | LA-01 | LA-02 | LA-03 | LA-04 | LA-08 | LA-09 | LA-10 | LA-13 |
|---------------------------|------|-------|-------|-------|-------|-------|-------|-------|-------|
| \( \alpha \)-thujene      | 924  | 0.00b | 0.00b | 0.43b | 0.27b | 0.00b | 0.00b | 0.00b | 0.00b |
| Sabinene                  | 969  | 0.00c | 0.00c | 0.00c | 0.15c | 0.00c | 0.64c | 0.00c | 4.39a |
| 1-Octen-3-ol              | 974  | 0.00b | 0.00b | 0.00b | 0.28b | 0.72a | 0.00b | 0.00b | 0.00b |
| 5-Methyl-6-hepten-2-one   | 981  | 0.00a | 0.00a | 0.46a | 0.41a | 0.34a | 0.00a | 0.00a | 0.00a |
| Myrcene                   | 988  | 0.00c | 0.76c | 2.78b | 2.85b | 0.31c | 0.00c | 0.00c | 0.00c |
| \( \alpha \)-Cymene        | 1022 | 0.00d | 0.00d | 0.11d | 0.32d | 0.00d | 0.00d | 0.00d | 0.00d |
| Limonene                  | 1024 | 0.00e | 0.00e | 10.24c | 0.17e | 0.00e | 0.00e | 45.35a |       |
| 1,8-Cineol                | 1026 | 7.22b | 0.00d | 0.00d | 0.00d | 0.00d | 9.22a | 0.00d | 0.00d |
| \( \gamma \)-terpinene    | 1054 | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| *cis*-sabinene hydrate    | 1065 | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| *cis*-linalool oxide      | 1067 | 0.86b | 0.00c | 0.00c | 0.00c | 1.20a | 0.00c | 0.00c | 0.00c |
| *trans*-linalool oxide    | 1084 | 0.65b | 0.00d | 0.00d | 0.00d | 0.98a | 0.00d | 0.00d | 0.00d |
| Linalool                   | 1095 | 84.73a| 32.14a| 29.78c | 30.28c | 31.09c | 0.00f | 29.32c | 0.00f |
| Geraniol                  | 1324 | 0.00d | 0.00d | 0.13c | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| Geranyl acetate           | 1379 | 0.00c | 0.00c | 0.29c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| Myrtenal                  | 1389 | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| \( \beta \)-caryophyllene | 1417 | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e |
| \( \alpha \)-guaiene       | 1437 | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| \( \gamma \)-muurolene    | 1478 | 0.62c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| *trans*-calamenene        | 1521 | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| Elemol                    | 1548 | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| Germacrene B              | 1559 | 0.57b | 0.00c | 0.00c | 0.00c | 0.00c | 0.28c | 0.00c | 0.00c |
| (E)-nerolidol             | 1561 | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e |
| Spathulenol               | 1577 | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| Caryophyllene oxide       | 1582 | 2.93d | 11.33c | 0.00e | 10.69c | 14.24c | 3.66d | 17.77b | 0.00e |
| Humulene epoxide II       | 1608 | 0.00d | 0.00d | 0.15d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| Essential oil content (%) |      |       |       |       |       |       |       |       |       |
| \( \alpha \)-thujene      | 924  | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| Sabinene                  | 969  | 0.00c | 0.00c | 0.00c | 0.71b | 0.00c | 0.29c | 0.00c | 0.64b |
| 1-Octen-3-ol              | 974  | 0.42a | 0.78a | 0.77a | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| 5-Methyl-6-hepten-2-one   | 981  | 1.03a | 0.91a | 0.58a | 0.00a | 0.38a | 0.00a | 0.00a | 0.00a |
| Myrcene                   | 988  | 3.07b | 0.67c | 0.45c | 0.76c | 0.84c | 0.00c | 0.00c | 0.21c |
| \( \alpha \)-Cymene        | 1022 | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| Limonene                  | 1024 | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e |
| 1,8-Cineol                | 1026 | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| \( \gamma \)-terpinene    | 1054 | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| *cis*-sabinene hydrate    | 1065 | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| Essential oil content (%) | LA-28 | LA-29 | LA-30 | LA-32 | LA-36 | LA-37 | LA-39 | LA-40 |
|---------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| cis-linalool oxide        | 1067  | 0.00c | 0.00c | 0.00c | 0.64b | 0.00c | 1.00a | 0.00c | 0.80b |
| trans-linalool oxide      | 1084  | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.23c | 0.00d | 0.61b |
| Linalool                   | 1095  | 0.83f | 1.43f | 0.83f | 57.69d | 7.27f | 84.45a | 49.38e | 75.79c |
| Perylene                  | 1102  | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| (E)-isocitral              | 1177  | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| Myrtenal                  | 1195  | 0.00c | 0.00c | 0.95a | 0.00c | 0.34c | 0.00c | 0.00c | 0.66b |
| Neral                     | 1235  | 31.98a | 28.91c | 31.22c | 11.51e | 28.98c | 0.00f | 16.59e | 0.58f |
| Geraniol                  | 1249  | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| Geranial                  | 1264  | 50.54a | 48.68a | 49.09a | 16.99e | 44.91a | 0.00f | 26.18e | 0.83f |
| Myrtyl acetate            | 1324  | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| Geranyl acetate           | 1359  | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| β-elemene                 | 1389  | 0.00d | 0.25d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.46d |
| γ-muurolere               | 1417  | 1.75b | 1.03c | 0.89c | 0.00d | 0.00d | 0.00d | 0.00d | 1.95b |
| α-thujene                 | 1437  | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| Sabinene                  | 1478  | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 1.60b |
| trans-calamenene          | 1521  | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| Elemol                    | 1548  | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| Germacrene B              | 1559  | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 1.26a |
| (E)-nerolidol             | 1561  | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e |
| Spathulenol               | 1577  | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e |
| Caryophyllene oxide       | 1582  | 10.35c | 16.86b | 14.04c | 3.18d | 14.63c | 4.35d | 4.14d | 0.00d |
| Humulene epoxide II       | 1608  | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| Essential oil content (%) | 1.09d | 1.04d | 0.89e | 1.33d | 0.76e | 2.53a | 2.50a | 2.26b |
| Compound                        | LA-41 | LA-42 | LA-43 | LA-44 | LA-45 | LA-49 | LA-52 | LA-53 |
|--------------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| α-thujene                      | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| Sabinene                       | 0.14c | 0.28c | 0.31c | 0.00c | 0.98b | 0.57b | 0.54b | 0.17c |
| 1-Octen-3-ol                   | 0.63a | 0.44a | 0.00b | 0.58a | 0.00b | 0.21b | 0.00b | 0.59a |
| 5-Methyl-6-hepten-2-one        | 0.74a | 0.00a | 0.43a | 0.51a | 0.30a | 0.26a | 0.30a | 0.34a |
| Myrcene                        | 1.47c | 2.04c | 0.71c | 0.42c | 8.47a | 0.00c | 0.21c | 0.00c |
| α-Cymene                       | 0.31d | 0.00d | 0.00d | 0.32d | 11.50a| 9.44b | 4.49c | 0.00d |
| Limonene                       | 0.00c | 0.00e | 7.46c | 0.00e | 0.00e | 0.00e | 3.86d | 0.00e |
| 1,8-Cineol                     | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| y-terpinene                    | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.98a | 0.00c | 0.00c |
| cis-sabinene hydrate           | 0.00c | 0.00c | 0.00c | 0.00c | 0.46b | 0.00c | 0.00c | 0.33b |
| cis-linalool oxide             | 0.15c | 0.00c | 0.00c | 0.00c | 0.00c | 0.27c | 0.00c | 0.00c |
| trans-linalool oxide           | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| Linalool                       | 0.85f | 2.22f | 0.74f | 0.73f | 1.33f | 0.33f | 0.00f | 0.57f |
| Perylene                       | 0.00b | 0.00b | 0.75a | 0.00b | 0.38a | 0.00b | 0.46a | 0.00b |
| (E)-isocitral                  | 0.00b | 0.00b | 0.75a | 0.00b | 0.38a | 0.00b | 0.46a | 0.00b |
| Myrtenal                       | 0.00c | 0.00c | 0.00c | 0.68b | 0.00c | 0.00c | 0.00c | 0.00c |
| Neral                          | 30.88c| 31.33c| 34.86a| 32.27a| 28.57c| 23.69c| 29.97c| 31.57a|
| Carvone                        | 0.00c | 0.00e | 3.56d | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e |
| Geraniol                       | 0.00c | 0.00c | 0.00c | 0.00c | 3.38a | 0.00c | 0.00c | 0.00c |
| Geranial                       | 48.69a| 48.59a| 51.18a| 49.88a| 46.36a| 39.39c| 46.22a| 48.37a|
| Myrtanyl acetate               | 0.00d | 0.00d | 0.00d | 0.50b | 0.00d | 0.00d | 0.00d | 0.00d |
| Geranyl acetate                | 0.27b | 0.00c | 0.00c | 0.40b | 1.03a | 0.00c | 0.00c | 0.00c |
| β-elemene                      | 0.79c | 1.75a | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| β-caryophyllene                | 0.88c | 1.23c | 0.00c | 0.00c | 2.84a | 1.15c | 1.60b | 0.00c |
| α-guaiene                      | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 1.66b |
| γ-muurolene                    | 0.00c | 0.00c | 0.00c | 0.00c | 0.33c | 0.38c | 0.00c | 0.00c |
| trans-calamenene               | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| Elemol                         | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| Germacrene B                   | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| (E)-nerolidol                  | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e |
| Spathulenol                    | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 3.21a |
| Caryophyllene oxide            | 12.46c| 11.66c| 0.00e | 13.43c| 5.37d | 19.89b| 6.05d | 5.05d |
| Humulene epoxide II            | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.66b | 0.34c | 1.45a |
| Essential oil content (%)      | 0.85e | 0.90e | 1.80c | 0.69e | 1.06d | 1.18d | 2.00c | 0.76e |
| α-thujene                      | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| Compound                    | LA-62 | LA-63 | LA-67 | LA-68 | LA-69 | LA-70 | LA-71 | LA-72 |
|-----------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| **Sabinene**                | 0.59b | 0.53b | 0.00c | 0.00c | 0.00c | 0.25c | 0.00c | 0.00c |
| **1-Octen-3-ol**            | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.67a | 0.52a | 0.00b |
| **5-Methyl-6-hepten-2-one** | 0.00a | 0.00a | 0.00a | 0.00a | 0.00a | 0.65a | 0.92a | 0.00a |
| **Myrcene**                 | 0.00c | 0.00c | 0.17c | 0.15c | 1.27c | 2.80b | 0.00c | 1.31c |
| **o-Cymene**                | 9.55b | 8.29b | 0.00d | 0.00d | 2.93c | 3.77b | 6.47b | 3.53c |
| **Limonene**                | 3.97d | 3.69d | 18.48b | 19.35b | 0.00e | 0.00e | 2.60b | 0.00e |
| **1,8-Cineol**              | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| **cis-sabinene hydrate**    | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| **cis-linalool oxide**      | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| **trans-linalool oxide**    | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| **Linalool**                | 0.00f | 0.00f | 0.32f | 0.19f | 2.83f | 2.31f | 0.00f | 2.30f |
| **Perylene**                | 0.00b | 0.00b | 0.00b | 0.00b | 0.14a | 0.13a | 0.00b | 0.00b |
| **(E)-isocitral**           | 0.85a | 0.44a | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| **Myrtenal**                | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| **Neral**                   | 29.99c | 30.98c | 0.00f | 0.00f | 33.20a | 33.93a | 33.46a | 35.31a |
| **Carvone**                 | 1239 | 0.00e | 0.00e | 77.74a | 77.20a | 0.00e | 0.00e | 0.00e |
| **Geraniol**                | 1437 | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| **Geranial**                | 1478 | 0.00c | 0.00c | 1.99b | 1.95b | 0.00c | 0.00c | 0.00c |
| **Myrtanylacetate**         | 1521 | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b | 0.00b |
| **Geranylacetate**          | 1548 | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d | 0.00d |
| **γ-elemene**               | 1559 | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c | 0.00c |
| **γ-caryophyllene**         | 1561 | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e |
| **α-thujene**               | 1577 | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e | 0.00e |
| **Spathulenol**             | 1582 | 7.54d | 5.96d | 0.00e | 0.00e | 5.00d | 2.59d | 4.85d |
| **Carvophyllene oxide**     | 1608 | 0.38c | 0.00d | 0.00d | 0.00d | 0.87b | 0.36c | 0.00d |
| **Essential oil content (%)** | 1.93c | 2.33b | 1.60c | 2.66a | 0.66e | 1.00d | 1.73c | 0.66e |

**Table 2:** Continued.
Table 2: Continued.

| Compound               | EUclidean distance | \( \beta \)-elemene  | \( \beta \)-caryophyllene | \( \gamma \)-muurolene | trans-calamenene | Elemol           | Germacrene B | (E)-nerolidol | Spathulenol | Caryophyllene oxide | Humulene epoxide II | Essential oil content (%) |
|------------------------|--------------------|-----------------------|---------------------------|------------------------|------------------|------------------|---------------|---------------|-------------|----------------------|--------------------------|----------------------------|
| (E)-isocitral          | 1177               | 0.63a                 | 0.98a                     | 0.44a                  | 0.00b            | 0.24b            | 0.00b         | 0.77a         | 0.58a       | RRI: relative retention index. Means followed by different letters in each row were significantly different by the Scott-Knott test \( (p < 0.05) \). |
| Myrtenal               | 1195               | 0.00c                 | 0.00c                     | 0.00c                  | 0.00c            | 0.00c            | 0.00c         | 0.00c         | 0.00c       |                      |                          |                            |
| Neral                  | 1235               | 31.36c                | 29.46c                    | 33.28a                 | 27.34c           | 29.05c           | 27.94c        | 36.14a        | 0.00f       |                      |                          |                            |
| Carvone                | 1239               | 5.27d                 | 1.06e                     | 0.00e                  | 0.29e            | 72.73b           | 0.00e         | 0.00e         | 0.00e       |                      |                          |                            |
| Geraniol               | 1249               | 0.00c                 | 0.00c                     | 0.00c                  | 0.00c            | 0.00c            | 0.00c         | 0.00c         | 0.00c       |                      |                          |                            |
| Geranial               | 1264               | 46.11a                | 45.12a                    | 49.53a                 | 45.36a           | 45.21a           | 0.00f         | 42.06c        | 54.63a      |                      |                          |                            |
| Myrtyl acetate         | 1324               | 0.00d                 | 0.00d                     | 0.00d                  | 0.00d            | 0.00d            | 0.00d         | 0.00d         | 0.00d       |                      |                          |                            |
| Geranyl acetate        | 1379               | 0.00c                 | 0.00c                     | 0.00c                  | 0.00c            | 0.00c            | 0.00c         | 0.00c         | 0.64a       |                      |                          |                            |
| \( \beta \)-elemene    | 1389               | 0.00d                 | 0.00d                     | 0.00d                  | 0.00d            | 0.00d            | 0.00d         | 0.00d         | 0.00d       |                      |                          |                            |
| \( \beta \)-caryophyllene | 1417           | 0.39c                 | 0.00c                     | 0.00c                  | 0.00c            | 0.00c            | 0.00c         | 0.12c         | 0.00c       |                      |                          |                            |
| \( \alpha \)-guaiene   | 1437               | 0.00d                 | 1.36c                     | 0.00d                  | 2.89a            | 1.58b            | 0.00d         | 0.00d         | 0.00d       |                      |                          |                            |
| \( \gamma \)-muurolene | 1478               | 0.00c                 | 0.00c                     | 0.26c                  | 0.00c            | 0.00c            | 2.57a         | 0.00c         | 0.00c       |                      |                          |                            |
| trans-calamenene       | 1521               | 0.00b                 | 0.00b                     | 0.00b                  | 0.00b            | 0.00b            | 0.00b         | 0.00b         | 1.24a       |                      |                          |                            |
| Elemol                 | 1548               | 0.00d                 | 0.00d                     | 1.54b                  | 0.00d            | 0.00d            | 0.00d         | 0.00d         | 0.00d       |                      |                          |                            |
| Germacrene B           | 1559               | 0.00c                 | 0.00c                     | 0.00c                  | 0.00c            | 0.00c            | 0.00c         | 0.00c         | 0.00c       |                      |                          |                            |
| (E)-nerolidol          | 1561               | 0.00e                 | 0.00e                     | 1.54c                  | 0.00e            | 0.00e            | 0.00e         | 0.00e         | 0.00e       |                      |                          |                            |
| Spathulenol            | 1577               | 0.00e                 | 2.85b                     | 0.00e                  | 2.59c            | 1.82d            | 0.00e         | 0.00e         | 0.00e       |                      |                          |                            |
| Caryophyllene oxide    | 1582               | 0.99e                 | 4.10d                     | 0.00e                  | 3.58d            | 4.59d            | 0.00e         | 9.28c         | 1.57e       |                      |                          |                            |
| Humulene epoxide II    | 1608               | 0.00d                 | 1.17a                     | 0.00d                  | 1.33a            | 0.36c            | 0.00d         | 0.71b         | 0.00d       |                      |                          |                            |

Essential oil content (%) | 1.59c | 0.66c | 2.80a | 1.23d | 1.17d | 1.95c | 1.46d | 1.20d |

Fig. 1: Two-dimensional dendrogram showing the similarity of the chemical compositions of 48 L. alba accessions obtained from the Active Germplasm Bank at the Federal University of Sergipe.
The variation in the concentrations of compounds among the accessions may have been a consequence of their origin, considering that in this experiment all of the accessions were grown in the same environment. Similar results were observed previously in studies with three chemotypes of *L. alba* from different Brazilian states (Rio de Janeiro, Ceará, and São Paulo) [15] and with accessions of *Pogostemon* sp. from the Active Germplasm Bank of the Federal University of Sergipe [16].

The chemical analysis (Table 2) indicated that the most abundant compounds among the accessions were 1,8-cineole, linalool, myrcene, limonene, carvone, geranial, and neral, leading to the formation of six clusters according to the obtained chemical compositions, which were differentiated through cluster analysis (Figure 1). The compound linalool, present in accessions LA-01 and LA-22 (84.73% and 84.45%, resp.), showed the highest abundance. A similar result was reported by [17]. Linalool is widely used in the perfume, cosmetic, and fragrance industries [12].

Considering the similarities of the chemical constituents of the essential oils of these 48 accessions, the clusters were classified as follows: Cluster 1 included LA-01, LA-09, LA-22, and LA-27, which contained the following major compounds: linalool, 1,8-cineole, and caryophyllene oxide. Cluster 2 was formed by accessions LA-20 and LA-24 and comprised the following major compounds: linalool, geranial, neral, 1,8-cineole, and caryophyllene oxide. Cluster 3 was formed by accession LA-13, with the following major compounds:
Geranial, Neral, and caryophyllene oxide. Cluster 6 consisted of accessions LA-03, LA-30, LA-36, LA-39, LA-43, LA-52, LA-53, LA-54, LA-55, LA-58, LA-59, LA-60, LA-61, LA-62, LA-63, LA-67, LA-68, LA-69, LA-71, and LA-72, which contained geranial, neral, o-cymene, limonene, and caryophyllene oxide (Figure 2).

According to the PCA (Figure 3), the first principal component accounted for 20.55% of the total variability in the data and was positively associated with 1,8-cineol ($r = 0.82$), cis-linalool oxide ($r = 0.79$), linalool ($r = 0.82$), and trans-linalool oxide ($r = 0.77$) and negatively associated with geranial ($r = 0.90$) and neral ($r = -0.89$).

The second principal component represented 12.39% of the total variation in the data and showed a positive correlation with 1-octen-3-ol ($r = 0.60$), myrtenal ($r = 0.69$), myrtanyl acetate ($r = 0.54$), and caryophyllene oxide ($r = 0.75$) and a negative correlation with carvone ($r = -0.49$) and limonene ($r = -0.63$).

### 4. Conclusions

Variability was observed in the chemical composition of the essential oils of *L. alba* accessions obtained from the AGB at UFS, resulting in the formation of six different groups.

The compounds characterizing the six groups were as follows: group 1: linalool, 1,8-cineole, and caryophyllene oxide; group 2: linalool, geranial, neral, 1,8-cineole, and caryophyllene oxide; group 3: limonene, carvone, and sabinene; group 4: carvone, limonene, g-muurolene, and myrcene; group 5: neral, geranial, and caryophyllene oxide; and group 6: geranial, neral, o-cymene, limonene, and caryophyllene oxide.

The most abundant compounds were 1,8-cineole, linalool, myrcene, limonene, carvone, geranial, and neral.

### Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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