

## Environmental Influence on Phenols and Essential Oils of *Myrciaria cauliflora* Leaves

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**Table S1.** Chemical characteristics<sup>a</sup> of *M. cauliflora* sampling sites

Constituent	Sampling sites					
	S1	S2	S3	S4	S5	S6
Clay (%)	16.0 b	30.0 ab	35.5 ab	41.5 a	42.0 a	19.0 b
Silt (%)	16.5 a	15.5 a	13.0 a	16.5 a	13.5 a	11.5 a
Sand (%)	67.5 a	54.5 a	51.5 a	42.0 a	44.5 a	69.5 a
Cu (mg dm <sup>-3</sup> )	0.9 abc	1.4 a	1.3 ab	0.9 abc	0.5 bc	0.8 bc
Fe <sup>b</sup> (mg dm <sup>-3</sup> )	44.3 bc	221.5 a	60.8 ab	33.4 de	24.1 e	37.1 cd
Mn <sup>b</sup> (mg dm <sup>-3</sup> )	17.4 bc	21.3 bc	37.7 ab	65.1 a	34.1 ab	9.4 c
Zn (mg dm <sup>-3</sup> )	0.6 b	1.5 ab	0.9 ab	3.0 a	2.6 ab	0.7 ab
Organic matter (%)	1.1 a	1.0 a	2.0 a	2.7 a	2.9 a	1.8 a
pH	5.0 a	4.8 a	5.0 a	5.2 a	5.2 a	5.0 a
P <sup>b</sup> (mg dm <sup>-3</sup> )	0.3 b	0.7 ab	0.3 b	11.8 a	1.2 ab	0.3 b
K <sup>b</sup> (mg dm <sup>-3</sup> )	35.0 bc	33.5 c	41.5 ab	77.5 a	64.0 a	36.0 bc
Ca <sup>b</sup> (mg dm <sup>-3</sup> )	1.2 c	1.3 bc	1.8 abc	4.2 ab	4.5 a	0.8 c
Mg (mg dm <sup>-3</sup> )	0.3 b	0.4 b	0.5 b	1.4 a	1.0 ab	0.3 b
H+Al (mg dm <sup>-3</sup> )	2.6 a	2.1 a	2.1 a	2.2 a	2.6 a	2.7 a
Al (mg dm <sup>-3</sup> )	0.1	0.0	0.0	0.0	0.0	0.1
CTC <sup>b</sup> (mg dm <sup>-3</sup> )	4.1 ab	3.9 b	4.5 ab	8.0 a	8.2 a	3.8 b

<sup>a</sup>Average based on original data. <sup>b</sup>Rank-transformed in ANOVA analysis (see Experimental section). Averages followed by the same letter in the rows did not share significant differences at 5% probability by Tukey's test.

**Table S2.** Chemical characteristics of *M. cauliflora* leaves from different sampling sites

Foliar parameter	Sampling sites					
	S1	S2	S3	S4	S5	S6
N (dag kg <sup>-1</sup> )	1.54	2.32	2.04	2.07	1.62	1.96
P (dag kg <sup>-1</sup> )	0.08	0.07	0.09	0.13	0.06	3.10
K (dag kg <sup>-1</sup> )	0.80	0.88	0.76	1.06	1.00	0.86
Ca (dag kg <sup>-1</sup> )	1.30	1.50	1.70	1.30	1.60	0.80
Mg (dag kg <sup>-1</sup> )	0.20	0.40	0.60	0.50	0.50	0.30
S (dag kg <sup>-1</sup> )	0.04	0.14	0.14	0.12	0.14	0.15
Cu (mg kg <sup>-1</sup> )	8.00	5.00	5.00	5.00	8.00	7.00
Fe (mg kg <sup>-1</sup> )	275.0	315.0	347.0	262.0	249.0	299.0
Mn (mg kg <sup>-1</sup> )	710.0	760.0	501.0	302.0	152.0	243.0
Zn (mg kg <sup>-1</sup> )	16.20	20.60	16.20	20.00	18.20	17.20

**Table S3.** Accumulated percentage<sup>a</sup> of volatile constituents from *M. cauliflora* leaves according to carbon skeletons

Carbon skeleton	Sampling sites					
	S1	S2	S3	S4	S5	S6
Pinane	1.58 ab	2.43 a	1.98 ab	0.91 b	1.26 ab	1.98 ab
Menthane <sup>b</sup>	1.02 ab	1.84 a	1.81 a	0.38 b	0.68 ab	1.69 a
Elemene	5.91 b	6.50 ab	6.74 ab	3.93 c	4.71 bc	7.87 a
Copaane	2.44 a	2.67 a	2.89 a	2.93 a	2.51 a	2.63 a
Bourbonane	1.56 a	1.77 a	1.69 a	0.22 c	0.75 bc	1.14 b
Caryophyllane	7.70 a	8.75 a	9.07 a	8.21 a	7.96 a	8.50 a
Guaiane <sup>c</sup>	0.69 a	0.27 a	1.12 a	0.68 a	0.02 a	0.89 a
Humulane <sup>b</sup>	1.30 ab	1.39 ab	1.54 a	1.35 ab	1.28 b	1.42 ab
Aromadendrane <sup>b</sup>	0.52 a	0.65 a	0.57 a	0.32 a	0.51 a	0.68 a
Germacrane	22.31 c	24.43 bc	26.31 b	29.80 a	28.58 ab	27.17 ab
Eudesmane	44.83 a	38.17 ab	35.37 b	38.75 ab	40.19 a	34.88 b
Bicyclogermacrane	6.41 b	6.86 b	7.16 ab	7.89 a	7.37 ab	7.71 ab
Cadinane	3.17 a	3.19 a	3.16 a	3.71 a	3.19 a	3.06 a
Eremophilane	0.56 a	1.09 a	0.58 a	0.93 a	0.98 a	0.37 a
Total	100.00	100.00	100.00	100.00	100.00	100.00

<sup>a</sup> Average based on original data. <sup>b</sup> Rank and <sup>c</sup> arcsine-transformed in ANOVA analysis (see Experimental section). Averages followed by the same letter in the rows did not share significant differences at 5% probability by Tukey's test.

**Table S4.** Percentages<sup>a</sup> and yields in essential oils and total phenol/tannin contents (mg g<sup>-1</sup>) of *M. cauliflora* clustered samples

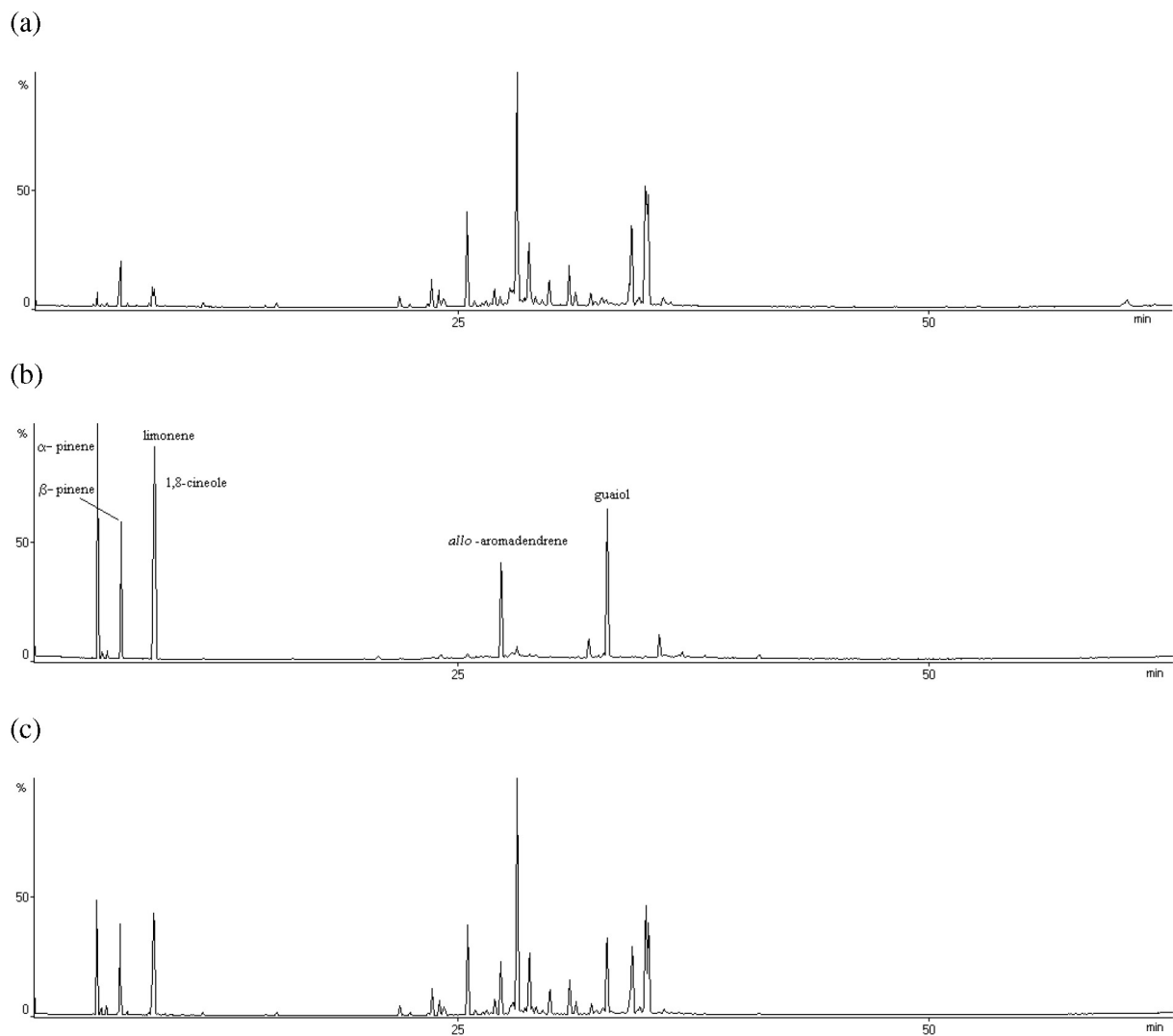
	Constituent	RI <sup>b</sup>	Clusters <sup>c</sup>			
			I	II	III	IV
1	$\alpha$ -Pinene	931	0.24 a	0.41 a	t	t
2	$\beta$ -Pinene	975	1.32 a	1.71 a	0.89 a	1.25 a
3	Limonene	1026	0.53 ab	0.97 a	0.36 b	0.22 b
4	1,8-Cineole	1029	0.48 a	0.78 a	t	0.45 a
5	$\delta$ -Elemene <sup>d</sup>	1337	1.28 b	1.57 ab	1.70 a	1.54 ab
6	$\alpha$ -Copaene <sup>d</sup>	1376	1.99 b	2.26 b	2.70 a	2.32 ab
7	$\beta$ -Bourbonene	1385	1.54 a	1.51 a	0.22 b	0.74 b
8	Unknown (M = 204)	1390	0.37 a	0.74 a	0.91 a	0.80 a
9	$\beta$ -Elemene <sup>c</sup>	1392	0.83 a	0.72 a	0.07 a	0.59 a
10	$\beta$ -Caryophyllene	1421	7.55 a	8.60 a	8.13 a	7.92 a
11	$\beta$ -Copaene	1429	0.41 a	0.41 a	0.20 a	0.18 a
12	6,9-Guaiadiene	1443	0.39 a	0.46 a	0.34 a	t
13	$\alpha$ -Humulene	1454	1.27 a	1.42 a	1.33 a	1.28 a
14	<i>allo</i> -Aromadendrene	1461	0.51 ab	0.63 a	0.32 b	0.51 ab
15	Germacrene D	1484	20.48 c	23.27 b	27.20 a	26.83 a
16	$\delta$ -Selinene	1492	0.09 a	0.07 a	0.30 a	t
17	Bicyclogermacrene	1498	6.29 b	7.09 a	7.82 a	7.33 a
18	$\alpha$ -Muurolole	1501	0.42 a	0.31 a	0.34 a	0.21 a
19	Germacrene A <sup>c</sup>	1506	0.07 a	0.63 a	0.52 a	t
20	$\delta$ -Cadinene	1524	2.69 b	2.77 b	3.32 a	2.96 ab
21	Elemol	1550	3.69 b	4.61 a	2.12 c	2.55 c
22	Germacrene B <sup>d</sup>	1558	1.34 c	1.49 b	1.79 a	1.59 ab
23	Unknown <sup>e</sup> (M = 220)	1578	1.04 b	1.29 a	0.38 c	0.46 c
24	Guaiol	1601	0.29 a	0.24 a	0.32 a	t
25	Eremoligenol	1630	0.54 a	0.70 a	0.91 a	0.97 a
26	$\gamma$ -Eudesmol	1634	11.55 a	8.94 b	7.81 b	8.75 b
27	$\beta$ -Eudesmol	1653	19.20 a	15.19 b	16.91 ab	17.46 ab
28	$\alpha$ -Eudesmol <sup>d</sup>	1656	12.72 ab	10.66 b	12.41 ab	12.94 a
Monoterpenes <sup>d</sup>			2.57 ab	3.88 a	1.27 b	1.93 b
Monoterpene hydrocarbons <sup>d</sup>			2.09 ab	3.09 a	1.26 b	1.48 b
Oxygenated monoterpenes			0.48 a	0.78 a	t	0.45 a
Sesquiterpenes			96.54 ab	95.57 b	98.08 a	97.98 a
Sesquiterpene hydrocarbons			47.50 b	53.95 a	57.22 a	54.83 a
Oxygenated sesquiterpenes			49.04 a	41.63 b	40.86 b	43.15 b
Oil yield (%)			0.48 a	0.39 ab	0.29 ab	0.26 ab
Total phenols			136.68 a	128.68 b	79.69 d	111.77 c
Tannins			60.72 a	58.57 a	34.04 c	44.51 b

<sup>a</sup> Average based on original data. <sup>b</sup> Retention index. <sup>c</sup> I (site 1,  $n = 7$ ); II (sites 2, 3 and 6,  $n = 18$ ); III (site 4,  $n = 7$ ); IV (site 5,  $n = 7$ ). <sup>d</sup> Rank and <sup>e</sup> arcsine-transformed in ANOVA analysis (see Experimental section). t = trace (< 0.05%). Averages followed by the same letter in the rows did not share significant differences at 5% probability by Tukey's test.

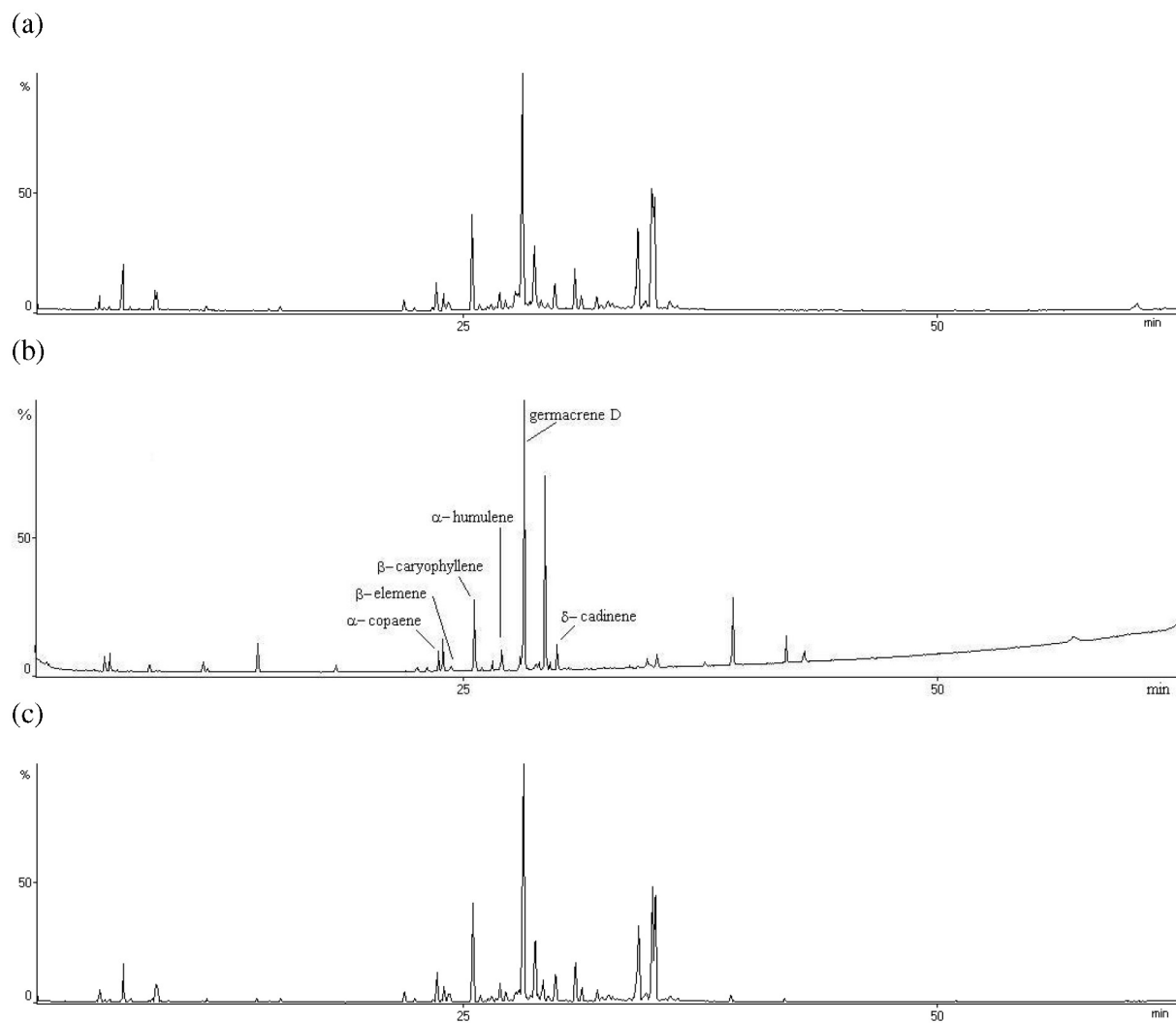
**Table S5.** Chemical characteristics<sup>a</sup> of *M. cauliflora* clustered sampling sites

Soil parameter	Clustered sampling sites			
	I	II	III	IV
Clay (%)	16.0 c	28.2 b	28.2 b	42.0 a
Silt (%)	16.5 a	13.3 a	13.3 a	13.5 a
Sand (%)	67.5 a	58.5 a	58.5 a	44.5 a
Cu (mg dm <sup>-3</sup> )	0.9 ab	1.1 a	1.1 ab	0.5 b
Fe <sup>b</sup> (mg dm <sup>-3</sup> )	44.3 ab	106.4 a	106.4 ab	24.1 b
Mn (mg dm <sup>-3</sup> )	17.4 b	22.8 b	22.8 a	34.1 ab
Zn (mg dm <sup>-3</sup> )	0.6 b	1.0 b	1.0 a	2.6 a
Organic matter (%)	1.1 b	1.6 ab	1.6 ab	2.9 a
pH	5.0 a	4.9 a	4.9 a	5.2 a
P <sup>b</sup> (mg dm <sup>-3</sup> )	0.3 a	0.4 a	0.4 a	1.2 a
K (mg dm <sup>-3</sup> )	35.0 d	37.0 c	37.0 a	64.0 b
Ca (mg dm <sup>-3</sup> )	1.2 b	1.3 b	1.3 a	4.5 a
Mg (mg dm <sup>-3</sup> )	0.3 b	0.4 b	0.4 a	1.0 a
H+Al (mg dm <sup>-3</sup> )	2.6 a	2.3 a	2.3 a	2.6 a
Al (mg dm <sup>-3</sup> )	0.1 a	0.0 a	0.0 a	0.0 a
CTC (mg dm <sup>-3</sup> )	4.1 b	4.0 b	4.0 a	8.2 a

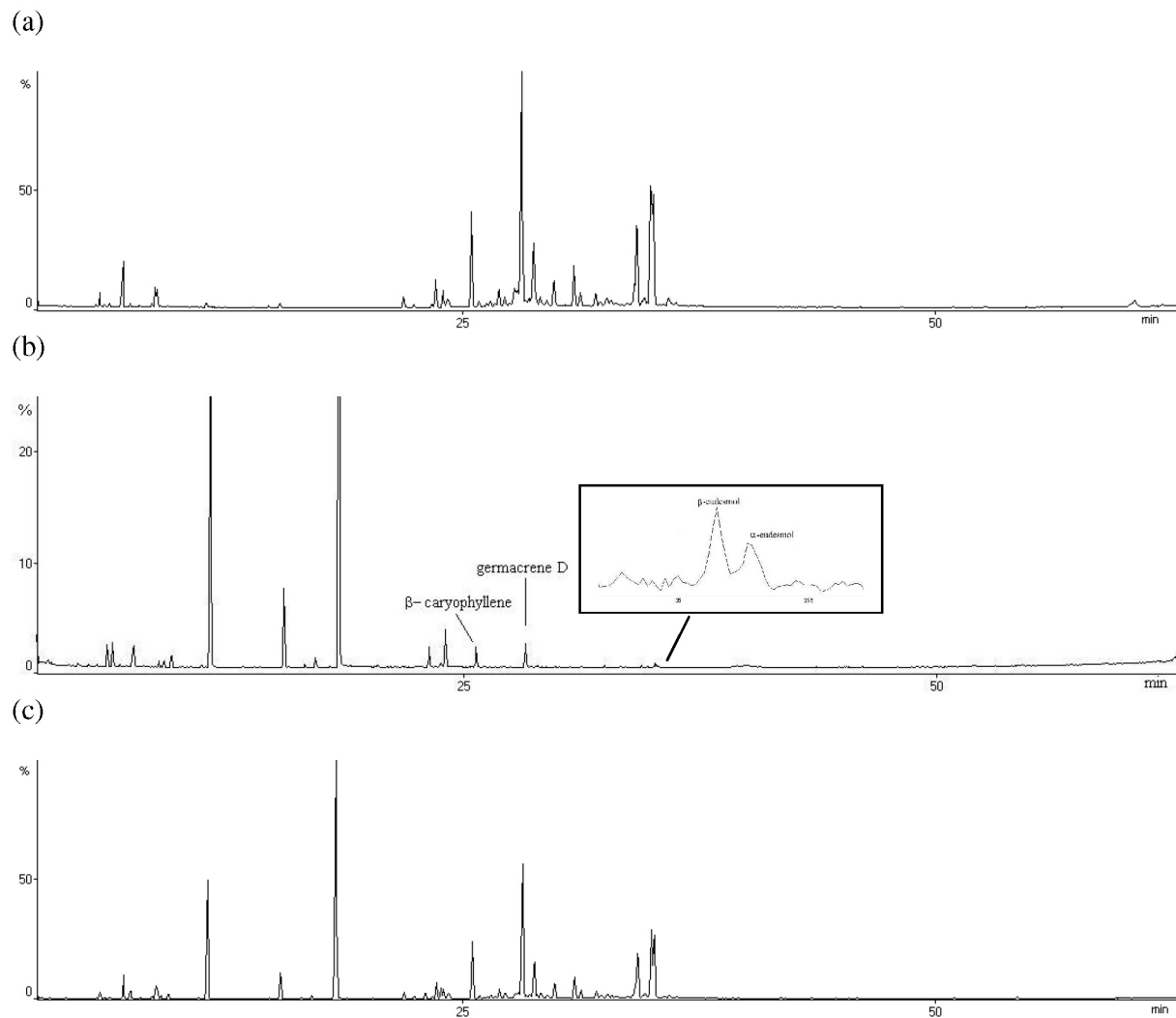
<sup>a</sup> Average based on original data. <sup>b</sup> Rank-transformed in ANOVA analysis (see Experimental section). Averages followed by the same letter in the rows did not share significant differences at 5% probability by Tukey's test.



**Figure S1.** (a) GC/MS of *M. cauliflora* leaves essential oil; (b) GC/MS standards; (c) Co-injection of both (a + b).



**Figure S2.** (a) GC/MS of *M. cauliflora* leaves essential oil; (b) GC/MS of ylang-ylang essential oil; (c) Co-injection of both (a + b).



**Figure S3.** (a) GC/MS of *M. cauliflora* leaves essential oil; (b) GC/MS of sage clary essential oil; (c) Co-injection of both (a + b).