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Supplementary Information

Chemotaxonomic Significance of Volatile Constituents in *Hypenia* (Mart. ex Benth.) R. Harley (Lamiaceae)

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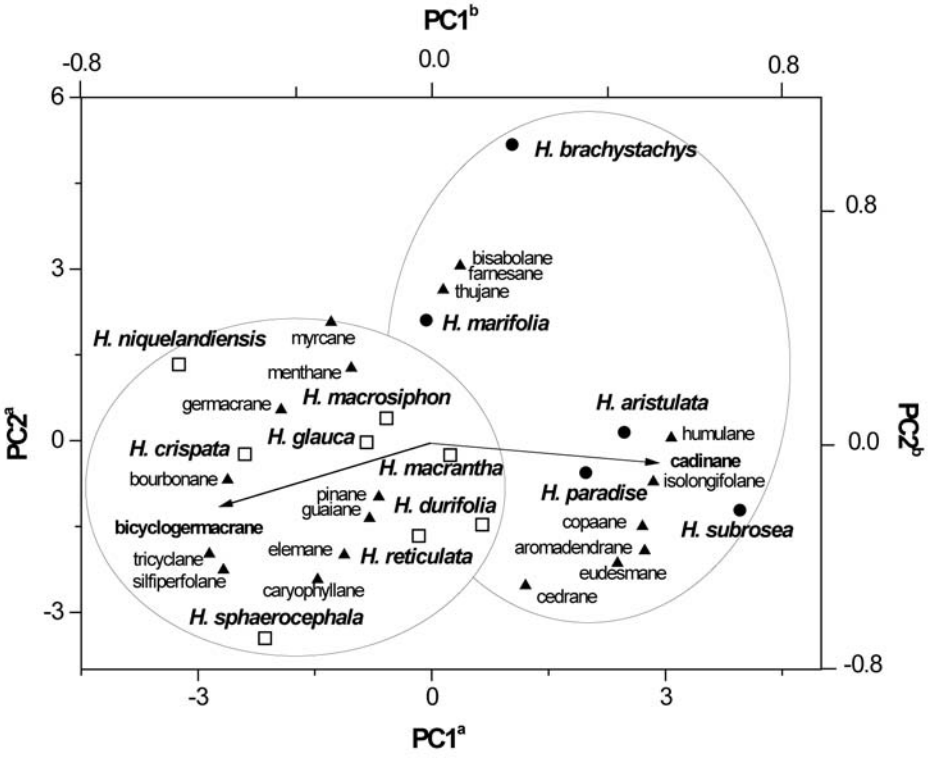

Figure S1. Biplot originating by PCA of *Hypenia* spp. based on carbon skeletons of volatiles to whose cluster it belongs: I (□); II (●). [a]Axes refer to scores from the samples. [b]Axes refer to loadings from carbon skeletons of oil constituents (Table S4) represented as shaded triangles, and discriminant variables are highlighted as vectors from the origin.

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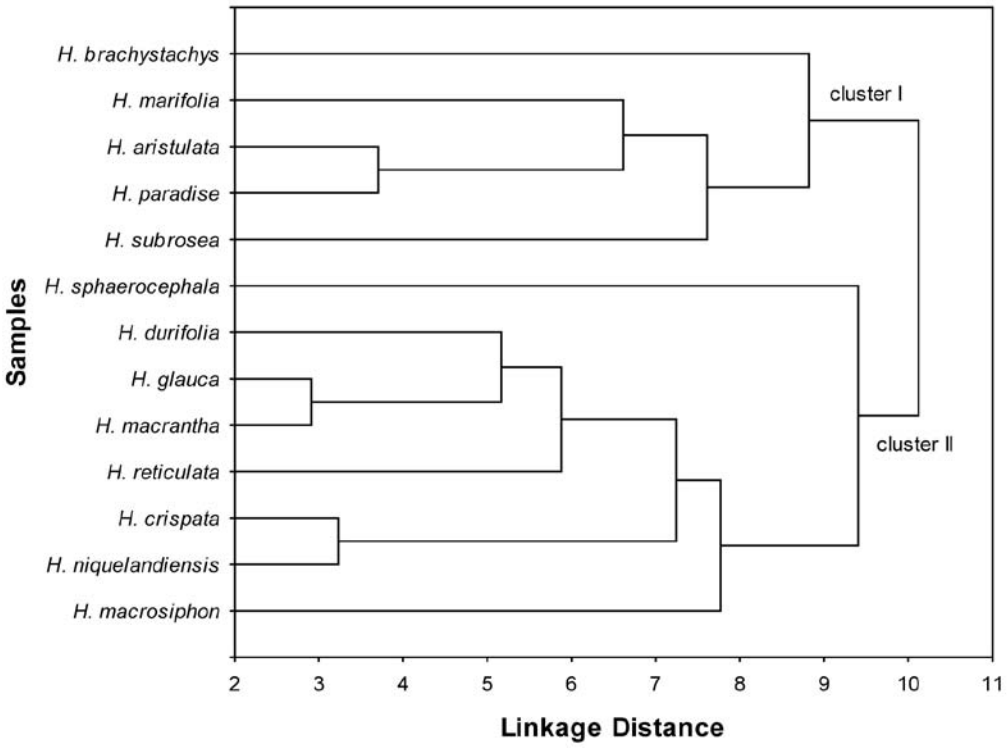

Figure S2. Dendrogram representing the similarity relationships among *Hypenia* spp. based on carbon skeleton of volatile constituents belonging to clusters I and II.

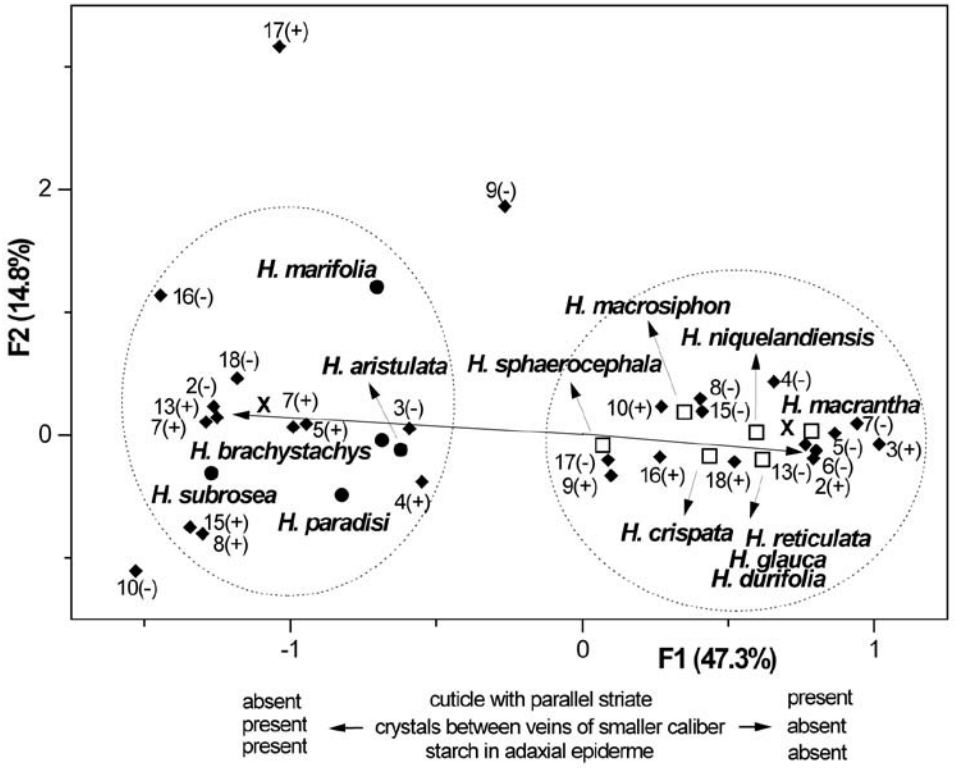

Figure S3. Biplot originating by multiple correspondence analysis of *Hypenia* spp. based on morphological and anatomical leaf characters to whose cluster it belongs: I (□); II (●). [a]Axes refer to scores from the samples. [b]Axes refer to loadings from morphological characters (see Table S6 for codes) represented as shaded losangles, and discriminant variables are highlighted as vectors from the origin. Crosses represent cluster centroids and values between parentheses refer to the explained variance on each principal component.

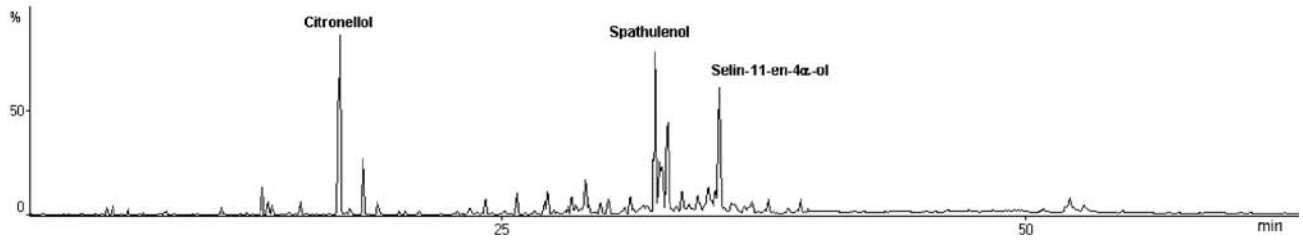

Figure S4. Total ion chromatogram of essential oil from *H. brachystachys*.

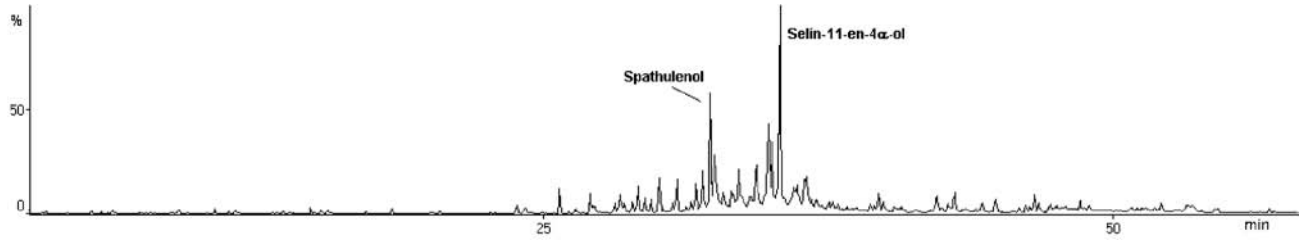

Figure S5. Total ion chromatogram of essential oil from *H. aristulata*.

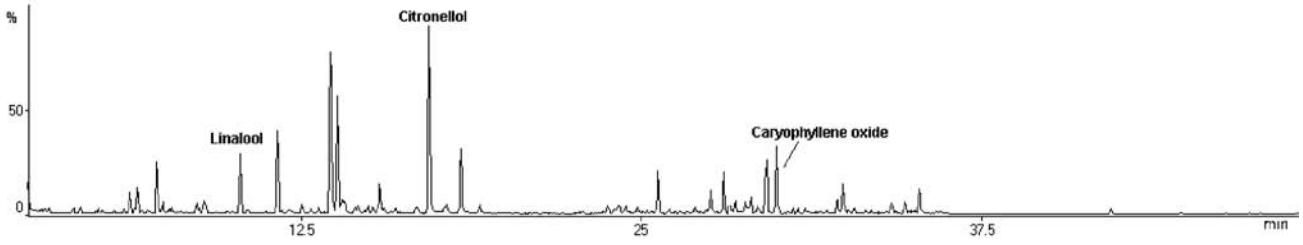

Figure S6. Total ion chromatogram of essential oil from *H. marifolia*.

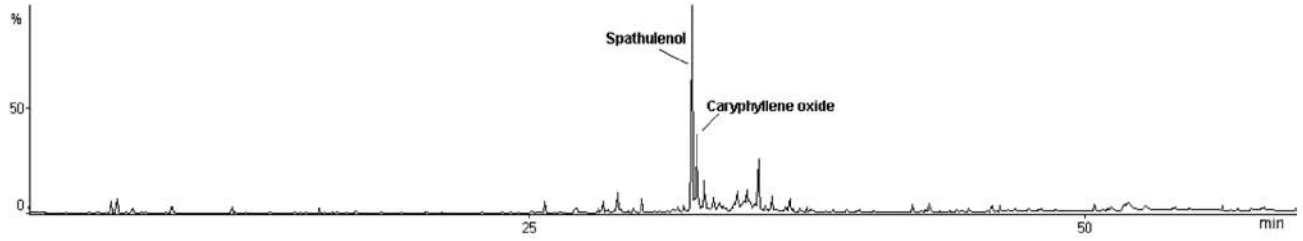

Figure S7. Total ion chromatogram of essential oil from *H. paradise*.

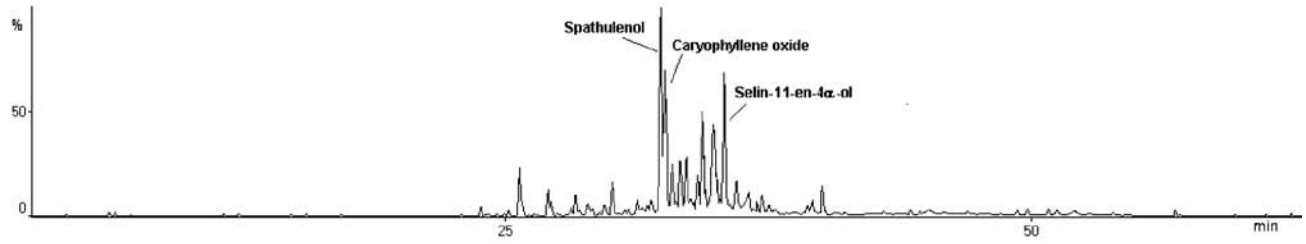

Figure S8. Total ion chromatogram of essential oil from *H. subrosea*.

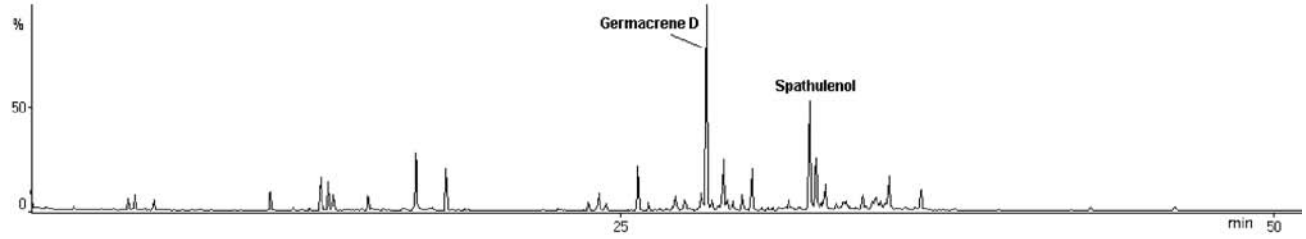

Figure S9. Total ion chromatogram of essential oil from *H. crispata*.

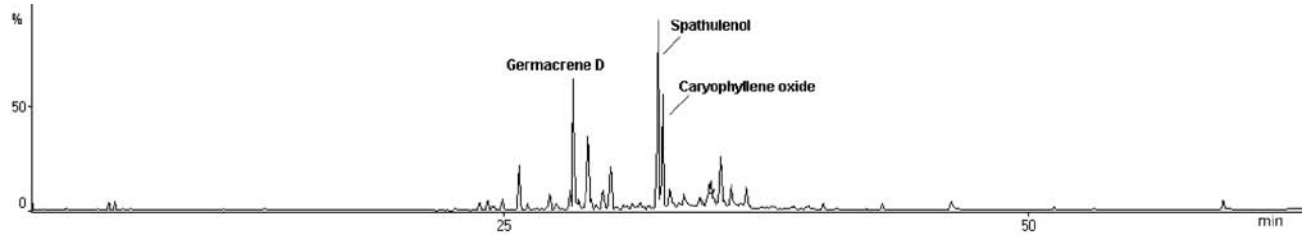

Figure S10. Total ion chromatogram of essential oil from *H. durifolia*.

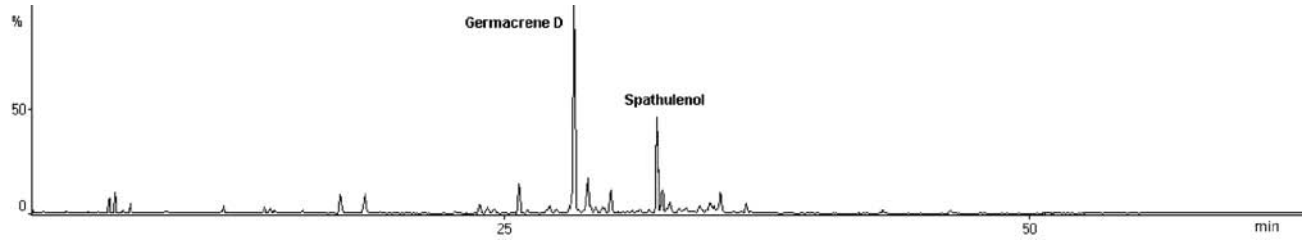

Figure S11. Total ion chromatogram of essential oil from *H. glauca*.

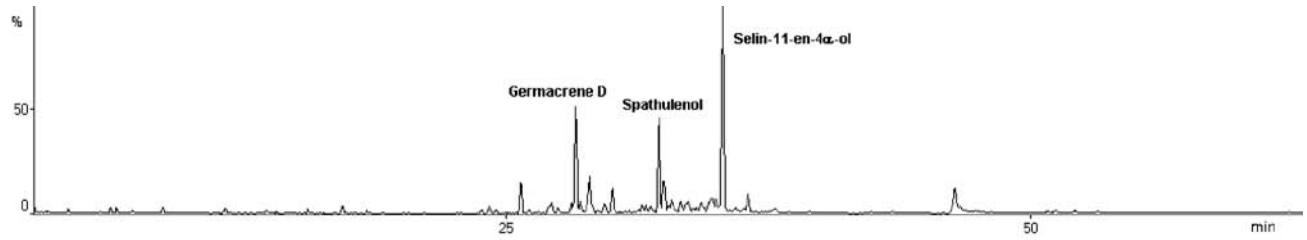

Figure S12. Total ion chromatogram of essential oil from *H. macrantha*.

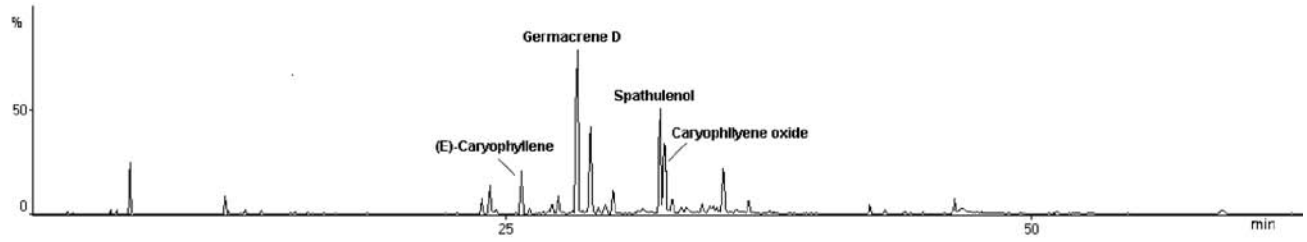

Figure S13. Total ion chromatogram of essential oil from *H. macrosiphon*.

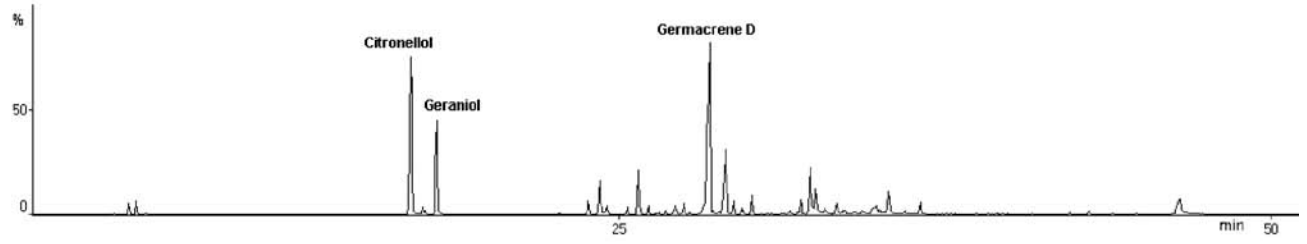

Figure S14. Total ion chromatogram of essential oil from *H. niquelandiensis*.

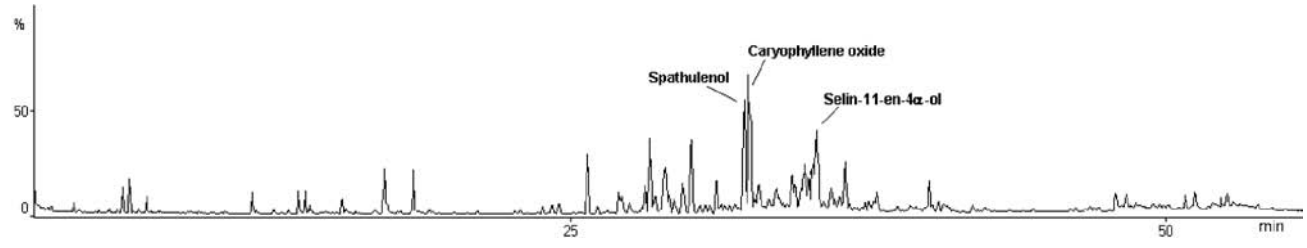

Figure S15. Total ion chromatogram of essential oil from *H. reticulata*.

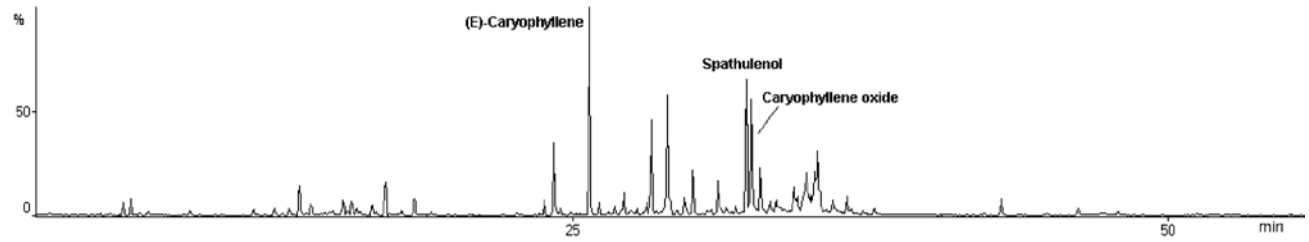

Figure S16. Total ion chromatogram of essential oil from *H. sphaerocephala*.

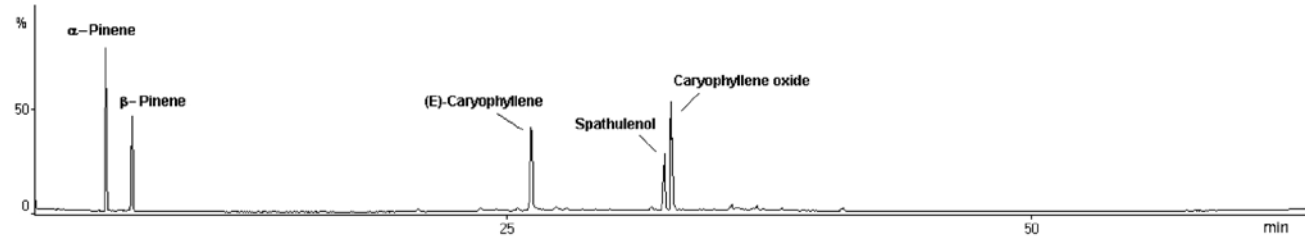

Figure S17. Total ion chromatogram of standards.

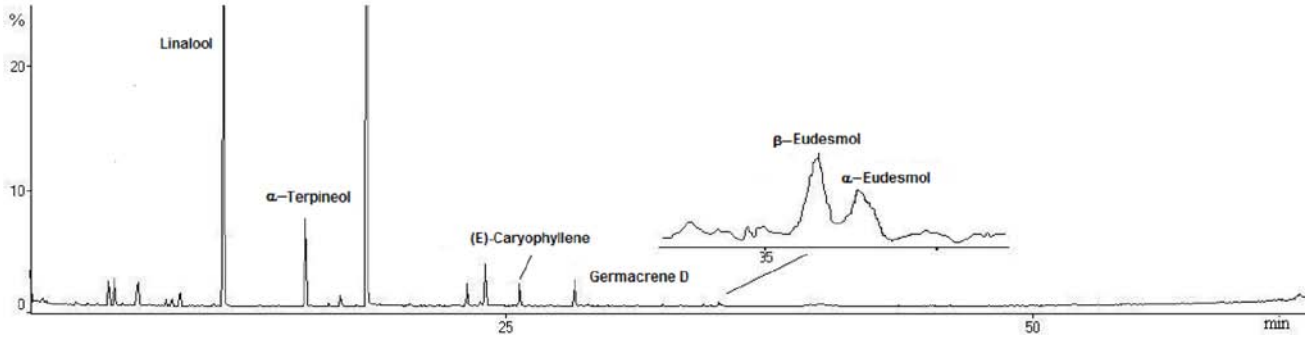

Figure S18. Total ion chromatogram of sage clary essential oil.

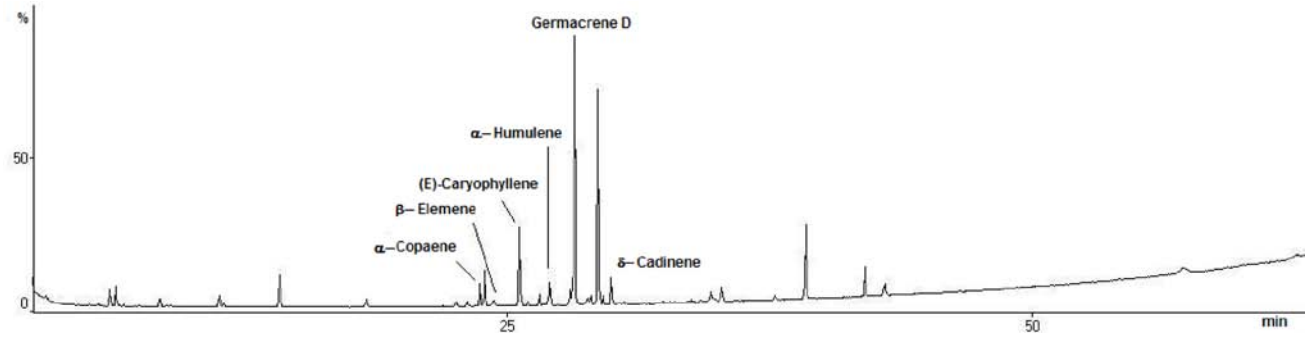

Figure S19. Total ion chromatogram of ylang-ylang essential oil.

Table S1. List of the *Hypenia* taxa with provenances and voucher specimens (UFG)

Hypenia Taxon	Locality	Coordinates	Date	Voucher
H. crispata (Pohl ex Benth.) R. Harley[a]	Serra Dourada, Mossamedes, 1021 m	S 16°4'25.8", W 50°11'12.8"	May, 2006	30815
H. brachystachys (Pohl ex Benth.) R. Harley	Serra dos Pireneus, Pirenópolis, 1070 m	S 15°50'22.2", W 48°46'15.8"	April, 2007	30815
H. marifolia (Benth.) R. Harley	Serra dos Pireneus, Pirenópolis, 1324 m	S 15°47'31.6", W 48°50'8.2"	August, 2006	30816
H. sphaerocephala (R. Atkinson) R. Harley	Serra dos Topázios, Cristalina, 1204 m	S 16°46'49.8", W 47°39'19.1"	September, 2007	30669
H. reticulata (Mart. ex Benth.) R. Harley	Vianópolis, 927 m	S 16°34'56", W 48°20'37.3"	October, 2007	30847
H. durifolia (Epl.) R. Harley	São João d'Aliança, 1166 m	S 15°39'32.1", W 47°33'17.2"	November, 2007	30809
H. glauca (St.-Hil. ex Benth.) R. Harley	Instituto Chico Mendes de Conservação da Biodiversidade, Silvânia, 938 m	S 16°38'37", W 48°39'7"	May, 2007	30668
H. macrantha (St.-Hil. ex Benth.) R. Harley	Luziânia, 958 m	S 16°15'48", W 47°56'15"	April, 2007	30821
H. paradisi Harley[a]	Chapada dos Veadeiros, Alto Paraíso, 1394 m	S 14°5'17", W 47°31'17"	April, 2007	30839
H. aristulata (Epl.) R. Harley[a]	Chapada dos Veadeiros, Alto Paraíso, 1196 m	S 14°12'33.4", W 47°29'18.8"	April, 2007	30829
H. subrosea Harley[a]	Chapada dos Veadeiros, Alto Paraíso, 1394 m	S 14°5'17", W 47°31'17"	April, 2007	30833
H. niquelandiensis (R. Atkinson) R. Harley	Chapada dos Veadeiros, Alto Paraíso, 1066 m	S 14°10'11", W 47°49'34"	May, 2007	30413
H. macrosiphon (Briq.) R. Harley	Serra Dourada, Mossâmedes, 1021 m	S 16°4'25.8", W 50°11'12.8"	May, 2006	30814

[a] Rare species.[6]

Table S2. Percentage of essential oil constituents of *Hypenia* spp. collected from central Brazilian Cerrado

Constituent	RI[a]	*Hypenia*												
		brachystachys	*aristulata*	*marifolia*	*paradise*	*subrosea*	*crispata*	*durifolia*	*glauca*	*macrantha*	*macrosiphon*	*niquelandiensis*	*reticulata*	*sphaerocephala*
Tricyclene	927	-	-	-	-	-	-	-	-	-	-	-	-	0.32
α-Pinene	934	-	-	-	-	-	-	-	-	-	0.90	-	-	-
Sabinene[b]	974	-	-	-	-	-	-	-	-	-	6.15	-	-	0.93
1-Octen-3-ol	977	-	-	4.22	-	-	-	-	0.68	-	-	-	-	-
β-Pinene	978	-	-	-	-	-	-	-	-	-	1.00	-	-	-
o-Cymene	1024	-	-	-	0.52	-	-	-	-	-	-	-	-	-
β-Phellandrene	1029	-	-	-	-	-	-	-	-	-	1.82	-	-	1.66
Acetophenone	1065	-	-	4.77	-	-	-	-	-	-	-	-	-	-
Linalool[b]	1100	-	-	5.52	1.24	-	1.40	-	0.61	-	0.96	0.72	1.29	-
1,3,8-ρ-Menthatriene	1111	-	-	0.34	-	-	-	-	-	-	-	-	-	-
trans-Thujone	1117	-	0.79	-	-	-	-	-	-	-	-	-	-	-
neo-Isopulegol[b]	1145	1.30	-	9.32	-	-	1.68	-	-	-	-	3.87	-	1.23
Isopulegol	1147	-	-	-	-	-	-	-	-	-	-	-	0.30	-
iso-Isopulegol[b]	1157	-	-	5.20	-	-	0.70	-	-	-	-	1.18	-	-
Menthol	1171	1.00	-	-	-	-	-	-	-	-	-	-	-	-
cis-Pinocamphone	1174	-	-	-	-	-	-	-	-	-	-	-	-	0.57
α-Terpineol	1185	-	-	-	-	0.90	-	-	-	-	-	-	-	-
trans-ρ-Mentha-1(7),8-dien-2-ol	1188	-	-	1.40	-	-	0.62	-	-	-	-	1.72	-	0.53
Citronellol[b]	1229	14.19	-	9.52	-	-	5.58	-	3.61	2.48	-	20.49	2.55	2.44
Geraniol[b]	1255	2.92	-	4.72	-	-	4.36	-	3.29	0.82	-	10.05	2.47	0.51
Neryl formate	1280	-	-	-	-	-	-	-	-	-	-	0.93	-	-
β-Bourbonene[b]	1387	0.72	-	-	-	-	3.25	-	0.92	-	1.71	4.45	0.75	3.97
β-Elemene	1392	-	-	-	0.77	-	-	-	-	-	-	-	2.79	-
Geosmin	1404	-	-	-	-	-	-	0.63	-	-	-	-	-	-
Dodecanal	1407	-	-	-	-	-	-	-	-	-	-	-	0.89	-
α-Cedrene	1410	-	-	-	-	-	-	-	-	-	-	-	0.82	-
(E)-Caryophyllene[b]	1420	1.93	2.42	3.56	2.83	2.89	6.19	2.72	5.36	4.80	7.92	4.64	6.52	18.57
α-*trans*-Bergamotene	1439	-	-	-	-	-	-	-	-	-	0.70	-	-	-
α-Humulene[b]	1456	1.15	-	-	-	-	-	0.86	-	0.60	4.48	-	-	-

Table S2. Continuation

Constituent	RI[a]	*Hypenia*												
		brachystachys	*aristulata*	*marifolia*	*paradise*	*subrosea*	*crispata*	*durifolia*	*glauca*	*macrantha*	*macrosiphon*	*niquelandiensis*	*reticulata*	*sphaerocephala*
trans-Prenyl limonene	1457	-	-	-	2.34	-	-	-	-	-	-	-	-	-
9-*epi*-(E)-Caryophyllene	1465	-	-	-	-	-	-	-	-	-	1.04	-	-	-
γ-Gurjunene	1478	-	-	-	1.62	-	-	-	-	-	-	-	-	-
γ-Muurolene[b]	1479	-	-	1.63	1.03	-	0.81	1.01	-	-	-	-	1.09	5.42
Germacrene D[b]	1484	-	-	3.25	0.87	1.57	31.48	17.20	31.20	17.22	17.18	25.25	5.02	-
β-Selinene[b]	1489	-	-	-	3.63	-	-	0.61	-	1.95	-	-	1.70	-
α-Selinene	1498	-	-	-	3.76	-	-	-	-	-	-	-	-	-
Bicyclogermacrene[b]	1500	1.39	-	-	1.36	1.87	8.03	5.93	6.00	6.24	6.55	8.79	6.53	5.14
α-Muurolene[b]	1501	0.72	2.60	-	1.67	-	-	0.62	-	-	-	-	1.95	-
Germacrene A	1506	-	-	-	0.85	-	-	-	-	-	-	-	3.21	-
α-Cadinene[b]	1516	-	-	2.59	1.10	-	0.73	1.55	-	2.56	2.12	-	2.35	0.48
7-*epi*-α-Selinene	1518	-	-	-	-	-	-	-	-	-	-	-	-	0.97
δ-Cadinene[b]	1524	0.56	4.20	3.98	3.58	2.81	3.56	3.61	3.35	1.82	3.86	1.02	5.58	2.99
α-Calacorene	1546	-	3.36	-	0.73	-	-	-	-	-	-	-	1.03	-
Elemol	1552	-	-	-	-	-	-	-	-	-	-	-	0.46	0.53
Silphiperfol-5-en-3-ol A	1554	-	-	-	-	-	-	-	-	-	-	-	-	0.86
Germacrene B	1560	-	-	-	-	-	0.60	-	-	-	-	0.86	-	-
Geranyl butanoate	1566	-	0.78	-	-	-	-	-	-	-	-	-	-	-
Palustrol	1572	-	-	-	-	-	-	-	-	-	-	2.71	-	-
Caryophyllenyl alcohol	1572	1.01	3.81	-	-	-	-	-	-	-	-	-	-	-
Spathulenol[b]	1578	13.97	11.27	5.23	26.18	30.25	11.29	31.55	25.57	16.50	14.66	4.49	11.94	12.59
trans-Sesquisabinene hydrate[b]	1583	7.20	-	-	-	-	-	-	-	-	-	-	-	-
Caryophyllene oxide[b]	1583	7.14	7.42	8.33	12.25	10.67	6.10	14.39	7.49	6.99	10.02	2.17	14.38	13.36
β-Copaen-4α-ol[b]	1586	-	-	-	-	8.39	-	-	-	-	-	-	-	-
Globulol	1593	2.62	-	-	-	-	-	-	-	-	-	-	-	0.84
Rosifoliol	1595	-	-	-	-	-	-	-	-	-	0.50	-	-	-
Guaiol	1596	-	-	-	-	-	1.78	1.29	-	-	-	-	-	-

Table S2. Continuation

Constituent	RI[a]	*Hypenia*												
		brachystachys	*aristulata*	*marifolia*	*paradise*	*subrosea*	*crispata*	*durifolia*	*glauca*	*macrantha*	*macrosiphon*	*niquelandiensis*	*reticulata*	*sphaerocephala*
Geranyl 2-methylbutanoate[b]	1596	8.09	-	6.01	-	-	-	-	-	-	-	-	-	-
Ledol	1604	-	1.38	-	-	-	-	-	-	-	-	-	-	-
Humulene epoxide II[b]	1613	0.65	3.91	-	4.64	1.82	-	1.75	-	-	2.55	-	-	-
trans-Isolongifolanone	1628	-	-	-	-	1.26	-	-	-	-	-	-	-	-
Muurola-4,10(14)-dien-1β-ol[b]	1631	0.66	5.88	5.51	2.34	5.11	0.88	-	-	-	-	-	1.08	2.85
Selina-1,3,7(11)-trien-8-one	1634	4.07	-	-	0.63	-	-	-	-	-	-	-	-	-
Caryophylla-4(12),8(13)-dien-5α-ol	1639	-	-	-	-	-	-	-	-	-	-	-	-	0.68
Caryophylla-4(12),8(13)-dien-5β-ol	1639	-	-	-	0.99	-	-	-	-	-	-	-	-	1.45
allo-Aromadendrene epoxide	1640	-	-	-	-	0.73	-	0.54	-	-	-	-	-	1.24
epi-α-Muurolol[b]	1644	0.73	6.86	-	-	-	-	-	-	-	-	-	-	0.93
α-Muurolol[b]	1645	2.40	10.54	4.45	4.93	6.95	-	-	-	0.71	-	-	0.77	0.75
Cubenol[b]	1649	1.80	3.77	-	1.17	1.18	-	-	-	-	-	-	0.36	-
β-Eudesmol	1654	-	-	-	-	-	-	-	-	-	-	-	0.73	1.17
α-Eudesmol	1655	-	-	-	-	-	-	-	-	-	-	-	-	1.99
α-Cadinol[b]	1656	0.66	-	3.19	4.23	-	-	1.98	-	-	-	1.28	-	-
Selin-11-en-4α-ol[b]	1659	8.41	25.20	-	5.17	11.06	4.39	6.90	5.33	34.80	5.81	2.12	12.20	5.47
ar-Turmerone	1665	0.68	-	-	-	-	-	-	-	-	-	-	-	-
14-hydroxy-9-*epi*-(E)-caryophyllene	1667	-	-	-	-	-	-	1.18	-	-	-	-	-	0.75
n-Tetradecanol	1670	-	-	-	-	-	-	-	-	-	-	-	3.28	-
5-*iso*-Cedranol	1671	-	-	-	-	-	-	1.23	-	-	-	-	-	-
Cadalene	1676	0.92	-	-	-	-	-	-	-	-	-	-	-	-
Khusinol	1676	-	-	-	1.24	0.68	-	-	-	-	-	-	-	-

Table S2. Continuation

Constituent	RI[a]	*Hypenia*												
		brachystachys	*aristulata*	*marifolia*	*paradise*	*subrosea*	*crispata*	*durifolia*	*glauca*	*macrantha*	*macrosiphon*	*niquelandiensis*	*reticulata*	*sphaerocephala*
Germacra-4(15),10(14)-trien-1α-ol	1688	-	-	-	-	-	-	-	-	-	0.77	-	-	-
Eudesma-4(15),7-dien-1β-ol[b]	1689	-	3.80	-	-	-	1.88	2.58	2.52	2.50	2.30	-	1.04	2.59
Eudesm-7(11)-en-4-ol	1695	-	-	-	1.16	-	-	-	-	-	-	-	-	-
β-Davanone-2-ol	1720	1.27	-	-	-	-	-	-	-	-	-	-	-	-
2-Hexyl-(E)-cinnamaldehyde	1747	2.00	-	-	-	-	-	-	-	-	-	-	-	-
Benzyl benzoate	1763	4.22	-	-	-	-	-	-	-	-	-	-	-	-
(Z)-Nerolidyl isobutyrate	1779	1.13	-	-	-	-	-	-	-	-	-	-	-	-
Monoterpene hydrocarbons		-	-	0.34	0.52	-	-	-	-	-	9.87	-	-	2.91
Oxygenated monoterpenes		19.41	0.79	35.68	1.24	0.90	14.34	-	7.51	3.30	0.96	38.03	6.61	5.28
Sesquiterpene hydrocarbons		6.47	9.22	15.01	25.41	9.14	54.05	34.11	46.83	35.19	45.56	44.15	38.31	37.54
Oxygenated sesquiterpenes		54.19	87.20	26.71	65.66	78.10	26.92	63.39	40.91	61.50	36.61	13.63	43.99	48.05
Others		15.44	0.78	15.00	-	-	-	0.63	0.68	-	-	0.93	4.17	-
Oil yield (wt.%/dry wt.)		0.032	0.012	0.092	0.010	0.105	0.129	0.088	0.098	0.103	0.118	0.019	0.078	0.043
Identified		95.51	97.99	92.74	92.83	88.14	95.31	98.13	95.93	99.99	93.00	96.74	93.08	93.78

[a]Retention Index. [b]Constituents selected for PCA (see Experimental section). – not detected.

Table S3. Percentage[a] of essential oils of clustered *Hypenia* spp. from central Brazilian Cerrado

	Constituent	RI[b]	RI[c]	Cluster I	Cluster II
1	Tricyclene	927	921	-	0.04 ± 0.11
2	α-Pinene	934	932	-	0.11 ± 0.32
3	Sabinene	974	969	-	0.89 ± 2.15
4	1-Octen-3-ol[d]	977	974	0.84 ± 1.89 a	0.09 ± 0.24 a
5	β-Pinene	978	974	-	0.13 ± 0.35
6	o-Cymene	1024	1022	0.10 ± 0.23	-
7	β-Phellandrene	1029	1025	-	0.44 ± 0.81
8	Acetophenone	1065	1065	0.95 ± 2.13	-
9	Linalool[e]	1100	1095	1.35 ± 2.39 a	0.62 ± 0.58 a
10	1,3,8-ρ-Menthatriene	1111	1108	0.07 ± 0.15	-
11	*trans*-Thujone	1117	1112	0.16 ± 0.35	-
12	*neo*-Isopulegol[e]	1145	1144	2.12 ± 4.06 a	0.85 ± 1.39 a
13	Isopulegol	1147	1145	-	0.04 ± 0.11
14	*iso*-Isopulegol[e]	1157	1155	0.18 ± 0.40	0.24 ± 0.45 a
15	Menthol	1171	1167	0.28 ± 0.63 a	-
16	*cis*-Pinocamphone	1174	1172	4.74 ± 6.70 a	0.07 ± 0.20
17	αTerpineol	1185	1186	0.18 ± 0.40	-
18	*trans*-ρ-Mentha-1(7),8-dien-2-ol	1188	1187	0.28 ± 0.63 a	0.36 ± 0.61 a
19	Citronellol	1229	1223	4.74 ± 6.70 a	4.64 ± 6.66 a
20	Geraniol	1255	1249	1.53 ± 2.19 a	2.69 ± 3.38 a
21	Neryl formate	1280	1280	-	0.12 ± 0.33
22	β-Bourbonene[e]	1387	1387	0.14 ± 0.32 b	1.88 ± 1.78 a
23	β-Elemene[e]	1392	1389	0.15 ± 0.34 a	0.35 ± 0.99 a
24	Geosmin	1404	1399	-	0.08 ± 0.22
25	Dodecanal	1407	1408	-	0.11 ± 0.31
26	α-Cedrene	1410	1410	-	0.10 ± 0.29
27	(E)-Caryophyllene[d]	1420	1417	2.73 ± 0.60 b	7.09 ± 4.88 a
28	α-*trans*-Bergamotene	1439	1432	-	0.09 ± 0.25
29	α-Humulene[e]	1456	1452	0.23 ± 0.51 a	0.74 ± 1.55 a
30	*trans*-Prenyl limonene	1457	1457	0.47 ± 1.05	-
31	9-*epi*-(E)-Caryophyllene	1465	1464	-	0.13 ± 0.37
32	γ-Gurjunene	1478	1475	0.32 ± 0.72	-
33	γ-Muurolene	1479	1478	0.53 ± 0.76 a	1.04 ± 1.83 a
34	Germacrene D[e]	1484	1484	1.14 ± 1.35 b	18.1 ± 11.4 a
35	β-Selinene	1489	1489	0.73 ± 1.62 a	0.53 ± 0.83 a
36	α-Selinene	1498	1498	0.75 ± 1.68	-
37	Bicyclogermacrene	1500	1500	0.92 ± 0.87 b	6.65 ± 1.19 a
38	α-Muurolene	1501	1500	1.00 ± 1.13 a	0.32 ± 0.69 a
39	Germacrene A[e]	1506	1508	0.17 ± 0.38 a	0.40 ± 1.13 a
40	α-Cadinene	1516	1513	0.74 ± 1.14 a	1.22 ± 1.05 a
41	7-*epi*-α-Selinene	1518	1520	-	0.12 ± 0.34
42	δ-Cadinene	1524	1522	3.03 ± 1.48 a	3.22 ± 1.37 a
43	α-Calacorene[e]	1546	1544	0.82 ± 1.46 a	0.13 ± 0.36 a
44	Elemol	1552	1548	-	0.12 ± 0.23
45	Silphiperfol-5-en-3-ol A	1554	1557	-	0.11 ± 0.30
46	Germacrene B	1560	1559	-	0.18 ± 0.34
47	Geranyl butanoate	1566	1562	0.16 ± 0.35	-
48	Palustrol	1572	1567	-	0.34 ± 0.96
49	Caryophyllenyl alcohol	1572	1570	0.96 ± 1.65	-

Table S3. Continuation

	Constituent	RI[b]	RI[c]	Cluster I	Cluster II
50	Spathulenol	1578	1577	17.4 ± 10.5 a	16.1 ± 8.60 a
51	*trans*-Sesquisabinene hydrate	1583	1577	1.44 ± 3.22	-
52	Caryophyllene oxide	1583	1582	9.16 ± 2.22 a	9.36 ± 4.45 a
53	β-Copaen-4α-ol	1586	1590	1.68 ± 3.75	-
54	Globulol[e]	1593	1590	0.52 ± 1.17 a	0.11 ± 0.30 a
55	Rosifoliol	1595	1600	-	0.06 ± 0.18
56	Guaiol	1596	1600	-	0.38 ± 0.72
57	Geranyl 2-methylbutanoate	1596	1601	2.82 ± 3.93	-
58	Ledol	1604	1602	0.28 ± 0.62	-
59	Humulene epoxide II	1613	1608	2.20 ± 2.02 a	0.54 ± 1.02 a
60	*trans*-Isolongifolanone	1628	1625	0.25 ± 0.56	-
61	Muurola-4,10(14)-dien-1β-ol	1631	1630	3.90 ± 2.29 a	0.60 ± 1.01 b
62	Selina-1,3,7(11)-trien-8-one	1634	1632	0.94 ± 1.77	-
63	Caryophylla-4(12),8(13)-dien-5α-ol	1639	1639	-	0.09 ± 0.24
64	Caryophylla-4(12),8(13)-dien-5β-ol	1639	1639	0.20 ± 0.44 a	0.18 ± 0.51 a
65	*allo*-Aromadendrene epoxide	1640	1639	0.15 ± 0.33 a	0.22 ± 0.45 a
66	*epi*-α-Muurolol[d]	1644	1640	1.52 ± 3.00 a	0.12 ± 0.33 a
67	α-Muurolol[e]	1645	1644	5.85 ± 3.08 a	0.28 ± 0.39 b
68	Cubenol	1649	1645	1.58 ± 1.38 a	0.05 ± 0.13 b
69	β-Eudesmol	1654	1649	-	0.24 ± 0.46
70	α-Eudesmol	1655	1652	-	0.25 ± 0.70
71	α-Cadinol	1656	1652	1.62 ± 1.97 a	0.41 ± 0.78 a
72	Selin-11-en-4α-ol	1659	1658	9.97 ± 9.46 a	9.63 ± 10.6 a
73	*ar*-Turmerone	1665	1668	0.14 ± 0.30	-
74	14-hydroxy-9-*epi*-(E)-caryophyllene	1667	1668	-	0.24 ± 0.46
75	n-Tetradecanol	1670	1671	-	0.41 ± 1.16
76	5-*iso*-Cedranol	1671	1672	-	0.15 ± 0.43
77	Cadalene	1676	1675	0.18 ± 0.41	-
79	Khusinol[d]	1676	1679	0.38 ± 0.56	-
80	Germacra-4(15),10(14)-trien-1α-ol	1688	1685	-	0.10 ± 0.27
81	Eudesma-4(15),7-dien-1β-ol	1689	1687	0.76 ± 1.70 a	1.93 ± 0.94 a
82	Eudesm-7(11)-en-4-ol	1695	1700	0.23 ± 0.52	-
83	β-Davanone-2-ol	1720	1718	0.25 ± 0.57	-
84	2-Hexyl-(E)-cinnamaldehyde	1747	1748	0.40 ± 0.89	-
85	Benzyl benzoate	1763	1759	0.84 ± 1.89	-
86	(Z)-Nerolidyl isobutyrate	1779	1783	0.23 ± 0.51	-
Monoterpene hydrocarbons[d]				0.17 ± 0.24 a	1.60 ± 3.49 a
Oxygenated monoterpenes				11.6 ± 15.7 a	9.50 ± 12.4 a
Sesquiterpene hydrocarbons				13.1 ± 7.6 b	42.0 ± 6.8 a
Oxygenated sesquiterpenes				62.4 ± 23.5 a	41.9 ± 16.7 a
Others[d]				6.24 ± 8.20 a	0.80 ± 1.41 a
Identified constituents				93.4 ± 3.7 a	95.8 ± 2.5 a

[a]Average based on original data. [b]Calculated Retention index. [c]Reported Retention index.[32] [d]Rank and [e]arcsine-transformed in ANOVA analysis (see Experimental section). - = not detected. Percentage values followed by the same letter in the rows did not share significant differences at 5% probability by Tukey's test.

Table S4. Percentage of essential oil constituents of *Hypenia* spp. according to their carbon skeletons

Carbon's skeleton	*Hypenia*												
	brachystachys	*aristulata*	*marifolia*	*paradise*	*subrosea*	*crispata*	*durifolia*	*glauca*	*macrantha*	*macrosiphon*	*niquelandiensis*	*reticulata*	*sphaerocephala*
Tricyclane	-	-	-	-	-	-	-	-	-	-	-	-	0.3
Pinane	-	-	-	-	-	-	-	-	-	2.8	-	-	0.6
Thujane	8.1	0.8	-	-	-	-	-	-	-	6.6	-	-	1.0
Menthane	2.6	-	19.4	3.1	1.0	3.2	-	-	-	2.0	7.0	0.3	3.7
Myrcane	29.5	0.8	30.8	1.3	-	11.9	-	7.9	3.3	1.0	33.3	7.1	3.2
Bourbonane	0.8	-	-	-	-	3.4	-	1.0	-	1.8	4.6	0.8	4.2
Elemane	-	-	-	0.8	-	-	-	-	-	-	-	3.7	0.6
Cedrane	-	-	-	-	-	-	1.3	-	-	-	-	0.9	-
Caryophyllane	11.3	13.9	14.2	17.3	15.4	12.9	18.8	13.5	11.8	20.4	7.0	23.5	37.1
Humulane	2.0	4.0	-	5.0	2.1	-	2.7	-	0.6	7.6	-	-	-
Guaiane	-	-	-	1.8	-	1.9	1.3	-	-	-	-	-	-
Cadinane	9.5	38.0	25.5	23.7	19.0	6.3	9.0	3.5	5.1	6.4	2.4	16.0	14.3
Germacrane	-	-	3.9	1.9	1.8	33.7	17.6	32.8	17.2	19.3	27.0	9.3	-
Eudesmane	14.0	29.6	-	15.5	12.6	6.6	10.4	8.2	39.3	9.3	2.2	17.6	13.0
Bicyclogermacrane	1.6	-	-	1.5	2.1	8.4	6.1	6.3	6.2	7.0	9.1	7.3	5.5
Silphiperfolane	-	-	-	-	-	-	-	-	-	-	-	-	0.9
Aromadendrane	18.6	12.9	6.2	28.2	35.2	11.9	32.9	26.9	16.5	15.8	7.4	13.4	15.6
Copaane	-	-	-	-	9.5	-	-	-	-	-	-	-	-
Isolongifolane	-	-	-	-	1.4	-	-	-	-	-	-	-	-
Bisabolane	0.8	-	-	-	-	-	-	-	-	-	-	-	-
Farnesane	1.4	-	-	-	-	-	-	-	-	-	-	-	-
Total	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

– not detected.

Table S5. Percentage[a] of essential oil constituents of clustered *Hypenia* spp. according to carbon skeletons

Carbon's skeleton	Cluster I	Cluster II
Tricyclane	-	0 ± 0.1
Pinane	-	0.4 ± 1.0
Thujane	1.8 ± 3.5 a	1.0 ± 2.3 a
Menthane[b]	5.2 ± 8.0 a	2.0 ± 2.5 a
Myrcane	12.5 ± 16.1 a	8.5 ± 10.8 a
Bourbonane[b]	0.2 ± 0.4 b	2.0 ± 1.9 a
Elemane[b]	0.2 ± 0.4 a	0.5 ± 1.3 b
Cedrane	-	0.3 ± 0.5
Caryophyllane[c]	14.4 ± 2.2 a	18.1 ± 9.3 a
Humulane	2.6 ± 1.9 a	1.4 ± 2.7 a
Guaiane	0.4 ± 0.8 a	0.4 ± 0.8 a
Cadinane[b]	23.1 ± 10.4 a	7.9 ± 4.9 b
Germacrane	1.5 ± 1.6 b	19.6 ± 11.5 a
Eudesmane	14.3 ± 10.5 a	13.3 ± 11.4 a
Bicyclogermacrane	1.0 ± 1.0 b	7.0 ± 1.2 a
Silphiperfolane	-	0.1 ± 0.3
Aromadendrane	20.2 ± 11.6 a	17.5 ± 8.3 a
Copaane	1.9 ± 4.3	-
Isolongifolane	0.3 ± 0.6	-
Bisabolane	0.2 ± 0.3	-
Farnesane	0.3 ± 0.6	-

[a]Average based on original data. [b]Arcsine and [c]rank-transformed in ANOVA analysis (see Experimental section). Percentage values followed by the same letter in the rows did not share significant differences at 5% probability by Tukey's test. - = not detected.

Table S6. Morphological characters of *Hypenia* spp. leaves collected in central Brazilian Cerrado

Character codes		*Hypenia*												
		brachystachys	*aristulata*	*marifolia*	*paradisi*	*subrosea*	*crispata*	*durifolia*	*glauca*	*macrantha*	*macrosiphon*	*niquelandiensis*	*reticulata*	*sphaerocephala*
1	Adaxial epidermal cells highest that abaxial epiderme	+	+	+	+	+	+	+	+	-	+	+	+	+
2	Cuticle with parallel striation	-	-	-	-	-	+	+	+	+	+	+	+	+
3	Abaxial epidermal cells with anticlinal straight wall	-	-	-	-	-	-	+	+	+	-	+	+	-
4	Abaxial epidermal cells with anticlinal sinuate wall	+	+	-	+	+	+	-	-	-	+	-	-	+
5	Druses in adaxial epiderme	+	+	+	+	+	-	-	-	-	-	-	-	+
6	Starch in adaxial epiderme	+	+	+	+	+	-	-	-	-	-	-	-	-
7	Crystals in adaxial epiderme	+	+	+	+	+	-	-	-	-	-	-	-	+
8	Crystals in abaxial epiderme	-	+	-	+	+	-	-	-	-	-	-	-	-
9	Anisocytic stomata	+	+	-	+	+	+	+	+	+	-	+	+	+
10	Convex-plane midrib	+	+	+	-	-	+	+	+	+	+	+	+	+
11	Midrib slightly convex-plane	-	-	-	-	-	-	-	-	+	-	-	-	-
12	Convex-convex midrib with triangular projection on adaxial face	-	-	-	-	+	-	-	-	-	-	-	-	-
13	Crystals between veins of smaller caliber	+	+	+	+	+	-	-	-	-	-	-	-	-
14	Marginal hydathodes	-	+	-	-	-	+	+	+	-	-	-	+	-
15	Cuticular flange at the midrib	+	-	-	+	+	-	-	-	-	-	-	-	-
16	Thick cuticle	+	+	-	+	-	+	+	+	+	+	+	+	+
17	Thin cuticle	-	-	+	-	-	-	-	-	-	-	-	-	-
18	Prismatic crystals in pith of midrid	-	-	-	+	-	+	+	+	+	+	+	+	+

+ Present. – Absent.