J. Braz. Chem. Soc., Vol. 23, No. 4, S1-S5, 2012.
Printed in Brazil - ©2012 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Supplementary Information

Influence of Spatial, Edaphic and Genetic Factors on Phenols and Essential Oils of *Myrciaria cauliflora* Fruits

Alessandra R. Duarte,[a] Suzana C. Santos,[a] José C. Seraphin[b] and Pedro H. Ferri*,[a]

[a]Laboratório de Bioatividade Molecular, Instituto de Química and [b]Núcleo de Estatística Aplicada, Instituto de Matemática e Estatística, Universidade Federal de Goiás, CP 131, 74001-970 Goiânia-GO, Brazil

Table S1. Cumulative percentage of essential oil constituents from *M. cauliflora* fruits according to carbon skeletons

Carbon skeleton	Sampling sites					
	S1	S2	S3	S4	S5	S6
Pinane	1.80 a	1.56 a	1.60 a	1.52 a	1.40 a	1.75 a
Myrcane	7.02 a	7.28 a	6.18 a	5.63 a	6.90 a	5.37 a
Mentane	8.45 a	7.30 abc	6.54 abc	5.04 c	6.00 bc	7.92 ab
Elemane	0.40 ab	0.40 b	0.74 ab	0.68 ab	0.80 a	0.45 ab
Copaane	0.56 ab	0.10 b	0.85 a	1.04 a	0.80 a	0.91 a
Caryophyllane	4.40 b	4.48 ab	5.66 ab	6.24 a	5.40 ab	5.21 ab
Humulane	0.64 a	0.81 a	0.94 a	0.97 a	0.90 a	0.80 a
Germacrane	4.96 bc	5.07 bc	5.08 bc	6.34 a	5.80 ab	3.99 c
Bicyclogermacrane	3.16 a	3.24 a	3.74 a	3.95 a	3.60 a	3.09 a
Cadinane	1.82 b	2.13 b	2.29 ab	3.41 a	2.30 ab	2.37 ab
Elemane	1.07 bc	1.11 abc	1.11 ab	0.36 d	0.80 cd	1.35 a
Aromadendrane	0.94 b	1.23 ab	1.55 a	1.63 a	1.50 a	1.40 ab
Cubebane	0.30 a	0.92 a	0.85 a	1.30 a	1.10 a	0.64 a
Eudesmane	64.5 a	64.4 a	62.9 a	61.9 a	63.0 a	64.7 a
Total	100	100	100	100	100	100

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

*e-mail: pedro@quimica.ufg.br

Table S2. Percentages in essential oil constituents, phenolics, reducing sugar and fruit acidity of *M. cauliflora* according to clustered sampling sites

Constituent	RI	Clusters			
		I	II	III	IV
α-Pinene	933	0.66 a	0.48 a	0.59 a	0.81 a
β-Pinene	976	0.99 a	0.95 a	0.99 a	0.94 a
β-Myrcene	990	0.46 a	0.21 a	0.28 a	0.32 a
α-Phellandrene	1005	0.40 a	0.25 a	0.34 a	0.34 a
Limonene	1028	5.01 a	3.38 b	3.96 ab	5.00 ab
1,8-Cineole	1031	0.52 b	0.12 c	0.26 bc	0.92 a
(Z)-β-Ocimene	1035	2.22 a	1.57 b	1.74 ab	1.54 b
(E)-β-Ocimene	1046	3.12 a	3.24 a	3.26 a	2.45 a
Linalool	1100	1.24 a	1.12 ab	0.80 b	1.04 ab
α-Terpineol	1191	1.81 a	1.67 a	1.84 a	1.63 a
δ-Elemene	1338	0.39 b	0.73 a	0.72 ab	0.45 ab
α-Copaene	1377	0.32 b	0.88 a	0.83 a	0.90
(E)-Caryophyllene	1421	4.36 b	5.70 a	5.53 a	5.18 ab
α-Humulene	1455	0.71 a	0.92 a	0.92 a	0.80 a
Germacrene D	1483	4.85 b	5.70 a	4.89 ab	3.97 b
δ-Selinene	1492	0.63 b	0.78 b	0.76	3.60 a
Bicyclogermacrene	1498	3.15 b	3.71 a	3.65 ab	3.08 ab
δ-Cadinene	1525	1.73 b	2.25 a	2.23 ab	1.87 ab
Elemol	1550	1.07 a	0.57 b	1.10 b	1.34
Germacrene B	1559	0.08 a	0.25 a	0.09 a	t
Globulol	1586	1.07 b	1.53 a	1.52 a	1.40 ab
Cubeban-11-ol	1596	0.60 a	1.20 a	0.84 a	0.64 a
10-*epi*-γ-Eudesmol	1622	1.65 a	1.64 a	1.79 a	0.61 b
γ-Eudesmol	1637	39.40 a	36.47 bc	36.95 b	34.36 c
Cubenol	1645	0.21 a	0.55 a	t	0.49 a
β-Eudesmol	1654	7.90 b	7.91 b	7.99 b	10.49 a
α-Eudesmol	1658	13.75 b	14.32 ab	14.10 ab	15.38 a
Monoterpenes		16.42 a	13.00 a	14.06 a	14.98 a
Monoterpene hydrocarbons		12.85 a	10.08 a	11.16 a	11.40 a
Oxygenated monoterpenes		3.57 a	2.92 a	2.91 a	3.58 a
Sesquiterpenes		81.86 a	85.10 a	83.94 a	84.58 a
Sesquiterpene hydrocarbons		16.22 b	20.91 a	19.63 ab	19.86 ab
Oxygenated sesquiterpenes		65.64 a	64.19 a	64.30 a	64.72 a
Total phenols / (mg mL^{-1})		1.73 a	1.43 ab	1.28 ab	1.20 b
Tannins / (mg mL^{-1})		0.62 a	0.33 b	0.40 b	0.47 ab
Anthocyanins / (mg mL^{-1})		0.28 a	0.23 a	0.22 a	0.13 b
Reducing sugar / (g *per* 100 g)		54.53 b	41.34 c	58.97 ab	66.81 a
Fruit acidity / (g *per* 100 g)		8.71a	8.34 ab	7.67 b	5.79 c

RI = Retention index; 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 S3. Percentages in essential oil constituents from *M. cauliflora* fruits in clustered sampling according to carbon skeletons

Carbon skeleton	Clusters			
	I	II	III	IV
Pinane	1.68 a	1.45 a	1.60 a	1.75 a
Myrcane	7.15 a	6.26 a	6.18 a	5.37 a
Mentane	7.88 a	5.53 b	6.54 ab	7.92 a
Elemane	0.40 b	0.75 a	0.74 ab	0.45 ab
Copaane	0.33 b	0.90 a	0.85 a	0.91 a
Caryophyllane	4.44 b	5.82 a	5.66 ab	5.21 ab
Humulane	0.72 a	0.94 a	0.94 a	0.80 a
Germacrane	5.01 b	6.07 a	5.08 b	3.99 c
Bicyclogermacrane	3.20 b	3.78 a	3.74 ab	3.09 b
Cadinane	1.98 a	2.87 a	2.29 a	2.37 a
Elemane	1.09 b	0.58 c	1.11 ab	1.35 a
Aromadendrane	1.09 b	1.56 a	1.55 a	1.40 ab
Cubebane	0.61 a	1.22 a	0.85 a	0.64 a
Eudesmane	64.42 a	62.29 a	62.87 a	64.72 a

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

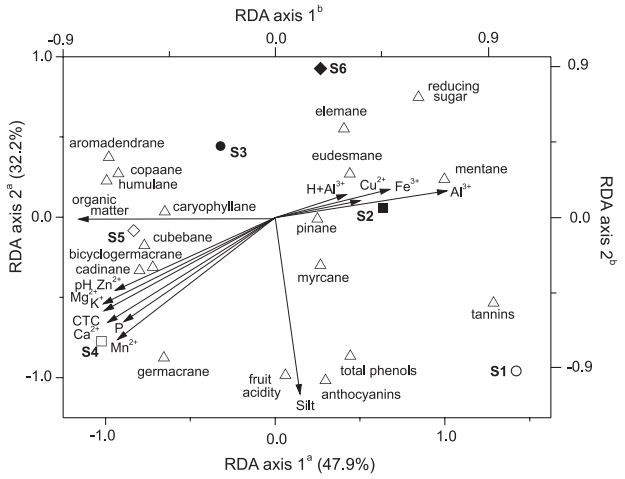

Figure S1. RDA ordination triplot of the first two axes showing distribution of *M. cauliflora* sampling sites (S1: ○, S2: ■, S3: ●, S4: □, S5: ◇, S6: ◆). Soil parameters were treated as environmental variables and are represented by long arrows from the origin. Oil constituents according to carbon skeletons, phenolics, reducing sugar and fruit acidity contents are represented by triangles instead of arrows and the triangle position is multiplied by 10 for clear visualization. [a]Axes refer to scores from samples; [b]axes refer to loadings from variables and values in brackets refer to the explained variance on each canonical axis.

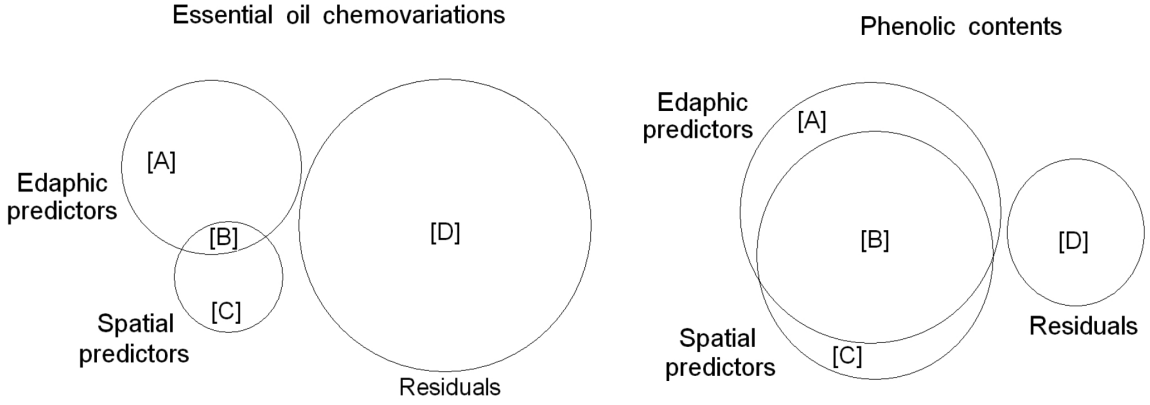

Figure S2. Venn diagrams illustrating percentages of variation in *M. cauliflora* fruit chemical composition that are attributable to two sets of explanatory variables: edaphic and spatial predictors. The overlap of the circles represents variation within and shared between sets of explanatory variables. Capital letters in brackets correspond to variation explained by each component of variation according to Table 2.

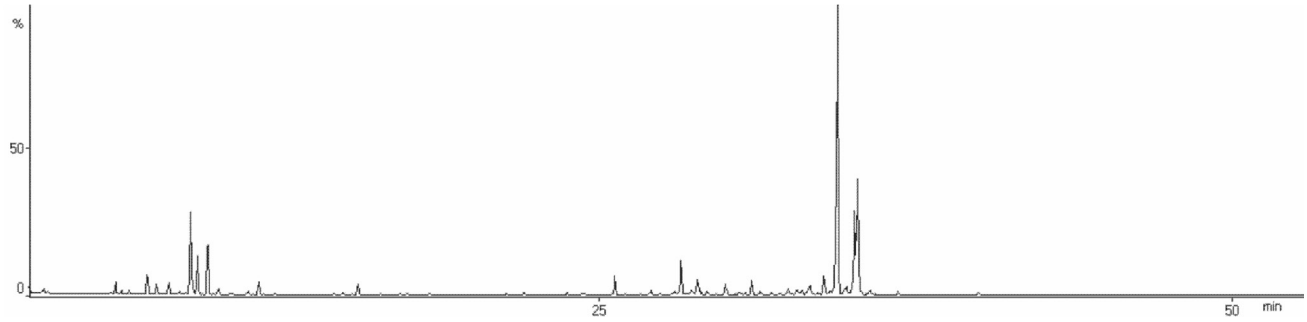

Figure S3. Total ion chromatogram (TIC) of representative essential oil from *M. cauliflora* fruit collected from S1 soil.

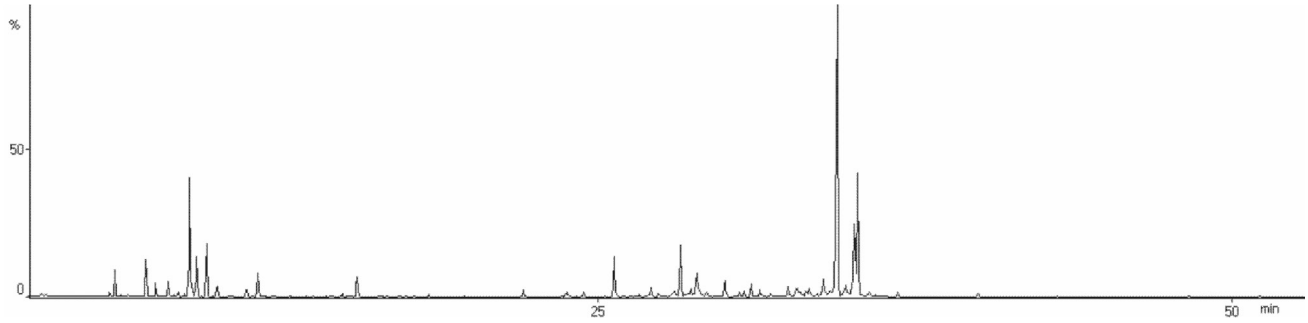

Figure S4. Total ion chromatogram (TIC) of representative essential oil from *M. cauliflora* fruit collected from S2 soil.

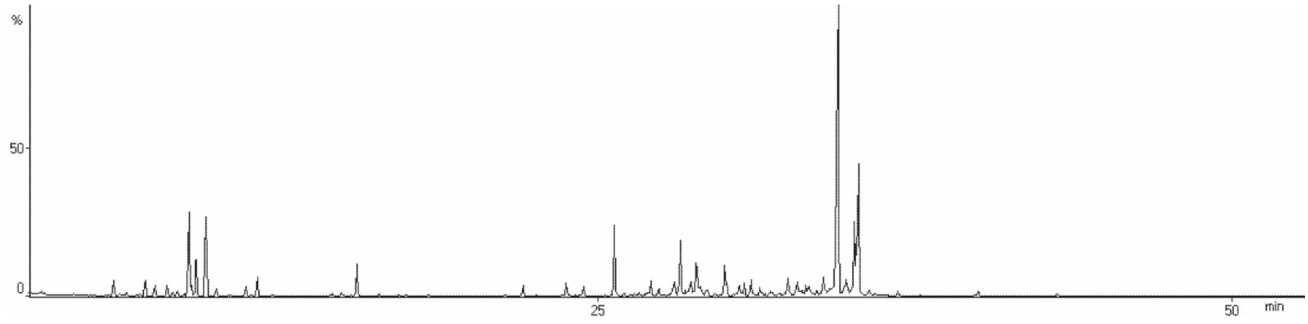

Figure S5. Total ion chromatogram (TIC) of representative essential oil from *M. cauliflora* fruit collected from S3 soil.

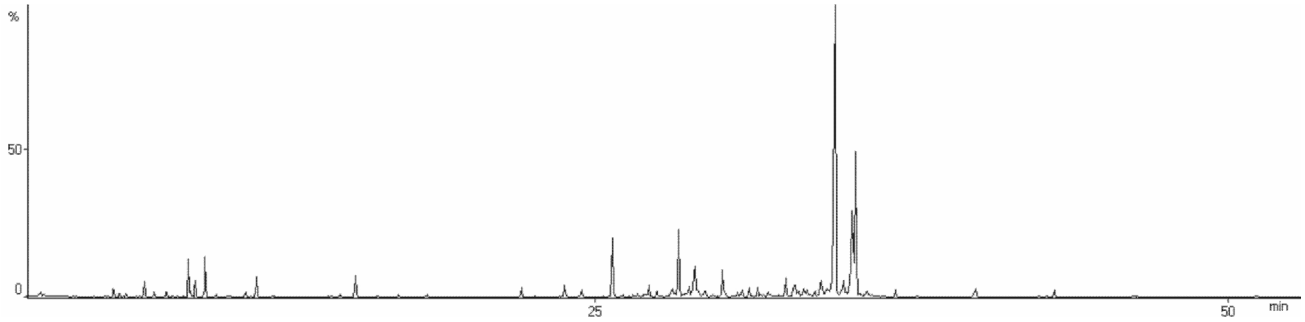

Figure S6. Total ion chromatogram (TIC) of representative essential oil from *M. cauliflora* fruit collected from S4 soil.

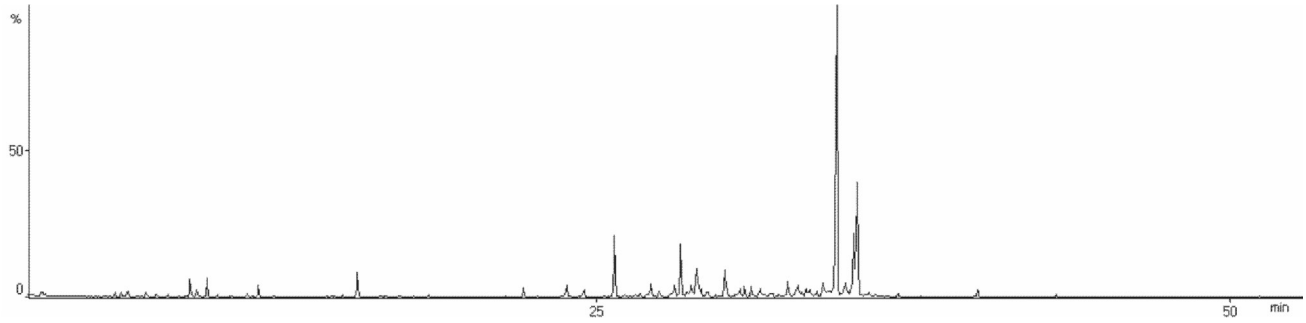

Figure S7. Total ion chromatogram (TIC) of representative essential oil from *M. cauliflora* fruit collected from S5 soil.

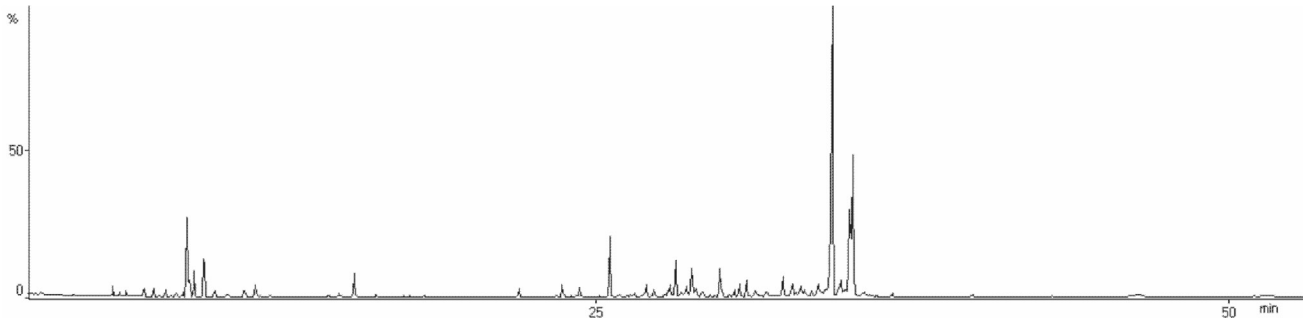

Figure S8. Total ion chromatogram (TIC) of representative essential oil from *M. cauliflora* fruit collected from S6 soil.