

Supplementary Information

Chemotaxonomy of *Marsypianthes* Mart. ex Benth. Based on Essential Oil Variability

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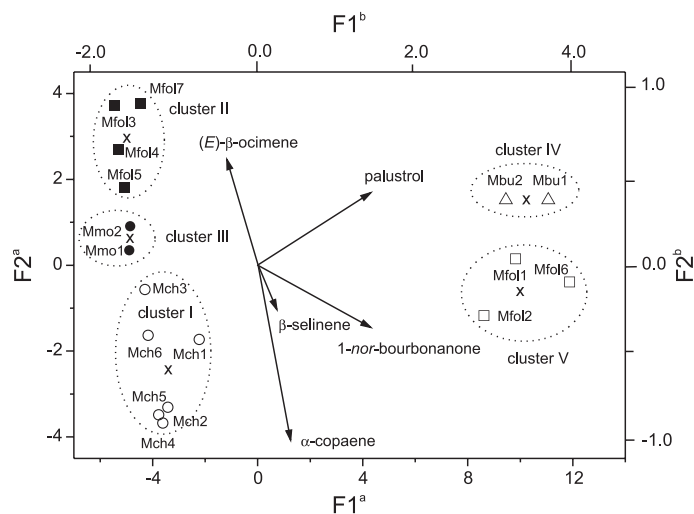


Figure S1. Biplot generated by the linear canonical discriminant analysis of *Marsypianthes* Mart. ex Benth. with (*E*)-β-ocimene, α-copaene, β-selinene, 1-nor-bourbonanone, and palustrol as predictor variables represented by vectors starting from the origin. Cluster centroids are represented by crosses. The first factorial plan represents 94.1% of total variability in the original data. *Marsypianthes* species: Mbu = *M. burchellii*, Mch = *M. chamaedrys*, Mfol = *M. foliolosa*, Mmo = *M. montana*.

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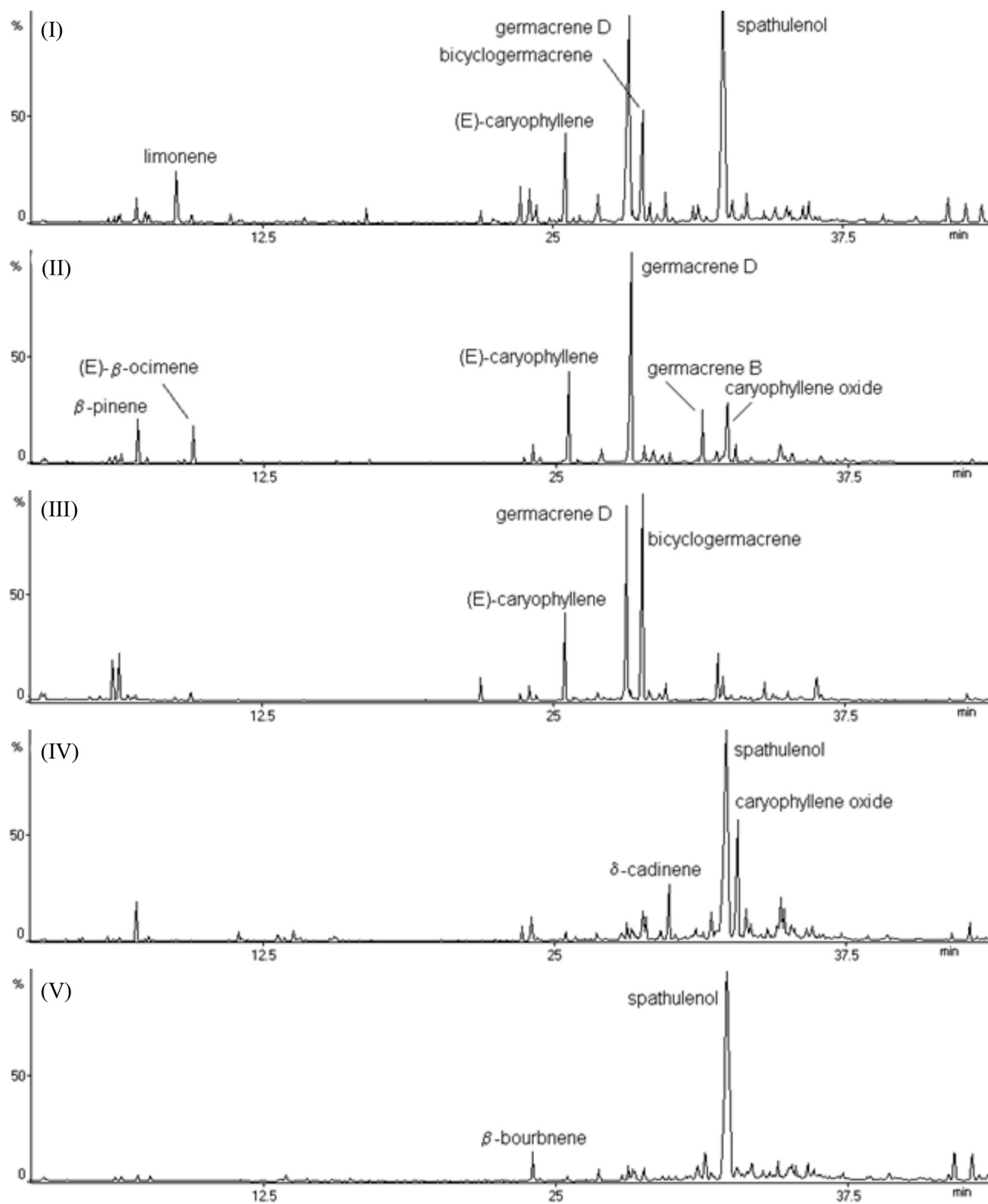


Figure S2. Total ion chromatograms (TICs) of the representative essential oils of clustered *Marsypianthes* Mart. ex Benth. (I-V), including the major oil constituents identified.

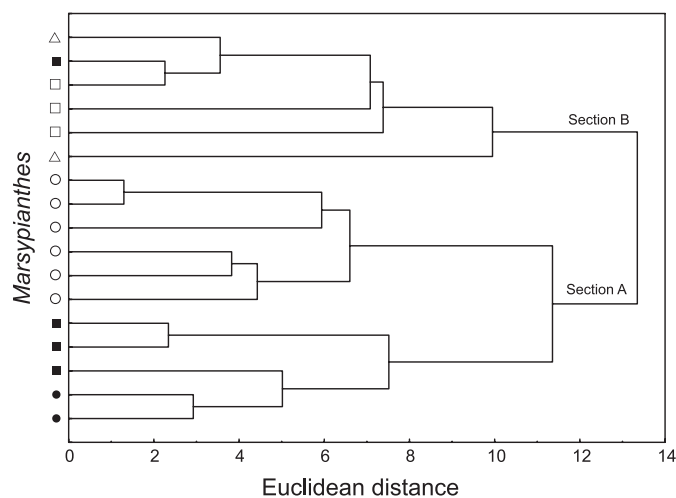


Figure S3. HCA dendrogram of similarity between *Marsypianthes* Mart. ex Benth. populations according to the biosynthetic carbon skeletons of essential oil constituents. Clusters I (O), II (■), III (●), IV (△), and V (□), and their chemical sections A and B.

Table S1. Species and provenance of *Marsypianthes* Mart. ex Benth. in Goiás State, Brazil

Taxon	Pop ^a	City/Goiás State	Geographic co-ordinates	UFG ^b
<i>M. burchellii</i> Epl.	Mbu1	Colinas do Sul	S 14° 11' 26", W 48° 7' 22", 533 m	47310
	Mbu2	Cavalcante	S 13° 47', W 47° 28', 823 m	47311
<i>M. chamaedrys</i> (Vahl) Kuntze	Mch1	Niquelândia	S 14° 9' 35", W 47° 46' 15", 583 m	45617
	Mch2	Trindade	S 16° 38' 52", W 49° 29' 53", 758 m	45934
	Mch3	Silvânia	S 16° 40' 5", W 48° 36' 26", 888m	47803
	Mch4	Pirenópolis	S 15° 50' 15", W 48° 58' 7", 820 m	47323
	Mch5	Cavalcante	S 13° 34' 57", W 47° 28' 14", 1052 m	47305
	Mch6	Colinas do Sul	S 14° 9' 20", W 48° 3' 58", 552 m	47308
<i>M. foliolosa</i> Benth.	Mfol1	Posse	S 16° 5', W 48° 48', 929 m	47802
	Mfol2	Rio Verde	S 18° 4', W 50° 30', 592 m	47801
	Mfol3	Alto Paraíso	S 13° 54' 52", W 47° 24' 53", 1395 m	47304
	Mfol4	Cavalcante	S 13° 48' 6", W 47° 27' 44", 804 m	47306
	Mfol5	Terezinha de Goiás	S 13° 36' 43", W 47° 13' 16", 754 m	47307
	Mfol6	Colinas do Sul	S 14° 11' 47", W 48° 5' 50", 562 m	47309
	Mfol7	Posse	S 14° 4' 32", W 46° 19' 1", 815 m	47800
<i>M. montana</i> Benth.	Mmo1	Mossâmedes	S 16° 8', W 50° 13', 1021 m	45935
	Mmo2	Alto Paraíso	S 14° 8' 1", W 47° 31' 17", 1253 m	30644

^aPopulation; ^bexsiccates from UFG's herbarium.

Table S2. Texture and physicochemical parameters of soil sampling sites

Pop. ^a	Clay / %	Sand / %	Silt / %	pH	Organic matter / %	P / (mg L ⁻¹)	K ⁺ / (mg L ⁻¹)	Ca ²⁺ / (cmol _c L ⁻¹)	Mg ²⁺ / (cmol _c L ⁻¹)	CEC / (cmol _c L ⁻¹)	H ⁺ +Al ³⁺ / (cmol _c L ⁻¹)	Al ³⁺ / (cmol _c L ⁻¹)	Cu ²⁺ / (mg L ⁻¹)	Fe ²⁺ / (mg L ⁻¹)	Mn ²⁺ / (mg L ⁻¹)	Zn ²⁺ / (mg L ⁻¹)
Mbu1	19.0	70.0	11.0	4.8	0.8	1.1	27.0	0.8	0.1	3.1	2.1	0.0	0.5	54.2	99.9	0.4
Nbu2	23.0	56.0	21.0	4.3	1.3	1.7	48.0	0.9	0.3	2.8	1.5	0.7	0.2	121.8	13.2	2.2
Mch1	20.0	65.0	15.0	5.4	2.1	1.1	54.0	2.7	1.0	5.2	1.4	0.0	0.2	30.4	22.9	3.0
Mch2	39.0	51.0	10.0	5.5	2.2	0.6	43.0	3.9	0.7	6.2	1.5	0.0	0.2	33.0	28.0	2.0
Mch3	33.0	44.0	23.0	5.3	3.7	2.0	63.0	4.1	1.5	7.7	1.9	0.0	1.6	77.2	94.0	3.2
Mch4	29.0	49.0	22.0	5.2	1.0	2.0	48.0	1.6	0.5	3.7	1.5	0.0	0.6	425.0	39.9	1.1
Mch5	23.0	56.0	21.0	4.3	1.3	1.7	48.0	0.9	0.3	2.8	1.5	0.7	0.2	121.8	13.2	2.2
Mch6	26.0	60.0	14.0	4.4	0.5	1.4	29.0	3.3	0.3	5.8	2.1	0.8	0.3	68.5	5.2	0.3
Mfol1	12.0	73.5	14.5	4.2	1.0	2.1	38.0	0.3	0.1	2.4	1.9	0.3	0.2	170.0	7.4	0.8
Mfol2	44.0	46.0	10.0	4.2	2.0	1.1	34.0	0.2	0.1	6.3	5.9	1.1	1.1	84.5	6.4	0.7
Mfol3	24.0	56.0	20.0	3.8	4.5	1.1	46.0	0.5	0.2	4.3	3.5	3.2	0.2	121.3	4.0	0.2
Mfol4	22.0	60.0	18.0	4.2	0.8	1.7	37.0	0.4	0.1	2.1	1.5	0.7	0.2	336.0	31.0	0.2
Mfol5	22.0	64.0	14.0	4.1	1.1	2.3	46.0	0.3	0.3	2.2	1.5	1.0	0.7	155.7	18.3	0.3
Mfol6	14.0	82.0	4.0	4.2	0.3	3.2	18.0	0.2	0.1	2.2	1.9	0.7	0.2	44.0	1.0	1.0
Mfol7	14.0	82.0	4.0	5.0	0.8	2.0	20.0	0.6	0.1	2.5	1.7	1.0	0.8	92.0	5.8	1.4
Mmo1	45.0	35.0	20.0	4.7	3.0	0.8	46.0	0.7	0.2	3.3	2.3	1.0	0.2	48.5	10.5	0.3
Mmo2	41.7	42.3	16.0	4.4	3.2	4.3	76.0	1.4	1.1	8.0	5.3	0.4	0.6	86.4	68.2	1.4

^aPopulation.**Table S3.** Chemical composition of essential oils from clustered samples of *Marsypianthes* Mart. ex Benth. according to PCA/HCA analyses

Constituent	Average		Standard deviation		<i>P</i> ^b	
	Cluster	Global	Cluster	Global		
Cluster I						
26	α -Copaene	3.13	1.44	1.00	1.45	0.000
34	α - <i>trans</i> -Bergamotene	0.50	0.18	0.30	0.30	0.001
27	β -Cubebene	0.51	0.22	0.28	0.28	0.001
44	Germacrene A	1.81	1.07	0.60	0.81	0.004
35	α -Humulene	2.18	1.32	0.78	1.00	0.005
8	Limonene	1.26	0.56	1.07	0.85	0.007
33	β -Copaene	0.24	0.13	0.15	0.15	0.014
29	β -Elemene	0.90	0.57	0.33	0.45	0.016
S	Sesquiterpenes	94.96	90.82	0.69	6.66	0.033
62	Muurolo-4,10(14)-dien-1 β -ol	1.38	0.78	1.37	1.04	0.044
25	δ -Elemene	0.96	0.53	0.74	0.75	0.045
32	(<i>E</i>)-Caryophyllene	11.49	8.42	3.69	5.44	0.048
Cluster II						
11	(<i>E</i>)- β -Ocimene	2.13	0.83	0.90	0.91	0.001
10	(<i>Z</i>)- β -Ocimene	0.13	0.05	0.06	0.07	0.002
64	<i>epi</i> - α -Cadinol	2.05	0.99	0.68	0.96	0.007
5	β -Pinene	2.39	1.21	1.40	1.11	0.009
71	Eudesma-4(15),7-dien-1 β -ol	0.63	0.31	0.38	0.35	0.021
MH	Monoterpene hydrocarbons	5.73	3.59	2.28	2.43	0.026

Table S3. continuation

Constituent	Average		Standard deviation		<i>p</i> ^b	
	Cluster	Global	Cluster	Global		
Cluster III						
42	Bicyclogermacrene	41.42	13.46	11.09	13.75	0.001
41	β-Selinene	1.24	0.38	0.47	0.45	0.002
37	<i>allo</i> -Aromadendrene	0.20	0.02	0.20	0.09	0.003
65	<i>allo</i> -Aromadendrene epoxide	0.21	0.03	0.21	0.10	0.003
70	Germacre-4(15),5,10(14)-trien-1α-ol	1.45	0.19	1.45	0.68	0.003
59	β-Atlantol	0.14	0.02	0.14	0.06	0.003
SH	Sesquiterpene hydrocarbons	85.38	54.35	8.55	25.61	0.038
Cluster IV						
53	Palustrol	2.20	0.39	0.13	0.76	0.000
57	Globulol	10.06	2.43	5.28	3.52	0.001
66	α-Muurolol	2.21	0.37	1.90	0.97	0.003
31	Acora-3,7(14)-diene	3.66	0.43	3.66	1.72	0.003
30	Longifolene	4.32	0.51	4.32	2.03	0.003
38	γ-Gurjunene	2.10	0.37	1.68	0.92	0.003
47	δ-Cadinene	3.88	1.73	1.34	1.30	0.008
58	Ledol	1.33	0.30	1.31	0.63	0.008
Cluster V						
51	1- <i>nor</i> -Bourbonanone	2.55	0.50	0.99	1.04	0.000
68	14-Hydroxy-9- <i>epi</i> -(<i>E</i>)-caryophyllene	1.36	0.56	0.16	0.50	0.001
61	1,10-di- <i>epi</i> -Cubanol	0.59	0.19	0.18	0.25	0.001
55	Caryophyllene oxide	14.38	7.59	2.08	4.34	0.002
OU	Others	3.32	0.78	2.65	1.66	0.002
69	Mustakone	1.13	0.46	0.29	0.47	0.004
OS	Oxygenated sesquiterpenes	65.86	36.47	12.44	23.56	0.010
28	β-Bourbonene	6.06	2.99	3.62	2.50	0.012
OM	Oxygenated monoterpenes	4.64	1.17	5.59	2.89	0.013
18	Borneol	1.77	0.33	2.40	1.21	0.014
46	6-Methyl-α-ionone	2.07	0.37	2.93	1.46	0.015
24	Isobornyl acetate	0.95	0.20	1.33	0.66	0.018
54	Spathulenol	36.34	18.54	14.56	16.00	0.020
3	Camphene	1.33	0.39	1.59	0.85	0.020
60	Humulene epoxide II	1.59	0.90	0.61	0.73	0.041

^aOther constituents did not differ at 5% probability; ^bprobability.

