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Supplementary Information

Chemotaxonomic Markers in Essential Oils of *Hypenia* (Mart. ex Benth.) R. Harley

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Table S1. *Hypenia* taxa with provenance and voucher specimens

Abbreviation	Taxon	Geographical coordinate	Voucher
Hcal1	*H. calycina* (Pohl ex Benth.) Harley	S 14°13'16", W 47°53'26", 774 m	45682
Hcal2		S 16°12'40", W 47°21'04", 923 m	45164
Hcha[a]	*H. chapadensis* Faria & Ferreira	S 14°06'29", W 47°31'27", 1101 m	45785
Hine	*H. inelegans* (Epl.) Harley	S 13°47'00", W 47°28'00", 823 m	45704
Hirr	*H. irregularis* (Benth. in DC.) Harley	S 14°09'31", W 46°36'24", 950 m	45736
Hjor1[a]	*H. jorgeana* Faria & Ferreira	S 14°12'48", W 47°29'17", 1216 m	45786
Hjor2		S 14°10'38", W 47°15'10", 1200 m	45785
Hmac	*H. macrantha* (St.-Hil. ex Benth.) R. Harley	S 14°32'49", W 46°51'16", 535 m	45725
Hpar	*H. paradisi* Harley	S 14°12'48", W 47°29'17", 1216 m	30839
Hpru1	*H. pruinosa* (Pohl ex Benth.) Harley	S 13°39'49", W 47°28'33", 1094 m	45709
Hpru2		S 15°27'58", W 47°30'25", 1179 m	45794
Hpru3		S 14°19'00", W 47°30'49", 1118 m	30684
Hpuc[a]	*H. puchra* Faria & Ferreira	S 14°12'48", W 47°29'17", 1216 m	45790
Hrup[a]	*H. rupestre* Faria & Ferreira	S 16°04'25", W 50°11'13", 881 m	45763

[a]New species.

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Table S2. Percentages of essential oil constituents from clustered *Hypenia* samples

	Constituent	Cluster I	Cluster II
1	Heptanal	–	0.11
2	Tricyclene	0.08	–
3	α-Pinene	0.25 a	0.06 a
4	(2*E*)-Heptenal	–	0.18
5	β-Pinene	0.83 a	0.07 a
6	Myrcene	0.13	–
7	ρ-Cymene	0.52 a	1.98 a
8	Limonene	–	1.39
9	β-Phellandrene	1.11	–
10	1,8-Cineole	1.08 a	0.24 a
11	γ-Terpinene	0.43	–
12	Acetophenone	–	2.68
13	Linalool	0.54 a	0.27 a
14	*trans*-Thujone	–	0.19
15	(2*E*)-Nonen-1-al	–	0.08
16	α-Copaene	3.67 a	2.85 a
17	Geranyl acetate	0.19	–
18	β-Bourbonene	1.72	1.60
19	β-Elemene	0.85 a	0.60 a
20	Methyl eugenol	–	0.11
21	Longifolene	–	0.08
22	α-Gurjunene	0.11	–
23	β-Funebrene	–	0.38
24	(*E*)-Caryophyllene	10.2 a	4.15 a
25	β-Copaene	0.06 a	0.08 a
26	α-*trans*-Bergamotene	–	0.47
27	α-Guaiene	–	0.07
28	Aromadendrene	0.28	–
29	Neryl propanoate	–	1.60
30	α-Humulene	1.45 a	2.17 a
31	Geranyl acetone	–	1.51
32	*allo*-Aromadendrene	–	0.49
33	*trans*-Cadina-1(6),4-diene	0.25 a	1.72 a
34	γ-Gurjunene	–	0.81
35	γ-Muurolene	9.90 a	9.02 a
36	γ-Himachalene	0.05 a	0.57 a
37	Germacrene D	11.0	–
38	β-Selinene	0.46 a	1.50 a
39	δ-Selinene	3.03 a	2.34 a
40	Indipone	–	0.88
41	Bicyclogermacrene	7.14 a	2.79 a
42	α-Muurolene	0.12 b	4.40 a
43	Germacrene A	0.29 a	0.48 a
44	γ-Cadinene	0.95 b	2.66 a
45	*trans*-Cycloisolongifol-5-ol	0.89	–
46	Cubebol	0.36 a	0.06 a
47	*trans*-Calamenene	–	2.03
48	δ-Cadinene	2.97 a	2.82 a
49	Zonarene	–	0.11
50	α-Cadinene	–	0.14
51	α-Calacorene	–	1.84
52	Italicene epoxide	0.11	–
53	Germacrene B	0.52 a	1.41 a
54	Caryophyllenyl alcohol	–	0.16
55	Caryolan-8-ol	–	1.22
56	Spathulenol[c]	18.1 a	3.97 b
57	*trans*-Sesquisabinene hydrate	–	1.40
58	Caryophyllene oxide	8.34 a	3.37 b
59	Globulol[b]	2.86 a	0.68 a
60	(*E*)-Dihydroapofarnesol	–	0.98
61	Guaiol	–	0.15
62	Ledol	–	0.23
63	Humulene epoxide	0.55 a	0.81 a
64	Junenol	–	0.26
65	α-Corocalene	–	0.11
66	1-*epi*-Cubenol	0.31 b	2.01 a
67	Muurola-4,10(14)-dien-1β-ol	–	0.62
68	γ-Eudesmol	–	0.08
69	*epi*-α-Cadinol	0.21 a	2.38 a
70	*allo*-Aromadendrene epoxide	0.18	–
71	Selina-3,11-dien-6α-ol	0.18 a	0.13 a
72	α-Muurolol	0.61 a	4.28 a
73	Cubenol	0.49 b	2.34 a
74	Pogostol	1.47	–
75	α-Cadinol	1.32 b	6.29 a
76	Selin-11-en-4α-ol	1.14 a	3.44 a
77	*cis*-Calamenen-10-ol	–	0.07
78	14-Hydroxy-9-*epi*-(*E*)-caryophyllene	0.57	–
79	Cadalene	–	1.32
80	Mustakone	0.38	–
81	Eudesma-4(15),7-dien-1β-ol	1.28 a	0.15 b
82	Eudesm-7(11)-en-4-ol	–	0.17
83	Benzyl benzoate	–	0.08
84	Hexahydrofarnesyl acetone	–	1.74
85	(5*E*,9*E*)-Farnesyl acetone	–	1.42
	Monoterpene hydrocarbons	2.92 a	3.51 a
	Oxygenated monoterpenes	2.05 a	0.69 a
	Sesquiterpene hydrocarbons	55.4 a	50.0 a
	Oxygenated sesquiterpenes	39.0 a	35.2 a
	Others	0.19 b	9.50 a
	Oil yield / %, m/m	0.04 a	0.05 a

Averages followed by the same letter in the rows did not share significant differences at 5% probability by Tukey's test; –: not detected.

Table S3. Percentages of essential oil constituents from clustered *Hypenia* species according to carbon skeletons

Constituent	Cluster I	Cluster II
Tricyclane	0.08	–
Pinane	1.11 a	0.13 a
Myrcane	0.87 a	1.88 a
Mentane	3.22 a	3.66 a
Thujane	–	0.19
Copaane	3.75 a	2.99 a
Bourbonane	1.73 a	1.62 a
Elemane	0.86 a	0.60 a
Longifolane	–	0.08
Isolongifolane	0.93	–
Cedrane	–	0.39
Caryophyllane	19.3 a	9.08 b
Guaiane	1.47 a	1.04 a
Aromadendrane	21.7 a	5.48 b
Humulane	2.01 a	3.04 a
Bicyclogermacrane	7.18 a	2.86 a
Germacrane	12.0 a	1.92 a
Cadinane	17.2 b	45.1 a
Eudesmane	6.22 a	8.14 a
Farnesane	–	1.00
Sesquisabinane	–	1.41
Italicane	0.11	–
Bergamotane	–	0.48
Indipane	–	0.90
Others	0.38 b	8.00 a

Percentages followed by the same letter in the rows did not share significant differences at 5% probability by Tukey's test; –:not detected.

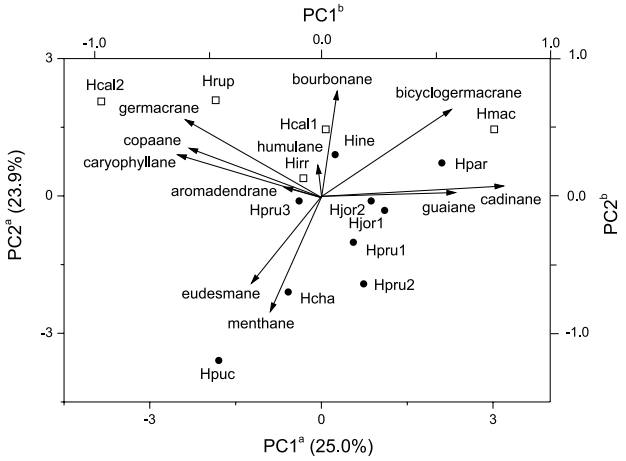

Figure S1. PCA biplot of *Hypenia* species based on carbon skeletons of essential oil constituents, according to the clusters they belong to: I (□); II (●). [a]Axes refer to scores from the samples. [b]Axes refer to loadings from carbon skeletons (Table S3) represented as vectors from the origin. *Hypenia* samples: Hcal = *H. calycina*; Hmac = *H. macrantha*; Hpuc = *H. puchra*; Hrup = *H. rupestre*; Hirr = *H. irregularis*; Hjor = *H. jorgeana*; Hpar = *H. paradisi*; Hpru = *H. pruinosa*; Hine = *H. inelegans*; Hcha = *H. chapadensis*.

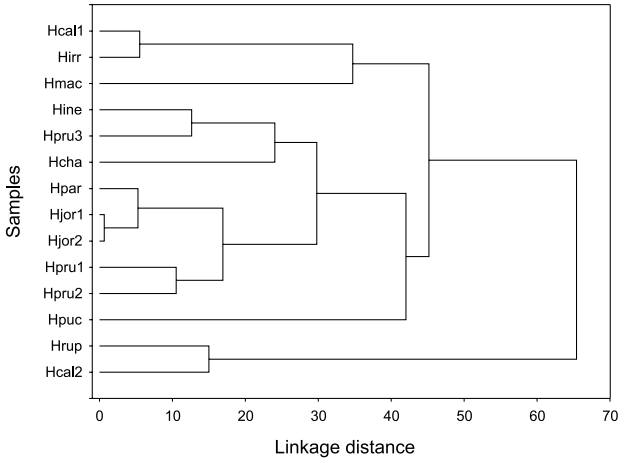

Figure S2. Dendrogram representing similarity relationships among *Hypenia* species based on carbon skeletons of essential oil constituents.

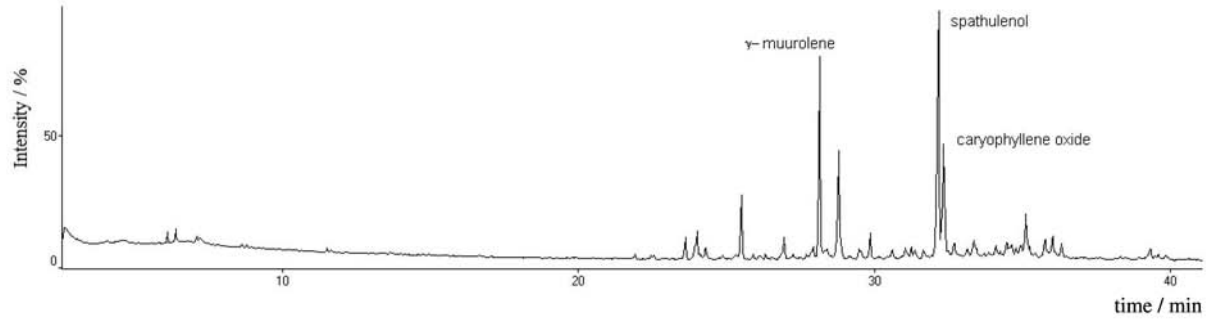

Figure S3. Total ion chromatogram (TIC) of essential oil from *H. calycina* (Hcal1).

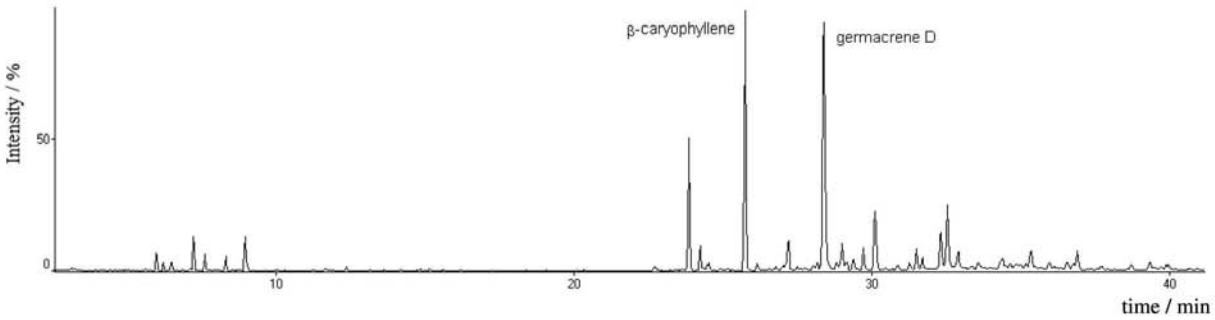

Figure S4. Total ion chromatogram (TIC) of essential oil from *H. calycina* (Hcal2).

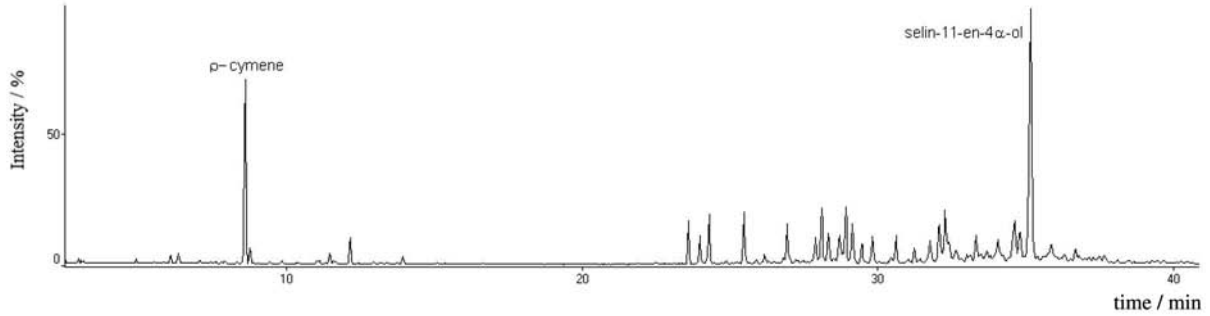

Figure S5. Total ion chromatogram (TIC) of essential oil from *H. chapadensis* (Hcha).

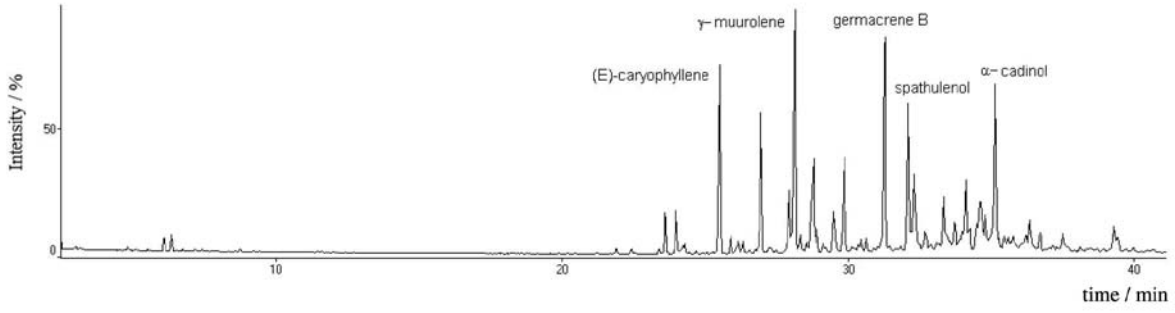

Figure S6. Total ion chromatogram (TIC) of essential oil from *H. inelegans* (Hine).

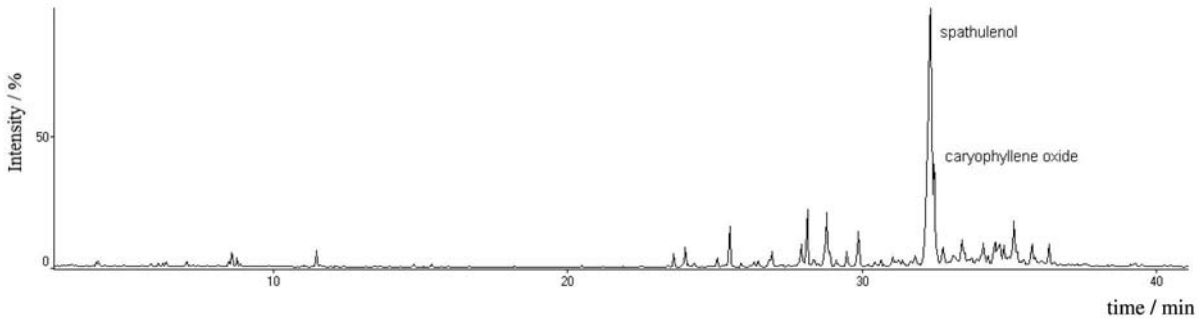

Figure S7. Total ion chromatogram (TIC) of essential oil from *H. irregularis* (Hirr).

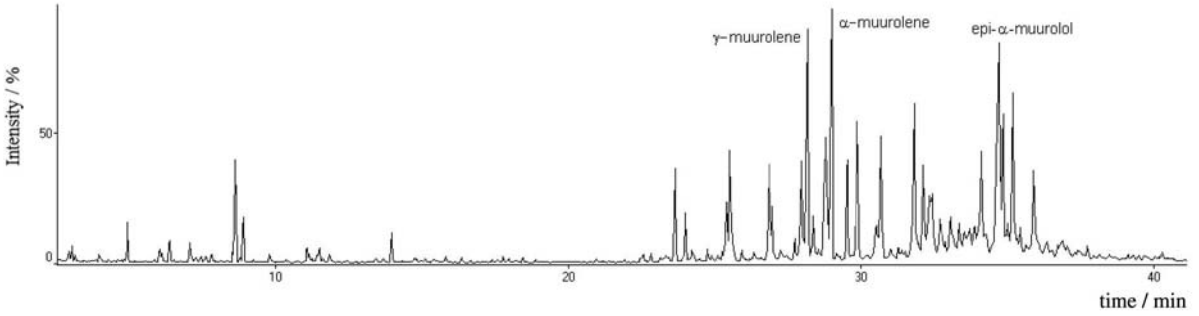

Figure S8. Total ion chromatogram (TIC) of essential oil from *H. jorgeana* (Hjor1).

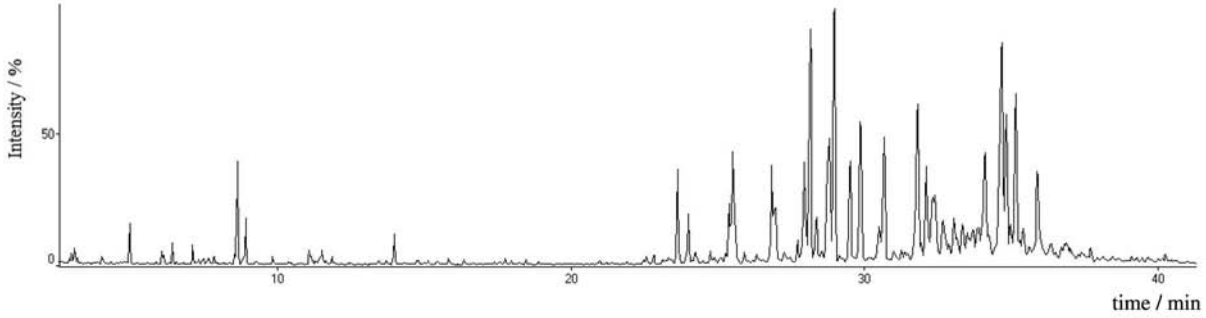

Figure S9. Total ion chromatogram (TIC) of essential oil from *H. jorgeana* (Hjor2).

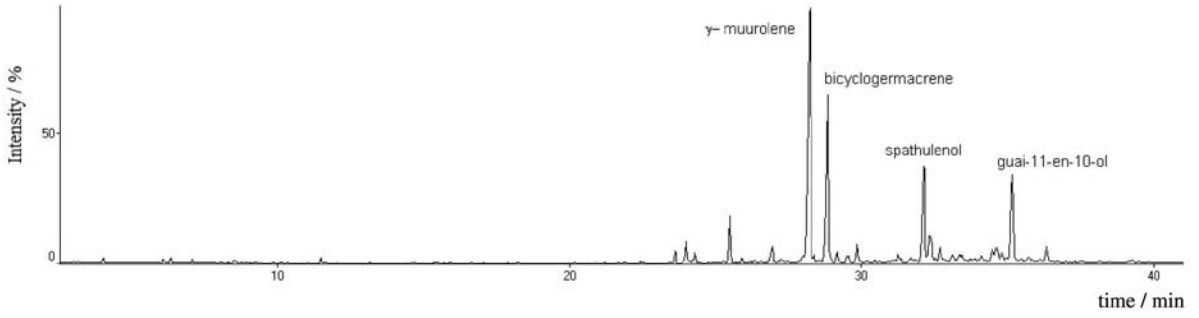

Figure S10. Total ion chromatogram (TIC) of essential oil from *H. macrantha* (Hmac).

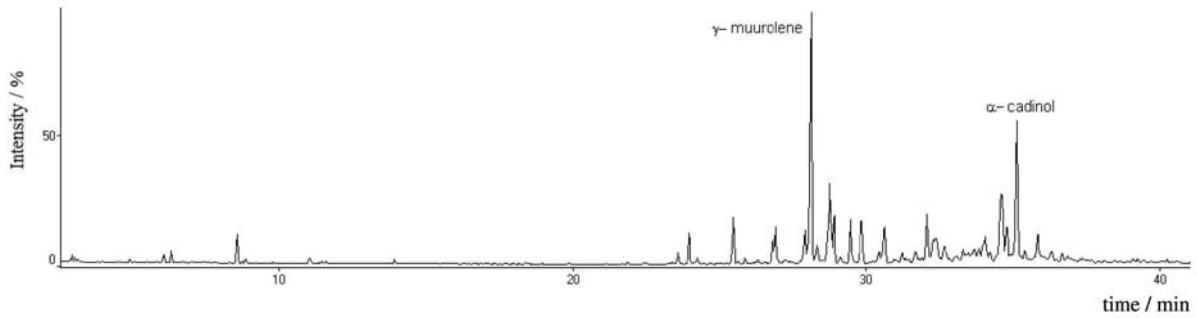

Figure S11. Total ion chromatogram (TIC) of essential oil from *H. paradisi* (Hpar).

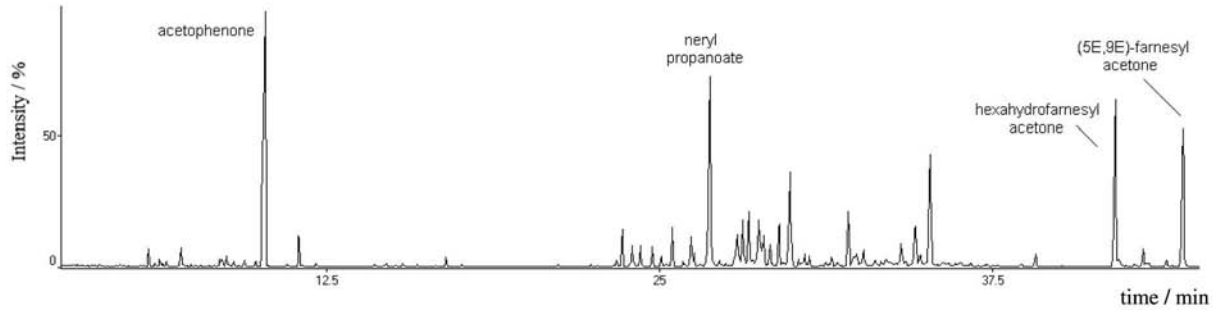

Figure S12. Total ion chromatogram (TIC) of essential oil from *H. pruinosa* (Hpru1).

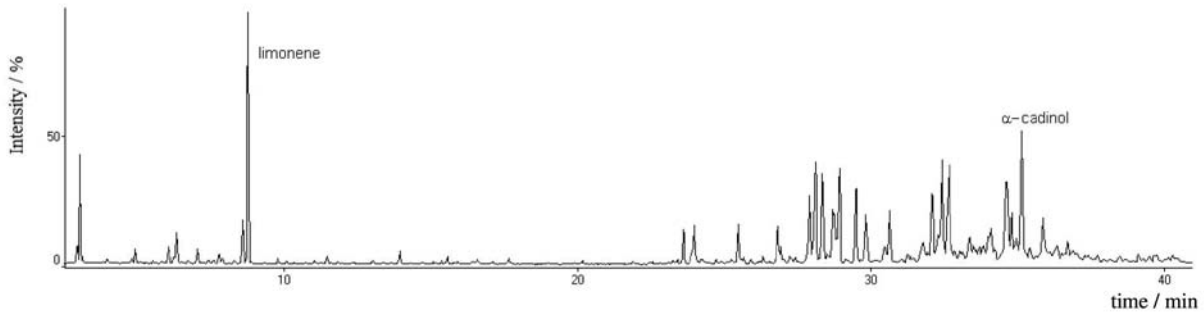

Figure S13. Total ion chromatogram (TIC) of essential oil from *H. pruinosa* (Hpru2).

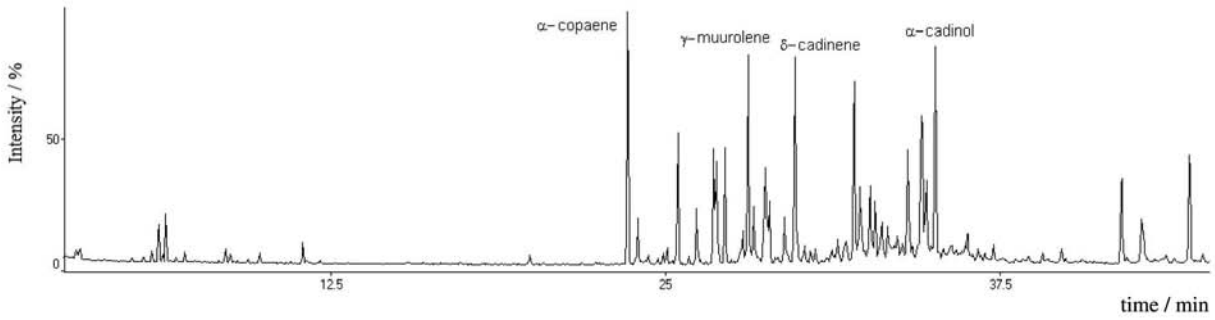

Figure S14. Total ion chromatogram (TIC) of essential oil from *H. pruinosa* (Hpru3).

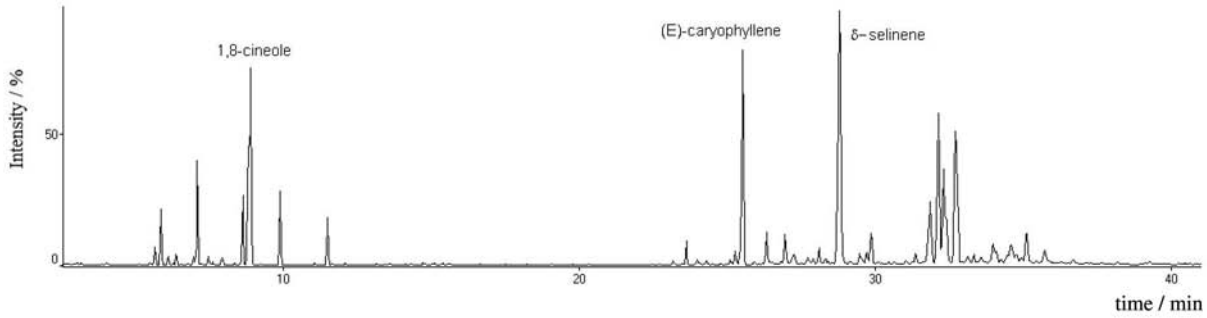

Figure S15. Total ion chromatogram (TIC) of essential oil from *H puchra* (Hpuc).

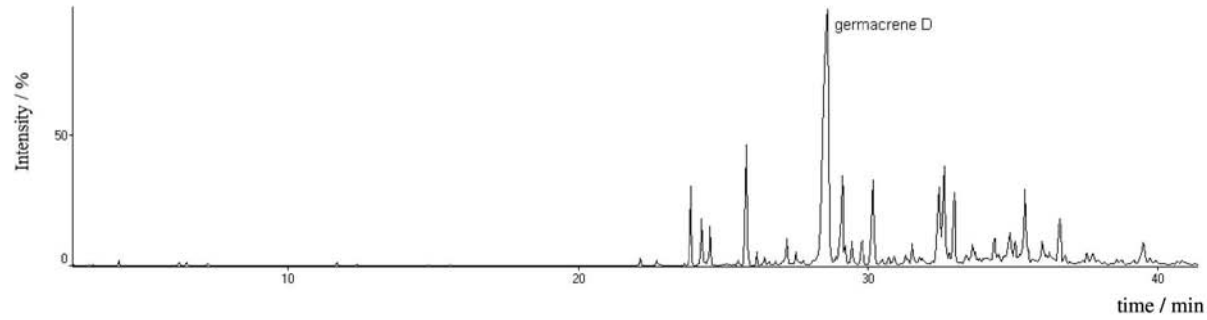

Figure S16. Total ion chromatogram (TIC) of essential oil from *H. rupestre* (Hrup).

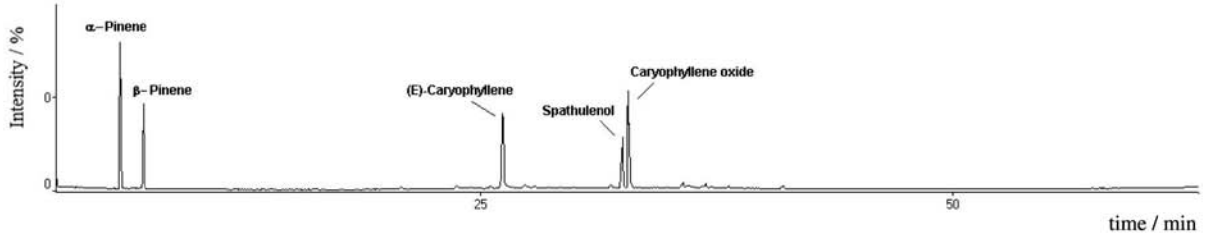

Figure S17. Total ion chromatogram (TIC) of standards.

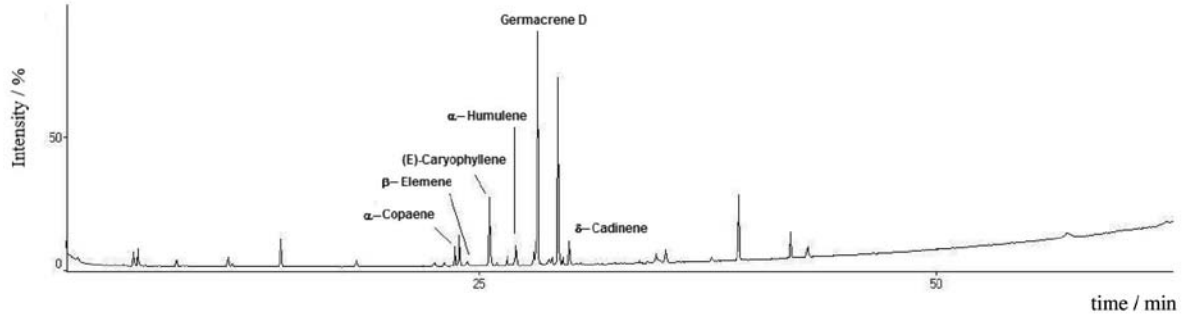

Figure S18. Total ion chromatogram (TIC) of ylang-ylang essential oil.

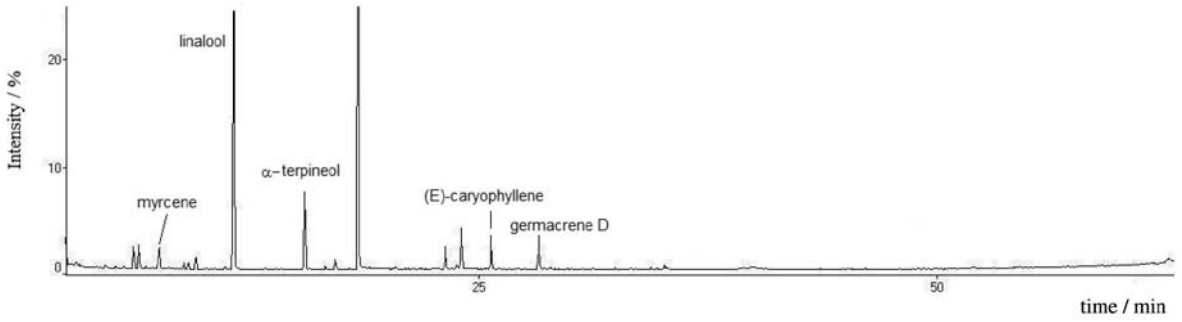

Figure S19. Total ion chromatogram (TIC) of sage clary essential oil.

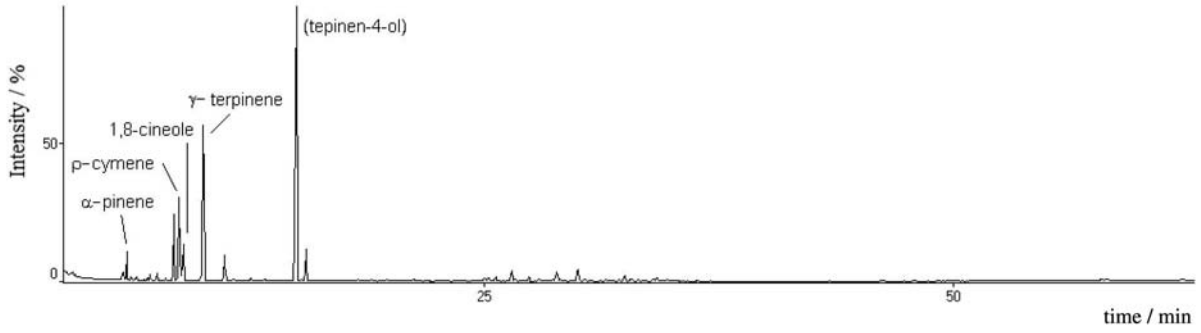

Figure S20. Total ion chromatogram (TIC) of tea-tree essential oil.