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Didjour Albert Kambiré, Kayatou Touré, Thierry Acafou Yapi, Mathieu Paoli, Ange Bighelli, et al.. Comparative Study of the Chemical Composition of Root, Stem and Leaf Essential Oils from *Synedrella nodiflora* (L.) Gaertn. *Compounds*, 2024, 4 (3), pp.521 - 533. <10.3390/compounds4030031>. <hal-05034510>

HAL Id: hal-05034510

<https://hal.science/hal-05034510v1>

Submitted on 15 Apr 2025

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Article

Comparative Study of the Chemical Composition of Root, Stem and Leaf Essential Oils from *Synedrella nodiflora* (L.) Gaertn

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Abstract: This study aims at investigating the chemical composition of root, stem and leaf essential oils from Ivorian *Synedrella nodiflora*, with the root oil being described for the first time. Sixty, fifty-one and forty-nine constituents were, respectively identified in the root, stem and leaf oils using a combination of GC(RI), GC-MS and ¹³C-NMR analyses. They accounted for 95.6–97.3%, 92.6–97.6% and 93.3–98.8% of the total composition, respectively. The main components of the root oil samples were γ -curcumene, (*E*)- β -caryophyllene, α -curcumene and curcuphenyl acetate. Three stem oil samples (S1, S2a, S3) were dominated by myrcene and limonene, while the most abundant components of sample S2b were thymol, germacrene D and β -elemene. (*E*)- β -caryophyllene and germacrene D were the major compounds of the leaf oil. Hierarchical cluster and principal component statistical analyses were performed and confirmed that the location does not influence the chemical composition. Group I consisted of the seven leaf oil samples, group II consisted of four stem oil samples and group III consisted of three root oil samples. The root oil composition differed considerably from the stem and leaf oil composition due to the presence of curcumene derivatives as major constituents. The leaf oil showed significant amounts of (*E*)- β -caryophyllene and germacrene D, while the stem oil stood out for its high myrcene, limonene and thymol contents.

Keywords: *Synedrella nodiflora*; essential oil; chemical composition; Côte d'Ivoire



Citation: Kambiré, D.A.; Touré, K.; Yapi, T.A.; Paoli, M.; Bighelli, A.; Boti, J.B.; Tomi, F. Comparative Study of the Chemical Composition of Root, Stem and Leaf Essential Oils from *Synedrella nodiflora* (L.) Gaertn.

Compounds **2024**, *4*, 521–533. <https://doi.org/10.3390/compounds4030031>

Academic Editor: Juan C. Mejuto

Received: 17 June 2024

Revised: 3 August 2024

Accepted: 13 August 2024

Published: 20 August 2024



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1. Introduction

Synedrella nodiflora (L.) Gaertn (synonyms *Ucacou nodiflorum* (L.) Hitchc. and *Verbesina nodiflora* L.) is a herbaceous, erect, branched, pubescent annual plant belonging to the genus *Synedrella*, which contains only one species from the Asteraceae family. It grows in ruderal and sometimes humid places and can reach 60 cm to 1 m in height [1]. The leaves have veins and are hairy, glabrous, elliptical or ovate, pinnate, an acuminate apex, are obtuse at the base end and toothed. Native to tropical America, this plant is widely distributed in the humid regions of West Africa [2,3].

The leaves of *S. nodiflora* are commonly eaten by cattle and humans. *S. nodiflora* is used in traditional medicine in various therapeutic indications. The sap from leaves is used to treat earaches, headaches and abdominal pain. Leaf infusion is taken orally as a laxative, and root decoction is used against cough. The whole plant is further used against arthritis, rheumatism, oedema, hematoma, leprosy, mycosis, gonorrhea, hemorrhoids, diarrhea, insect pests and to stop bleeding [1–7]. In tropical regions of the world (Africa, Asia, Caribbean and Latin America) the plant is used as an anti-inflammatory, emmenagogue, diuretic, contraceptive and against varicose ulcers, wounds, leprosy, heart diseases and

colds. The aqueous extract is drunk to treat epilepsy, hiccups and as an anti-abortion measure [8].

Investigations into solvent extracts, essential oil composition and the biological activity of *S. nodiflora* were previously reported. Phytochemical screenings revealed the presence of alkaloids, steroids, triterpenoids, coumarins, tannins and other phenolic compounds [3–11]. Antioxidant, anti-inflammatory, insecticidal, antimicrobial and antibacterial activities were also evidenced for some solvent extracts [1,4,6,7,9,10]. The chemical composition of the plant essential oil from India is dominated by farnesene, β -caryophyllene, δ -cadinene and germacrene D [12]. The essential oil of leaves from islands in Fiji showed high amounts of β -caryophyllene followed by β -farnesene, germacrene D and β -cubebene [13], while limonene, α -santalene, *n*-tetradecane and *n*-hexadecane are the main compounds of the stem essential oil from Nigeria [14]. In Côte d'Ivoire, the composition of a single sample of leaf oil was previously described, with a predominance of β -caryophyllene, germacrene D, caryophyllene oxide and β -elemene [15].

This study is part of our works on the chemical characterization of essential oils from Côte d'Ivoire [16–20]. We report the determination and the comparison of the chemical composition of the essential oil of three organs (root, stem and leaf) of *S. nodiflora* in three locations characterized by diverse pedoclimatic conditions, littoral humid forests and wooded savannah. The essential oil composition of the root is being reported here for the first time, to our knowledge.

2. Materials and Methods

2.1. Plant Material and Essential Oil Isolation

The fresh roots, stems and leaves of *S. nodiflora* were collected from the edge of the following two forests: Adiopodoumé Forest, Region of Lagunes, southern Côte d'Ivoire, geographical coordinates 5°19'57.7'' N and 4°08'02.0'' W (Location 1); Yapo-Abbé Forest, Region of Agneby-Tiassa, southern Côte d'Ivoire, geographical coordinates 5°40'43.1'' N and 4°05'56.0'' W (Location 2); and nearby Korhogo, Region of Poro, northern Côte d'Ivoire, geographical coordinates 9°25'20.7'' N and 5°38'18.3'' W (Location 3). The harvest took place during the dry season (January and February 2021), and plant material was authenticated by botanists from the Centre Suisse de Recherches Scientifiques (CSRS) and the Centre National de Floristique (CNF, Abidjan, Côte d'Ivoire) in accordance with voucher specimens available at the CNF. The fresh leaves, stems and root samples were hydrodistilled for 3 h each using a Clevenger-type apparatus. Essential oil yields were calculated from fresh plant material (*w/w*) and are reported in Table 1.

Table 1. Plant material and essential oil extraction data.

Sample	Harvest Site Elevation (m)	Organ	Weight (g)		Yield (%)
			Plant Material	Essential Oil	
R1	Adiopodoumé Forest: littoral humid forest 32	Roots	109.7	0.0443	0.040
S1		Stems	462.4	0.0869	0.019
L1a		Leaves	628.1	0.0692	0.011
L1b			612.7	0.0857	0.014
R2	Yapo-Abbé Forest: littoral humid forest 80	Roots	459.3	0.2297	0.050
S2a		Stems	911.4	0.1458	0.016
S2b			898.0	0.2104	0.023
L2a		Leaves	840.8	0.3335	0.040
L2b			835.9	0.1976	0.024
L2c			877.2	0.2543	0.029
R3	Korhogo: wooded savannah 376	Roots	428.7	0.1839	0.043
S3		Stems	926.1	0.2039	0.022
L3a		Leaves	812.4	0.3005	0.037
L3b			817.0	0.2861	0.035

2.2. Gas Chromatography

Analyses were performed on a Clarus 500 PerkinElmer Chromatograph (PerkinElmer, Courtaboeuf, France) equipped with a flame ionization detector (FID) and two fused-silica capillary columns (50 m $\times$ 0.22 mm, film thickness 0.25 μ m), BP-1 (polydimethylsiloxane) and BP-20 (polyethylene glycol). The oven temperature was programmed from 60 °C to 220 °C at 2 °C/min and then held isothermal at 220 °C for 20 min; the injector temperature was 250 °C; the detector temperature was 250 °C; the carrier gas was hydrogen (0.8 mL/min); the split was 1/60; and the injected volume was 0.5 μ L. Retention indices (RI) were determined relative to the retention times of a series of n-alkanes (C8–C29) with linear interpolation (“Target Compounds” software 2013 from PerkinElmer). The quantification of the volatile compounds was obtained using a relative response factor (RRF) and calculated according to the International Organization of the Flavor Industry (IOFI). The relative proportion of each compound (expressed in g/100 g) was calculated using the weight of the essential oil and reference (methyl octanoate), the peak area and relative response factors [21].

2.3. Gas Chromatography–Mass Spectrometry in Electron Impact Mode

The essential oil samples were analyzed with a Clarus SQ8S PerkinElmer TurboMass detector (quadrupole) directly coupled with a Clarus 580 PerkinElmer Autosystem XL (PerkinElmer, Courtaboeuf, France) equipped with a BP-1 (polydimethylsiloxane) fused-silica capillary column (60 m $\times$ 0.22 mm i.d., film thickness 0.25 μ m). The oven temperature was programmed from 60 to 230 °C at 2°/min and then held isothermal for 45 min. Additionally, the injector temperature was 250 °C; the ion-source temperature was 250 °C; the carrier gas was He (1 mL/min); the split ratio was 1:80; the injection volume was 0.2 μ L; and the ionization energy was 70 eV. The electron ionization (EI) mass spectra were acquired over the mass range 35–350 Da.

2.4. Nuclear Magnetic Resonance

The ^{13}C -NMR spectra of 14 samples (root, stem, leaf) were recorded on a Bruker AVANCE 400 Fourier transform spectrometer (Bruker, Wissembourg, France) operating at 100.623 MHz for ^{13}C , equipped with a 5 mm probe, in CDCl_3 , with all shifts referring to the internal TMS. The following parameters were used: pulse width = 4 μ s (flip angle 45°); relaxation delay D1 = 0.1 s, acquisition time = 2.7 s for 128 K data table with a spectral width of 25,000 Hz (250 ppm); CPD mode decoupling; digital resolution = 0.183 Hz/pt. The number of accumulated scans was 3000 for each sample (40 mg, when available, in 0.5 mL of CDCl_3).

A laboratory-made software compares the chemical shift of every carbon in the experimental spectrum with the spectra of pure compounds listed in our in-house data library [22,23]. Each compound was identified taking into account the following:

- The number of observed carbons with respect to the number of expected signals;
- The number of overlapped signals of carbons which possess fortuitously the same chemical shift;
- The difference of chemical shift of each signal in the mixture spectrum and in the reference.

These three parameters are directly available from the computer program. A compound was considered as identified when at least 50% of its signals belonging solely to that molecule and 70% of all its signals was observed.

2.5. Identification of Individual Components

Identification of the individual components was achieved as follows: (i) by comparison of their GC retention indices (RI) on apolar and polar columns with those of reference compounds [24–26]; (ii) through computer matching against digital mass spectral libraries [24,27,28]; (iii) through comparison of the signals in the ^{13}C -NMR spectra of the samples with those of reference spectra compiled in the laboratory spectral library with

the help of laboratory-made software [22,23]. This method allowed for the identification of individual components of the essential oil at contents as low as 0.4–0.5%.

2.6. Statistical Analysis

The chemical compositions of the 14 essential oil samples from *S. nodiflora* were submitted to hierarchical cluster analysis (HCA) and principal component analysis (PCA) using XLSTAT 2016 software (Addinsoft, Paris, France) [29]. Only constituents in a concentration of 1.0% and higher were used as variables for the PCA analysis. The XLSTATS-3DPlot module was used to afford 3D PCA using the principal factors F1, F2 and F3. The aptitude of the complete correlation matrix was checked by the Kaiser–Meyer–Olkin criterion. The HCA and dendrogram were made with dissimilarity matrices calculated through the Euclidean distance, and the average link was the aggregation method systematically chosen.

3. Results and Discussion

The chemical compositions of the essential oils from three organs of *S. nodiflora* growing wild in Côte d’Ivoire were determined. Essential oils were isolated by hydrodistillation of fresh plant material collected from the edge of the Yapo-Abbé and the Adiopodoumé forests, both in Southern Côte d’Ivoire and nearby Korhogo (north of the country). The oil extraction yields calculated on a weight (*w/w*) basis varied poorly at 0.040–0.050% (root oil samples), 0.016–0.023% (stem oil samples) and 0.011–0.040% (leaf oil samples). A combination of GC(RI)(non-polar and polar columns), GC-MS (non-polar column) and ¹³C-NMR, following a computerized method developed at the University of Corsica [22,23], was used to analyze the oil samples.

3.1. Chemical Composition of the Root’s Essential Oil

The root essential oil from *S. nodiflora* is characterized for the first time. The analysis of three oil samples led to the identification of 60 compounds, accounting for 95.6–97.3% of the whole chemical composition. They primarily consist of hydrocarbon sesquiterpenes (59.4–72.3%) followed by oxygenated sesquiterpenes (13.3–18.7%). Hydrocarbon monoterpenes and oxygenated monoterpenes accounted for 2.7–11.5% and 3.3–10.2%, respectively. Rich in curcumen derivatives, this essential oil is dominated by γ -curcumen (22.2–24.8%), (*E*)- β -caryophyllene (11.7–22.2%), α -curcumen (11.6–12.4%) and curcumenyl acetate (5.6–10.7%). The majority of compounds are followed by xanthorrhizyl acetate (1.3–6.2%) and neryl isovalerate (1.2–6.2%). Other compounds are also present in significant proportions, such as β -pinene (1.0–4.6%), α -pinene (1.0–4.4%), cyclosativene (2.1–3.6%) and cyprene (1.0–3.5%) (Table 2). The harvest sites have a negligible influence on the chemical composition of the root essential oil from *S. nodiflora* due to the geographic areas (littoral humid forests and wooded savannah) of the three harvest sites being distant (around 550 km).

Table 2. Chemical composition of root essential oil from *Synedrella nodiflora*.

N°	Compounds	RIa ^L	RIa	RIp	RRF	A (%) R1	Y-A (%) R2	K (%) R3	Identification
1	α -Pinene	934	931	1020	0.765	4.4	1.7	1.0	RI, MS, ¹³ C-NMR
2	Camphene	947	945	1071	0.765	0.1	0.2	tr	RI, MS
3	Sabinene	968	966	1127	0.765	0.1	0.2	0.1	RI, MS
4	β -Pinene	973	971	1116	0.765	2.2	4.6	1.0	RI, MS, ¹³ C-NMR
5	Myrcene	983	981	1166	0.765	0.4	2.4	0.3	RI, MS, ¹³ C-NMR
6	α -Phellandrene	999	998	1170	0.765	0.1	0.1	-	RI, MS
7	<i>p</i> -Cymene	1015	1012	1276	0.698	0.1	tr	tr	RI, MS
8	β -Phellandrene *	1021	1022	1215	0.765	0.2	0.3	0.1	RI, MS
9	Limonene *	1024	1022	1206	0.765	0.5	1.7	0.2	RI, MS, ¹³ C-NMR
10	(<i>E</i>)- β -Ocimene	1038	1035	1254	0.765	-	0.3	-	RI, MS

Table 2. Cont.

N°	Compounds	RIa ^L	RIa	RIp	RRF	A (%) R1	Y-A (%) R2	K (%) R3	Identification
11	α-Terpineol	1175	1174	1697	0.809	0.1	0.1	tr	RI, MS
12	Neral	1220	1215	1682	0.817	-	-	0.2	RI, MS
13	Geraniol	1238	1236	1848	0.809	0.1	tr	0.2	RI, MS
14	Geranial	1247	1244	1732	0.817	-	-	0.3	RI, MS
15	Thymol	1271	1268	2188	0.755	0.7	0.1	0.4	RI, MS, ¹³ C-NMR
16	Bornyl acetate	1270	1270	1582	0.849	0.8	0.5	0.3	RI, MS, ¹³ C-NMR
17	α-Cubebene	1352	1350	1458	0.751	tr	-	0.2	RI, MS
18	Longicyclene	1371	1366	1489	0.751	0.2	0.3	0.2	RI, MS
19	Cyclosativene	1368	1369	1483	0.751	2.1	3.6	3.1	RI, MS, ¹³ C-NMR
20	α-Copaene	1375	1375	1493	0.751	0.4	0.7	0.6	RI, MS, ¹³ C-NMR
21	β-Elemene	1388	1387	1591	0.751	0.8	1.9	0.4	RI, MS, ¹³ C-NMR
22	Cyperene	1398	1399	1528	0.751	3.5	3.3	1.0	RI, MS, ¹³ C-NMR
23	α-Gurjunene	1405	1409	1531	0.751	0.4	0.6	0.5	RI, MS, ¹³ C-NMR
24	cis-α-Bergamotene	1410	1411	1573	0.751	0.1	0.1	0.1	RI, MS
25	(E)-β-Caryophyllene	1419	1417	1598	0.751	11.7	17.1	22.2	RI, MS, ¹³ C-NMR
26	Precocene	1428	1433	2070	0.815	0.2	0.3	0.3	RI, MS
27	α-Guaiene	1442	1435	1608	0.751	0.1	0.1	tr	RI, MS
28	(E)-β-Farnesene	1449	1446	1669	0.751	0.6	0.5	0.5	RI, MS, ¹³ C-NMR
29	α-Humulene	1449	1449	1669	0.751	0.9	1.1	1.2	RI, MS, ¹³ C-NMR
30	α-Curcumene	1471	1470	1776	0.707	11.6	12.4	11.9	RI, MS, ¹³ C-NMR
31	γ-Curcumene	1472	1472	1694	0.751	24.8	22.2	23.6	RI, MS, ¹³ C-NMR
32	Germacrene D	1476	1474	1709	0.751	0.5	1.0	0.2	RI, MS, ¹³ C-NMR
33	β-Selinene	1481	1478	1719	0.751	0.1	0.3	3.9	RI, MS, ¹³ C-NMR
34	γ-Humulene	1483	1481	1728	0.751	0.1	0.1	0.1	RI, MS
35	4- <i>epi</i> -Cubebol	1489	1485	1881	0.787	0.1	0.1	0.1	RI, MS
36	α-Selinene	1489	1490	1723	0.751	0.3	0.5	0.2	RI, MS, ¹³ C-NMR
37	α-Muurolene	1491	1492	1732	0.751	0.1	0.2	0.3	RI, MS
38	β-Bisabolene	1500	1500	1727	0.751	0.2	0.4	0.7	RI, MS, ¹³ C-NMR
39	γ-Cadinene	1506	1506	1761	0.751	0.2	0.1	0.3	RI, MS
40	δ-Cadinene	1514	1513	1757	0.751	0.5	0.8	0.8	RI, MS, ¹³ C-NMR
41	Italicene oxide	1525	1521	1858	0.791	0.1	0.1	0.2	RI, MS
42	Geranyl 2-methylbutyrate	1562	1558	1861	0.819	1.7	0.9	0.4	RI, MS, ¹³ C-NMR
43	Spathulenol	1566	1563	2120	0.791	0.1	0.1	0.1	RI, MS
44	Neryl isovalerate	1568	1564	1881	0.819	6.2	2.6	1.2	RI, MS, ¹³ C-NMR
45	Caryophyllene oxide	1570	1569	1978	0.791	1.4	1.1	2.9	RI, MS, ¹³ C-NMR
46	Globulol	1578	1573	2061	0.781	0.1	0.3	0.2	RI, MS
47	Viridiflorol	1580	1591	2080	0.781	0.1	0.4	0.8	RI, MS, ¹³ C-NMR
48	neo-Intermedeol	1601	1603	2145	0.781	tr	0.1	tr	RI, MS
49	1,10- <i>diepi</i> -Cubenol	1605	1610	2054	0.781	0.1	0.1	0.1	RI, MS
50	Intermedeol	1636	1637	2247	0.781	0.2	0.3	0.3	RI, MS
51	Geranyl tiglate	1649	1647	2070	0.829	0.2	0.1	0.2	RI, MS
52	Neryl tiglate	1652	1656	2091	0.829	0.4	0.2	0.1	RI, MS
53	α-Bisabolol	1668	1665	2213	0.781	0.5	0.3	0.7	RI, MS, ¹³ C-NMR
54	Curcphenol	1684	1676	2600	0.746	1.9	1.3	1.2	RI, MS, ¹³ C-NMR
55	Curcuphenyl acetate	1694	1690	2626	0.781	6.4	5.6	10.7	RI, MS, ¹³ C-NMR
56	Pentadecanal	1695	1694	2041	0.764	-	0.2	0.2	RI, MS
57	Xanthorrhizol	1728	1737	-	0.746	0.5	0.2	0.1	RI, MS, ¹³ C-NMR
58	Xanthorrhizyl acetate	1767	1743	-	0.781	6.2	3.3	1.3	RI, MS, ¹³ C-NMR
59	Falcarinol	2000	1983	-	0.797	-	0.2	-	RI, MS
60	(E)-Phytol	2099	2097	2614	0.748	0.2	-	0.1	RI, MS

Table 2. Cont.

N°	Compounds	RIa ^L	RIa	RIp	RRF	A (%) R1	Y-A (%) R2	K (%) R3	Identification
	Hydrocarbon monoterpenes					8.1	11.5	2.7	
	Oxygenated monoterpenes					10.2	4.5	3.3	
	Hydrocarbon sesquiterpenes					59.4	67.6	72.3	
	Oxygenated sesquiterpenes					17.7	13.3	18.7	
	Other compounds					0.2	0.4	0.3	
	Total identified					95.6	97.3	97.3	

Order of elution and percentages are given on an apolar column (BP-1), except components with an asterisk (*), where percentages are taken on a polar column (BP-20). RIa^L: apolar column retention indices from the literature [24–26]; RIa, RIp: retention indices measured on an apolar and polar capillary column, respectively. RRF: relative response factors calculated using methyl octanoate as internal standard. The relative proportions of constituent are expressed in g/100 g. tr: traces level (<0.05%). A: Adiopodoumé Forest; Y-A: Yapo-Abbé Forest; K: Korhogo.; (-): not detected.

3.2. Chemical Composition of Stem Essential Oil

The chemical composition of the stem essential oil from *S. nodiflora* is dominated by hydrocarbon monoterpenes (23.2–61.1%) and hydrocarbon sesquiterpenes (22.9–49.5%). Fifty-one constituents representing 92.6–97.6% of the chemical composition were identified. Samples S1, S2a and S3 are rich in myrcene (19.6–22.6%) and limonene (18.3–22.1%), followed by β -pinene (5.1–11.5%), germacrene D (0.2–10.5%), β -elemene (7.6–9.2%), (*E*)- β -caryophyllene (7.1–8.1%), α -pinene (2.5–4.5%) and bicyclogermacrene (0.3–4.0%). As for sample S2b, the main constituents are thymol (12.7%), germacrene D (12.2%), β -elemene (11.8%), limonene (9.0%), (*E*)- β -caryophyllene (9.0%), myrcene (8.5%) and bicyclogermacrene (7.6%) (Table 3). Thus, two chemical compositions appear for the stem essential oil, differing by the presence of thymol in appreciable content in one of the four oil samples. This difference could be related to the vegetative stage of the plant, since samples S2a and S2b from the same location do not have the same composition.

The stem essential oil sample from Nigeria, dominated by limonene (14.9%), α -santalene (9.0%), *n*-hexadecane (3.0%) and *n*-tetradecane (3.0%), differs from those of the present study [14]. Indeed, α -santalene, *n*-hexadecane and *n*-tetradecane are absent from our samples, while, in the Nigerian oil sample, thymol, β -pinene, germacrene D, β -elemene, bicyclogermacrene and α -pinene were not detected; additionally, there was a relatively low content of myrcene (1.5%) and (*E*)- β -caryophyllene (1.5%). Thus, the stem essential oil from *S. nodiflora* of an Ivorian origin showed original chemical compositions.

Table 3. Chemical composition of stem essential oil from *Synedrella nodiflora*.

N°	Compounds	RIa ^L	RIa	RIp	RRF	A (%) S1	Y-A (%) S2a	S2b	K (%) S3	Identification
1	α -Pinene	934	931	1020	0.765	4.5	2.9	0.5	2.5	RI, MS, ¹³ C-NMR
2	Camphene	947	945	1071	0.765	0.4	0.3	0.1	0.2	RI, MS
3	Sabinene	968	966	1127	0.765	0.6	0.8	0.2	0.5	RI, MS, ¹³ C-NMR
4	β -Pinene	973	971	1116	0.765	9.9	11.5	3.2	5.1	RI, MS, ¹³ C-NMR
5	Myrcene	983	981	1166	0.765	22.6	19.6	8.5	21.2	RI, MS, ¹³ C-NMR
6	α -Phellandrene	999	998	1170	0.765	0.1	0.1	tr	-	RI, MS
7	α -Terpinene	1010	1010	1186	0.765	-	0.1	0.3	-	RI, MS
8	<i>p</i> -Cymene	1015	1012	1276	0.698	-	-	0.4	0.4	RI, MS
9	β -Phellandrene *	1021	1022	1215	0.765	1.2	1.4	0.7	1.8	RI, MS, ¹³ C-NMR
10	Limonene *	1024	1022	1206	0.765	21.5	18.3	9.0	22.1	RI, MS, ¹³ C-NMR
11	(<i>E</i>)- β -Ocimene	1038	1035	1254	0.765	0.2	0.2	0.1	0.4	RI, MS

Table 3. Cont.

N°	Compounds	RIa ^L	RIa	RIp	RRF	A (%) S1	Y-A (%) S2a	S2b	K (%) S3	Identification
12	γ-Terpinene	1050	1049	1250	0.765	-	tr	0.2	-	RI, MS
13	Terpinolene	1079	1079	1278	0.765	0.1	-	-	0.4	RI, MS
14	Terpinen-4-ol	1164	1163	1603	0.809	-	0.1	0.3	0.4	RI, MS
15	α-Terpineol	1175	1174	1697	0.809	-	0.1	0.2	0.2	RI, MS
16	Nerol	1216	1209	1793	0.809	-	-	tr	0.3	RI, MS
17	Neral	1220	1215	1682	0.817	-	-	0.1	2.5	RI, MS, ¹³ C-NMR
18	Geraniol	1238	1236	1848	0.809	-	-	0.2	0.3	RI, MS
19	Geranial	1247	1243	1732	0.817	-	-	0.1	2.9	RI, MS, ¹³ C-NMR
20	Thymol	1271	1268	2188	0.755	-	0.2	12.7	0.2	RI, MS, ¹³ C-NMR
21	Bornyl acetate	1270	1270	1582	0.849	0.4	0.3	-	0.1	RI, MS
22	Bicycloelemene	1336	1334	1482	0.751	-	0.1	0.3	0.5	RI, MS, ¹³ C-NMR
23	α-Cubebene	1352	1348	1459	0.751	-	tr	0.2	0.2	RI, MS
24	Cyclosativene	1368	1369	1483	0.751	-	0.6	tr	-	RI, MS, ¹³ C-NMR
25	α-Copaene	1375	1375	1493	0.751	0.6	0.2	0.2	0.2	RI, MS, ¹³ C-NMR
26	β-Cubebene *	1383	1387	1540	0.751	0.6	0.4	0.4	0.8	RI, MS, ¹³ C-NMR
27	β-Elemene *	1388	1387	1591	0.751	9.2	8.0	11.8	7.6	RI, MS, ¹³ C-NMR
28	α-Isocomene	1388	1389	1536	0.751	tr	tr	-	0.6	RI, MS, ¹³ C-NMR
29	Cyperene	1398	1399	1528	0.751	-	0.5	tr	-	RI, MS, ¹³ C-NMR
30	α-Gurjunene	1405	1409	1531	0.751	-	0.1	0.1	-	RI, MS
31	(E)-β-Caryophyllene	1419	1417	1598	0.751	7.1	7.1	9.0	8.7	RI, MS, ¹³ C-NMR
32	Precocene	1428	1433	2070	0.815	-	0.6	0.3	tr	RI, MS, ¹³ C-NMR
33	(E)-β-Farnesene	1449	1446	1669	0.751	-	0.2	0.2	0.5	RI, MS, ¹³ C-NMR
34	α-Humulene	1449	1449	1669	0.751	0.8	0.7	1.0	0.6	RI, MS, ¹³ C-NMR
35	α-Curcumene	1471	1470	1776	0.707	-	1.8	0.7	0.3	RI, MS, ¹³ C-NMR
36	γ-Curcumene	1472	1472	1694	0.751	0.4	3.9	0.8	0.7	RI, MS, ¹³ C-NMR
37	Germacrene D	1476	1474	1709	0.751	10.5	6.3	12.2	0.2	RI, MS, ¹³ C-NMR
38	β-Selinene	1481	1481	1719	0.751	0.6	0.4	1.6	0.5	RI, MS, ¹³ C-NMR
39	4- <i>epi</i> -Cubebol	1489	1485	1881	0.787	-	0.1	0.1	0.1	RI, MS
40	Bicyclogermacrene	1490	1491	1733	0.751	4.0	4.0	7.6	0.3	RI, MS, ¹³ C-NMR
41	β-Bisabolene	1500	1500	1727	0.751	1.5	1.2	2.3	1.1	RI, MS, ¹³ C-NMR
42	δ-Cadinene	1514	1513	1757	0.751	0.2	0.4	0.8	0.1	RI, MS, ¹³ C-NMR
43	β-Elemol	1536	1534	2077	0.781	-	-	0.6	tr	RI, MS, ¹³ C-NMR
44	Spathulenol	1566	1563	2119	0.791	-	0.4	0.7	3.4	RI, MS, ¹³ C-NMR
45	Neryl isovalerate	1568	1564	1881	0.819	-	0.5	-	0.9	RI, MS, ¹³ C-NMR
46	Caryophyllene oxide	1570	1569	1978	0.791	-	0.3	0.7	5.0	RI, MS, ¹³ C-NMR
47	Intermedeol	1636	1637	2247	0.781	0.6	0.6	1.2	1.0	RI, MS, ¹³ C-NMR
48	Curcuphenyl acetate	1694	1690	2626	0.781	-	1.6	0.3	0.1	RI, MS, ¹³ C-NMR
49	Benzyl benzoate	1733	1722	2620	0.770	-	tr	2.0	0.2	RI, MS, ¹³ C-NMR
50	Xanthorrhizyl acetate	1767	1743	-	0.781	tr	tr	tr	1.0	RI, MS, ¹³ C-NMR
51	(E)-Phytol	2099	2097	2614	0.748	-	0.2	0.7	1.3	RI, MS, ¹³ C-NMR
Hydrocarbon monoterpenes						61.1	55.2	23.2	54.6	
Oxygenated monoterpenes						0.4	1.2	13.6	7.8	
Hydrocarbon sesquiterpenes						35.5	36.5	49.5	22.9	
Oxygenated sesquiterpenes						0.6	3.0	3.6	10.6	
Other compounds						0.0	0.2	2.7	1.5	
Total identified						97.6	96.1	92.6	97.4	

Order of elution and percentages are given on an apolar column (BP-1), except components with an asterisk (*), where percentages are taken on a polar column (BP-20). RIa^L: apolar column retention indices from the literature [24–26]; RIa, RIp: retention indices measured on an apolar and polar capillary column, respectively. RRF: relative response factors calculated using methyl octanoate as the internal standard. The relative proportions of constituent are expressed in g/100 g. tr: traces level (<0.05%). A: Adiopodoumé Forest; Y-A: Yapo-Abbé Forest; K: Korhogo; (-): not detected.

3.3. Chemical Composition of Leaf Essential Oil

Forty-nine compounds, accounting for 93.3–98.8% of the whole chemical composition of the seven leaf essential oil samples, were identified. This essential oil mainly consists of hydrocarbon sesquiterpenes (59.1–86.1%) and lower contents of hydrocarbon monoterpenes (3.4–27.1%). (*E*)- β -caryophyllene (20.0–30.3%) and Germacrene D (7.7–33.6%) are the predominant compounds, followed by bicyclogermacrene (2.4–7.2%), β -cubebene (2.7–7.2%) and β -elemene (3.3–5.2%). However, only samples L1a and L1b from Adiopodoumé Forest contain thianthrene (2.8 and 0.6%, respectively). They also have an interesting amount of α -isocomene (6.7 and 1.1%, respectively), while L2a, L2b and L2c from Yapo-Abbé Forest exhibit appreciable thymol contents (3.0–8.7%). Sample L2c exhibited significant proportions of limonene (12.1%) and myrcene (8.0%). Samples L3a and L3b from Korhogo showed a relatively low content of germacrene D (10.0 and 7.7%, respectively vs. 21.2–33.6% for L1a–L2c). Significant amounts of (*E*)-phytol, a diterpene, have also been identified in samples L2a, L2c, L3a and L3b (2.2, 3.6, 4.7 and 5.1%, respectively) (Table 4). Hence, despite the predominance of (*E*)- β -caryophyllene and Germacrene D, quantitative differences are observable between the samples. The harvest sites and vegetative stage of the plant could be possible factors in this chemical variation.

Although a previous study conducted in Côte d'Ivoire on a single sample of leaf essential oil reported similar chemical composition with β -caryophyllene (19.5%), germacrene D (17.63%), caryophyllene oxide (10.5%) and β -elemene (9.80%) as major compounds, notable quantitative and qualitative variations are observable. Indeed, there is a low proportion of caryophyllene oxide in our samples (0.7–4.2%) compared to the previous study (10.5%). Qualitatively, some compounds that featured significantly in our samples, such as myrcene, thymol, α -isocomene, precocene, benzyl benzoate, thianthrene and (*E*)-phytol, were not detected in the previous study [15]. These quantitative and qualitative variations could be explained by differences in harvest sites and seasons. Moreover, the leaf essential oil from Côte d'Ivoire differs from those of Fiji and India. Germacrene D (21.2–33.6% in our samples) accounted only for 7.6 and 1.27% in oils from Fiji and India, respectively, whereas (*E*)- β -farnesene (11.9 and 22.75%, respectively Fiji and India) did not exceed 1.2% in our samples. Also, qualitative variations were observable through many compounds detected in our samples but absent from the Fiji and India chemical compositions, and conversely [12,13]. Combined factors, like differences in climate, vegetation, relief and harvest season, could be responsible for the observed variations.

Table 4. Chemical composition of leaf essential oil from *Synedrella nodiflora*.

N°	Compounds	RIa ^L	RIa	RIp	RRF	A (%)		Y-A (%)			K (%)		Identification
						L1a	L1b	L2a	L2b	L2c	L3a	L3b	
1	α -Pinene	934	931	1020	0.765	0.2	0.6	0.2	0.2	1.7	0.8	1.4	RI, MS, ¹³ C-NMR
2	Camphene	947	945	1071	0.765	-	0.3	tr	tr	0.3	0.1	0.2	RI, MS
3	Sabinene	968	966	1127	0.765	-	0.2	0.1	tr	0.4	0.2	0.2	RI, MS, ¹³ C-NMR
4	β -Pinene	973	971	1116	0.765	0.4	1.4	0.7	0.5	3.6	1.0	1.8	RI, MS, ¹³ C-NMR
5	Myrcene	983	981	1166	0.765	1.6	3.6	2.0	1.1	8.0	4.4	6.0	RI, MS, ¹³ C-NMR
6	<i>p</i> -Cymene	1015	1012	1276	0.698	-	-	0.1	0.1	0.1	0.1	0.2	RI, MS
7	β -Phellandrene *	1021	1022	1215	0.765	0.1	0.3	0.2	0.1	0.8	0.8	0.5	RI, MS, ¹³ C-NMR
8	Limonene *	1024	1022	1206	0.765	2.0	5.1	2.2	1.4	12.1	4.4	4.8	RI, MS, ¹³ C-NMR
9	(<i>E</i>)- β -Ocimene	1038	1035	1254	0.765	-	tr	tr	-	0.1	-	0.1	RI, MS
10	Terpinolene	1079	1079	1278	0.765	2.3	0.4	tr	-	-	0.2	0.1	RI, MS, ¹³ C-NMR
11	Nerol	1216	1 210	1793	0.809	-	-	-	-	0.1	0.1	-	RI, MS
12	Neral	1220	1 215	1682	0.817	-	-	tr	tr	0.3	1.7	tr	RI, MS, ¹³ C-NMR
13	Geraniol	1238	1234	1849	0.809	-	-	0.1	0.1	0.3	0.5	0.1	RI, MS, ¹³ C-NMR
14	Geranial	1247	1242	1731	0.817	-	-	tr	tr	0.5	2.7	-	RI, MS, ¹³ C-NMR
15	Thymol	1271	1268	2188	0.755	0.5	0.2	8.7	4.8	3.0	0.2	0.2	RI, MS, ¹³ C-NMR

Table 4. Cont.

N°	Compounds	RIa ^L	RIa	RIp	RRF	A (%)		Y-A (%)			K (%)		Identification
						L1a	L1b	L2a	L2b	L2c	L3a	L3b	
16	Bornyl acetate	1270	1270	1582	0.849	0.2	0.3	-	0.1	0.6	0.1	0.1	RI, MS, ¹³ C-NMR
17	Bicycloelemene	1336	1334	1482	0.751	-	0.2	0.3	0.4	0.2	0.1	0.1	RI, MS
18	α-Cubebene	1352	1347	1472	0.751	1.5	0.2	0.1	0.1	0.1	0.1	0.1	RI, MS, ¹³ C-NMR
19	α-Copaene	1375	1375	1493	0.751	1.0	0.9	0.6	0.6	0.5	0.9	1.7	RI, MS, ¹³ C-NMR
20	β-Bourbonene	1381	1385	1520	0.751	0.8	0.8	0.9	1.1	0.3	3.7	2.9	RI, MS, ¹³ C-NMR
21	β-Cubebene *	1383	1387	1540	0.751	4.0	4.6	3.9	4.5	2.7	7.2	3.9	RI, MS, ¹³ C-NMR
22	β-Elemene *	1388	1387	1591	0.751	5.2	4.3	3.9	4.3	3.3	3.5	3.6	RI, MS, ¹³ C-NMR
23	α-Isocomene	1388	1389	1536	0.751	6.7	1.1	-	-	-	0.1	tr	RI, MS, ¹³ C-NMR
24	α-Gurjunene	1405	1409	1531	0.751	3.2	0.5	0.2	0.2	0.1	0.2	0.4	RI, MS, ¹³ C-NMR
25	(E)-β-Caryophyllene	1419	1417	1598	0.751	24.3	26.0	25.2	30.3	20.0	26.9	29.4	RI, MS, ¹³ C-NMR
26	β-Copaene	1427	1428	1582	0.751	0.2	0.3	0.3	0.4	0.2	0.7	0.7	RI, MS, ¹³ C-NMR
27	Precocene	1428	1433	2070	0.815	1.3	0.4	0.2	0.3	1.9	1.5	0.8	RI, MS, ¹³ C-NMR
28	(E)-β-Farnesene	1449	1446	1669	0.751	0.9	1.2	0.7	0.8	0.7	0.9	0.7	RI, MS, ¹³ C-NMR
29	α-Humulene	1449	1449	1669	0.751	2.9	2.9	2.5	3.1	2.2	2.6	3.1	RI, MS, ¹³ C-NMR
30	Germacrene D	1476	1474	1709	0.751	28.1	33.6	27.7	29.7	21.2	10.0	7.7	RI, MS, ¹³ C-NMR
31	β-Selinene	1481	1481	1719	0.751	-	-	-	0.3	0.3	0.2	0.6	RI, MS, ¹³ C-NMR
32	4- <i>epi</i> -Cubebol	1489	1485	1881	0.787	-	-	0.2	0.3	0.2	0.3	1.0	RI, MS, ¹³ C-NMR
33	Bicyclogermacrene	1490	1491	1733	0.751	5.2	6.4	6.4	7.2	4.5	2.4	3.2	RI, MS, ¹³ C-NMR
34	α-Murolene	1491	1492	1732	0.751	-	-	-	0.4	0.3	0.2	0.6	RI, MS, ¹³ C-NMR
35	(E,E)-α-Farnesene	1496	1498	1751	0.751	0.4	0.5	0.4	0.2	tr	0.2	0.2	RI, MS, ¹³ C-NMR
36	β-Bisabolene	1500	1500	1727	0.751	-	-	0.4	0.3	0.2	0.7	1.0	RI, MS, ¹³ C-NMR
37	δ-Cadinene	1514	1513	1757	0.751	0.4	0.4	0.5	0.7	0.4	0.5	3.1	RI, MS, ¹³ C-NMR
38	β-Elemol	1536	1534	2077	0.781	-	-	0.4	0.3	0.1	0.4	0.5	RI, MS, ¹³ C-NMR
39	Spathulenol	1566	1563	2119	0.791	0.4	0.1	0.6	0.1	0.6	1.2	1.1	RI, MS, ¹³ C-NMR
40	Neryl isovalerate	1568	1566	1882	0.819	tr	tr	0.1	0.1	0.1	0.9	0.9	RI, MS, ¹³ C-NMR
41	Caryophyllene oxide	1570	1569	1978	0.791	0.8	0.7	0.8	0.9	0.8	4.1	4.2	RI, MS, ¹³ C-NMR
42	Isospathulenol	1625	1619	2195	0.791	-	-	0.2	0.1	0.1	0.3	0.3	RI, MS
43	τ-Cadinol	1626	1626	2167	0.781	-	-	0.3	0.2	tr	tr	0.6	RI, MS, ¹³ C-NMR
44	Curcuphenol	1684	1677	2600	0.746	-	-	0.2	0.1	-	1.1	1.0	RI, MS, ¹³ C-NMR
45	Benzyl benzoate	1733	1722	2620	0.770	-	-	1.2	1.0	-	0.1	tr	RI, MS, ¹³ C-NMR
46	Thianthrene	1883	1876	-	0.890	2.8	0.6	-	-	-	-	-	RI, MS, ¹³ C-NMR
47	Cembrene A	1959	1954	2245	0.744	-	-	0.6	0.3	0.1	0.3	0.2	RI, MS, ¹³ C-NMR
48	Falcarinol	2000	1983	-	0.797	-	-	0.5	tr	-	-	-	RI, MS
49	(E)-Phytol	2099	2097	2614	0.748	0.8	0.7	2.2	0.5	3.6	4.7	5.1	RI, MS, ¹³ C-NMR
Hydrocarbon monoterpenes						6.6	11.9	5.5	3.4	27.1	12.0	15.3	
Oxygenated monoterpenes						0.7	0.5	8.9	5.1	4.9	6.2	1.3	
Hydrocarbon sesquiterpenes						86.1	84.3	74.2	84.9	59.1	62.6	63.8	
Oxygenated sesquiterpenes						1.2	0.8	2.7	2.0	1.8	7.4	8.7	
Other compounds						3.6	1.3	4.5	1.8	3.7	5.1	5.3	
Total identified						98.2	98.8	95.8	97.2	96.6	93.3	94.4	

Order of elution and percentages are given on an apolar column (BP-1), except components with an asterisk (*), where percentages are taken on a polar column (BP-20). RIa^L: apolar column retention indices from the literature [24–26]; RIa, RIp: retention indices measured on an apolar and polar capillary column, respectively. RRF: relative response factors calculated using methyl octanoate as the internal standard. The relative proportions of constituent are expressed in g/100 g. tr: traces level (<0.05%). A: Adiopodoumé Forest; Y-A: Yapo-Abbé Forest; K: Korhogo; (-): not detected.

3.4. Discussion about Statistical Analyses

Statistical analyses were carried out on the 14 essential oil compositions through hierarchical cluster analysis (HCA) and principal component analysis (PCA) to confirm the observed chemical variability. The dendrogram from the HCA displayed three distinct chemical compositions within the 14 investigated oil samples, as follows: group I (seven

leaf oil samples and stem oil sample S2b), group II (three stem oil samples) and group III (three root oil samples). The first and second principal factors of the PCA (F1: 47.40% and F2: 35.16%, respectively) accounted for 82.56% of the total variance of the chemical composition. The PCA map relative to the principal axes F1 and F2 confirmed the three groups observed in the dendrogram (Figure 1). Groups II and III are more homogenous than group I. However, considering the third main factor (F3: 9.17%), in a 3D PCA projection, principal axes F1, F2 and F3 account then for 91.74% of the total variance of the chemical composition, and stem oil sample S2b fits well into group II (Figure 2).

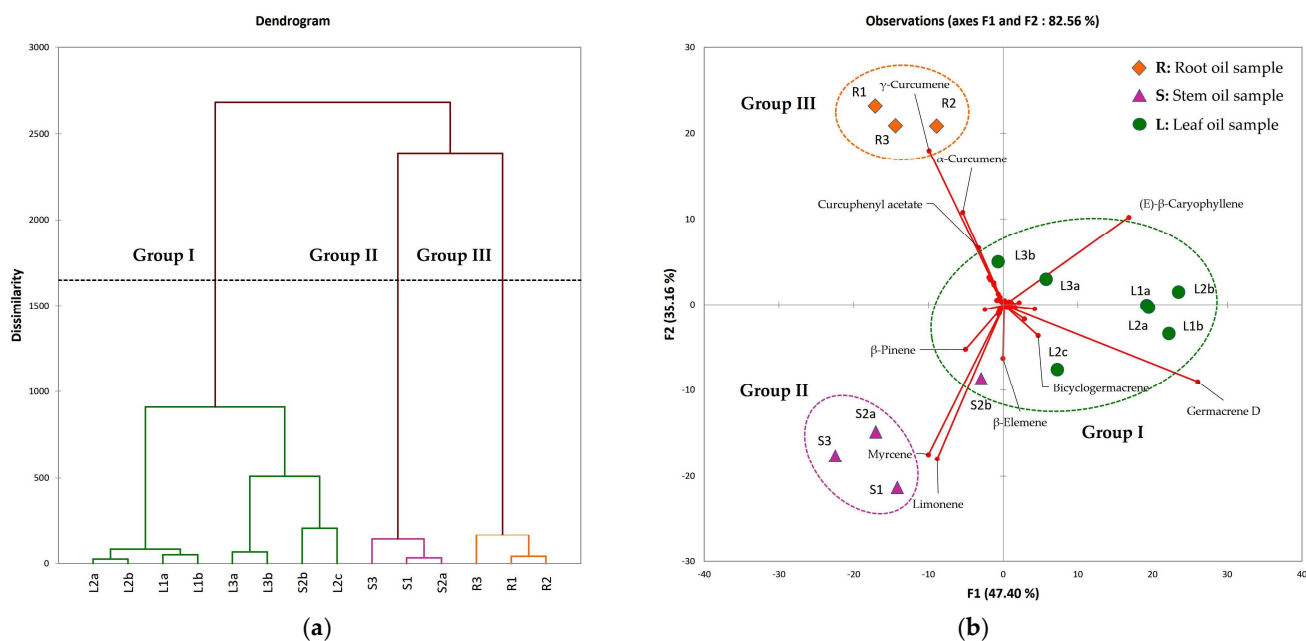


Figure 1. HCA dendrogram and PCA map of the 14 oil samples from *S. nodiflora*. **(a)** Hierarchical Cluster Analysis (HCA); **(b)** Principal Component Analysis (PCA) and biplot.

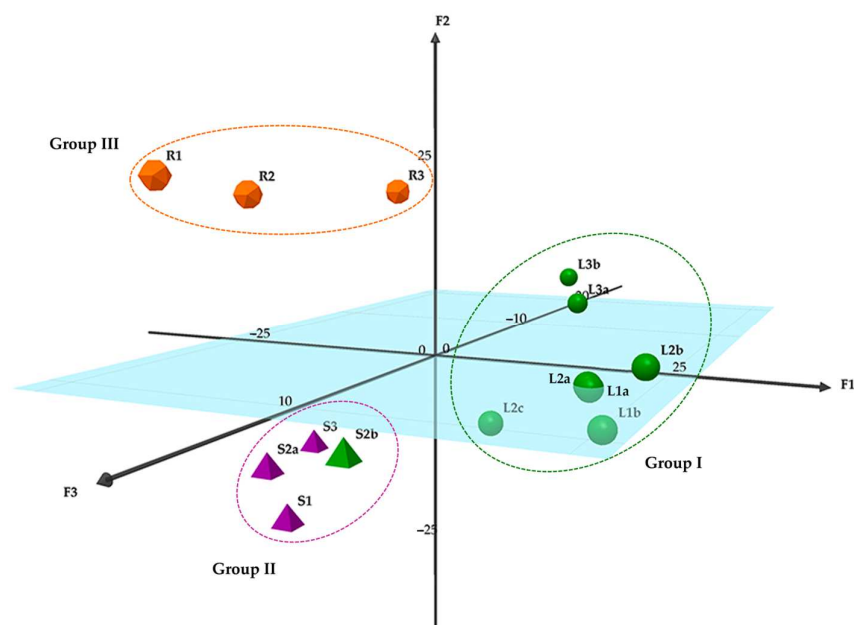


Figure 2. 3D PCA map of the 14 oil samples from *S. nodiflora*.

The mean contents (M) and the standard deviation (SD) of the major compounds of the different groups are reported on Table 5. The chemical composition of each organ is

homogeneous and appears to be not deeply influenced by the location. However, Korhogo leaf oil samples L3a and L3b and the Yapo-Abbé forest stem oil sample S2b exhibited slightly different chemical compositions.

Table 5. Main compounds of the three groups related to the three organs of *S. nodiflora*.

Component ^[a]	Group I			Group II			Group III		
	M% ± SD	Min	Max	M% ± SD	Min	Max	M% ± SD	Min	Max
α-Pinene	0.7 ± 0.6	0.2	1.7	2.6 ± 1.6	0.5	4.5	2.4 ± 1.8	1.0	4.4
β-Pinene	1.3 ± 1.1	0.4	3.6	7.4 ± 3.9	3.2	11.5	2.6 ± 1.8	1.0	4.6
Myrcene	3.8 ± 2.5	1.1	8.0	18.0 ± 6.4	8.5	22.6	1.0 ± 1.2	0.3	2.4
Limonene	4.6 ± 3.6	1.4	12.1	17.7 ± 6.1	9.0	22.1	0.8 ± 0.8	0.2	1.7
Thymol	2.5 ± 3.3	0.2	8.7	3.3 ± 6.3	-	12.7	0.4 ± 0.3	0.1	0.7
β-Cubebene *	4.4 ± 1.4	2.7	7.2	0.6 ± 0.2	0.4	0.8	-	-	-
β-Elemene *	4.0 ± 0.6	3.3	5.2	9.2 ± 1.9	7.6	11.8	1.0 ± 0.8	0.4	1.9
(E)-β-Caryophyllene	26.0 ± 3.4	20.0	30.3	8.0 ± 1.0	7.1	9.0	17.0 ± 5.3	11.7	22.2
α-Curcumene	-	-	-	0.7 ± 0.8	-	1.8	12.0 ± 0.4	11.6	12.4
γ-Curcumene	-	-	-	1.5 ± 1.6	0.4	3.9	23.5 ± 1.3	22.2	24.8
Germacrene D	22.6 ± 10.1	7.7	33.6	7.3 ± 5.3	0.2	12.2	0.6 ± 0.4	0.2	1.0
Bicyclgermacrene	5.0 ± 1.8	2.4	7.2	4.0 ± 3.0	0.3	7.6	-	-	-
Neryl isovalerate	0.3 ± 0.4	-	0.9	0.4 ± 0.4	-	0.9	3.3 ± 2.6	1.2	6.2
Curcuphenyl acetate	-	-	-	0.5 ± 0.7	-	1.6	7.6 ± 2.7	5.6	10.7
Xanthorrhizyl acetate	-	-	-	0.3 ± 0.5	tr	1.0	3.6 ± 2.5	1.3	6.2
(E)-Phytol	2.5 ± 2.0	0.5	5.1	0.6 ± 0.6	-	1.3	0.1 ± 0.1	-	0.2

^[a] Order of elution and percentages on apolar column (BP-1), except components with an asterisk (*), percentages on polar column (BP-20); M% ± SD: mean percentage and standard deviation; tr: traces level (<0.05%); (-): not detected.

Group I, consisting of the seven leaf oil samples, is dominated by (E)-β-caryophyllene (26.0 ± 3.4%) and germacrene D (22.6 ± 10.1%), followed by bicyclgermacrene (5.0 ± 1.8%). The four stem oil samples (group II) are characterized by monoterpene hydrocarbons such as myrcene (18.0 ± 6.4%), limonene (17.7 ± 6.1%) and β-pinene (7.4 ± 3.9%). In contrast, the root oil samples (group III) are characterized by the presence of γ-curcumene (23.5 ± 1.9%) and α-curcumene (12.0 ± 0.6). Other compounds, such as curcuphenyl acetate (7.6 ± 2.7%), xanthorrhizyl acetate (3.6 ± 2.5%) and neryl isovalerate (3.3 ± 2.6%), are present in significant amounts. Apart from neryl isovalerate, all these compounds were not detected in leaf oil samples.

4. Conclusions

The chemical compositions of the root, stem and leaf essential oils from *S. nodiflora* were investigated, with the root oil composition being reported for the first time. A combination of GC(RI), GC-MS and ¹³C-NMR was used for the identification and quantification of the constituents, and different chemical profiles were observed for the three organs of the plant. The location did not deeply influence the chemical composition. Leaf oil samples were dominated by sesquiterpene hydrocarbons such as (E)-β-caryophyllene and germacrene D, while stem oil samples showed monoterpene hydrocarbons, myrcene and limonene as being the most abundant constituents. The root oil samples were characterized by the high amounts of γ-curcumene and α-curcumene.

Author Contributions: Conceptualization, D.A.K., T.A.Y. and F.T.; methodology, D.A.K., K.T. and F.T.; software, D.A.K. and M.P.; validation, J.B.B., A.B. and F.T.; formal analysis, D.A.K. and K.T.; data analysis, D.A.K., T.A.Y. and F.T.; essential oil investigation, D.A.K. and K.T.; writing—original draft preparation, D.A.K. and F.T.; writing—review and editing, D.A.K., T.A.Y., J.B.B. and F.T.; visualization, D.A.K. and M.P.; supervision, T.A.Y., A.B. and F.T. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: Data and samples of the essential oils are available from the authors.

Acknowledgments: The authors gratefully acknowledge H. Téré for his valuable help in the plant identification.

Conflicts of Interest: The authors declare no conflicts of interest.

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