

Genetic and Environmental Influence on Essential Oil Composition of *Eugenia dysenterica*

Alessandra R. Duarte,^a Ronaldo R. Naves,^b Suzana C. Santos,^a
 José C. Seraphin^c and Pedro H. Ferri^{*,a}

^aInstituto de Química, ^bEscola de Agronomia e de Engenharia de Alimentos and ^cInstituto de Matemática e Estatística, Universidade Federal de Goiás, CP 131, 74001-970 Goiânia-GO, Brazil

Table S1. Percentages^a of essential oil constituents in *E. dysenterica* clustered samples from wild and adjacently-cultivated individuals from seeds originated from Senador Canedo (SC) and Campo Alegre de Goiás (CA) to which subclusters IA/IB and cluster II it belongs

Constituent	Clusters		
	IA	IB	II
1 α -Pinene	9.0 $\pm$ 2.5 a	6.6 $\pm$ 3.6 a	6.4 $\pm$ 3.3 a
2 β -Pinene	9.3 $\pm$ 2.8 a	5.9 $\pm$ 3.8 ab	4.1 $\pm$ 2.3 b
3 Myrcene ^b	1.0 $\pm$ 0.5 a	3.8 $\pm$ 4.4 a	0.74 $\pm$ 0.58 a
4 Limonene ^b	7.8 $\pm$ 5.9 a	12 $\pm$ 10 a	1.9 $\pm$ 1.5 c
5 (Z)- β -Ocimene	5.9 $\pm$ 4.5 a	t	2.4 $\pm$ 3.2 b
6 (E)- β -Ocimene	1.9 $\pm$ 1.1 a	0.05 $\pm$ 0.10	0.57 $\pm$ 0.65 b
7 Linalool	0.50 $\pm$ 0.15 a	0.04 $\pm$ 0.06 a	0.40 $\pm$ 0.31 a
8 α -Terpineol	0.27 $\pm$ 0.24 ab	0.16 $\pm$ 0.24 b	0.80 $\pm$ 0.55 a
9 α -Copaene ^c	2.3 $\pm$ 1.3 b	0.44 $\pm$ 0.75 c	9.6 $\pm$ 3.3 a
10 β -Caryophyllene	18 $\pm$ 7 a	16 $\pm$ 7 a	24 $\pm$ 8 a
11 α -Guaiene ^b	0.40 $\pm$ 0.43 a	0.51 $\pm$ 1.2 a	1.6 $\pm$ 2.6 a
12 6,9-Guaiadiene ^b	1.6 $\pm$ 1.0 a	1.1 $\pm$ 0.3 a	0.18 $\pm$ 0.38 b
13 α -neo-Clovane	1.9 $\pm$ 0.8 b	3.1 $\pm$ 0.7 a	0.36 $\pm$ 0.49 c
14 α -Humulene	11 $\pm$ 5 a	7.3 $\pm$ 8.9 a	13 $\pm$ 7 a
15 γ -Murolene	0.47 $\pm$ 0.29 a	0.40 $\pm$ 0.34 a	0.70 $\pm$ 0.40 a
16 α -Amorphene	0.03 $\pm$ 0.05	t	t
17 β -Selinene ^c	0.75 $\pm$ 1.2 a	0.15 $\pm$ 0.33 a	0.46 $\pm$ 0.74 a
18 δ -Selinene ^b	2.1 $\pm$ 2.7 a	0.19 $\pm$ 0.43 a	2.1 $\pm$ 4.4 a
19 α -Selinene	0.63 $\pm$ 1.1 a	t	0.59 $\pm$ 0.85 a
20 Bicyclogermacrene	0.53 $\pm$ 0.20 a	0.54 $\pm$ 0.61 a	0.04 $\pm$ 0.14
21 α -Murolene ^b	2.6 $\pm$ 2.6 a	0.06 $\pm$ 0.13 a	0.55 $\pm$ 0.35 a
22 α -Bulnesene ^b	0.18 $\pm$ 0.19 a	0.79 $\pm$ 1.9 a	2.1 $\pm$ 3.4 a
23 δ -Amorphene	0.13 $\pm$ 0.13 a	0.10 $\pm$ 0.23 a	t
24 γ -Cadinene	11 $\pm$ 5 b	27 $\pm$ 5 a	0.81 $\pm$ 1.6 c
25 7- <i>epi</i> - α -Selinene	0.87 $\pm$ 1.4 a	t	1.1 $\pm$ 2.3 a
26 δ -Cadinene ^c	4.4 $\pm$ 1.9 b	2.1 $\pm$ 1.7 b	13 $\pm$ 5 a
27 Caryophyllene oxide	1.6 $\pm$ 0.7 b	7.4 $\pm$ 5.1 a	4.5 $\pm$ 3.2 b
28 Humulene epoxide II ^c	0.82 $\pm$ 0.42 a	1.2 $\pm$ 1.8 a	2.7 $\pm$ 2.0 a
29 Muurola-4,10(14)-dien-1 β -ol ^c	0.52 $\pm$ 0.62 b	0.30 $\pm$ 0.47 b	1.8 $\pm$ 1.2 a
Monoterpene hydrocarbons	35 $\pm$ 8 a	29 $\pm$ 11 a	16 $\pm$ 6 b
Oxygenated monoterpenes	0.78 $\pm$ 0.28 a	0.19 $\pm$ 0.27 b	1.2 $\pm$ 0.6 a
Sesquiterpene hydrocarbons	59 $\pm$ 8 b	60 $\pm$ 11 b	70 $\pm$ 7 a
Oxygenated sesquiterpenes ^c	2.9 $\pm$ 1.3 b	8.9 $\pm$ 5.5 a	9.0 $\pm$ 4.3 a

^aAverage based on original data $\pm$ standard deviation. ^bRank- and ^carcsine-transformed in ANOVA analysis. t: trace. IA (n = 6): only cultivated samples from SC seed origin; IB (n = 6): majority wild samples from SC origin; II (n = 19): all samples from CA origin regardless of population (see text). Percentages followed by the same letter in a row did not share significant differences at 5% probability by Tukey's test.

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

Table S2. Soil minerals and climatic data^a in sampling sites of *E. dysenterica* clustered samples from wild and adjacently-cultivated individuals from seeds originated from Senador Canedo (SC) and Campo Alegre de Goiás (CA) to which subclusters IA/IB and cluster II it belongs

Edapho-climatic variable	Clusters		
	IA	IB	II
P / (mg dm ⁻³)	2.2 ± 0.0	1.4 ± 0.4 b	2.0 ± 0.3 a
Zn ^b / (mg dm ⁻³)	1.4 ± 0.0	4.5 ± 1.5 a	1.8 ± 0.7 b
Cu ^b / (mg dm ⁻³)	1.4 ± 0.0	3.4 ± 1.0 a	1.6 ± 0.4 b
Fe / (mg dm ⁻³)	34.8 ± 0.0	47.3 ± 6.1 a	41.8 ± 10.6 a
Mn / (mg dm ⁻³)	8.3 ± 0.0	14.0 ± 2.8 a	10.1 ± 2.7 b
Temperature ^b / (°C)	19.3 ± 0.0	24.6 ± 2.6 a	20.2 ± 1.3 b
Precipitation / mm	0.0 ± 0.0	12.5 ± 6.1 a	3.2 ± 4.8 b

^aAverage based on original data ± standard deviation. ^bRank-transformed in ANOVA analysis. IA (n = 6): only cultivated samples from SC seed origin; IB (n = 6): majority wild samples from SC origin; II (n = 19): all samples from CA origin regardless of population (see text). Percentages followed by the same letter in a row did not share significant differences at 5% probability by Tukey's test.

**Figure S1.** Map of Goiás State in central Brazilian Cerrado, showing the locations of *E. dysenterica* sampling sites: Senador Canedo (SC) and Campo Alegre de Goiás (CA), as well as Corumbá River, which geographically separates SC wild from CA wild populations. UFG's experimental field is the location of the adjacently-cultivated samples originated from wild plants' seed propagations.

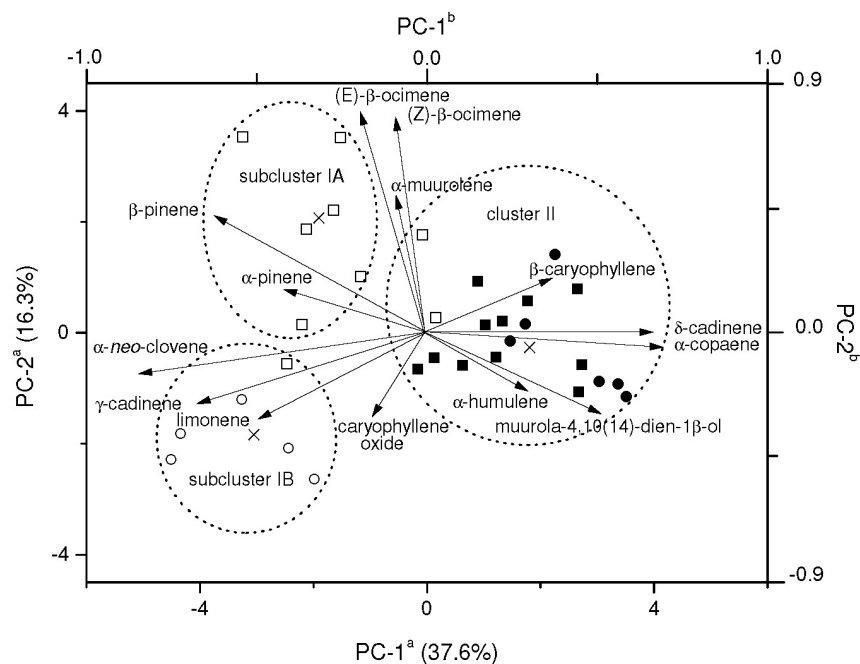


Figure S2. Principal component scatterplot of *E. dysenterica* wild samples (circle symbols) and adjacently-cultivated individuals (square symbols) from seeds originated from Senador Canedo (SC; unshaded symbols) and Campo Alegre de Goiás (CA; shaded symbols) to which subclusters IA/IB and cluster II it belongs. ^aAxes refer to scores from samples. ^bAxes refer to loadings from oil constituents represented as long arrows from origin. Crosses represent cluster centroids and values between parentheses refer to the explained variance on each principal component.

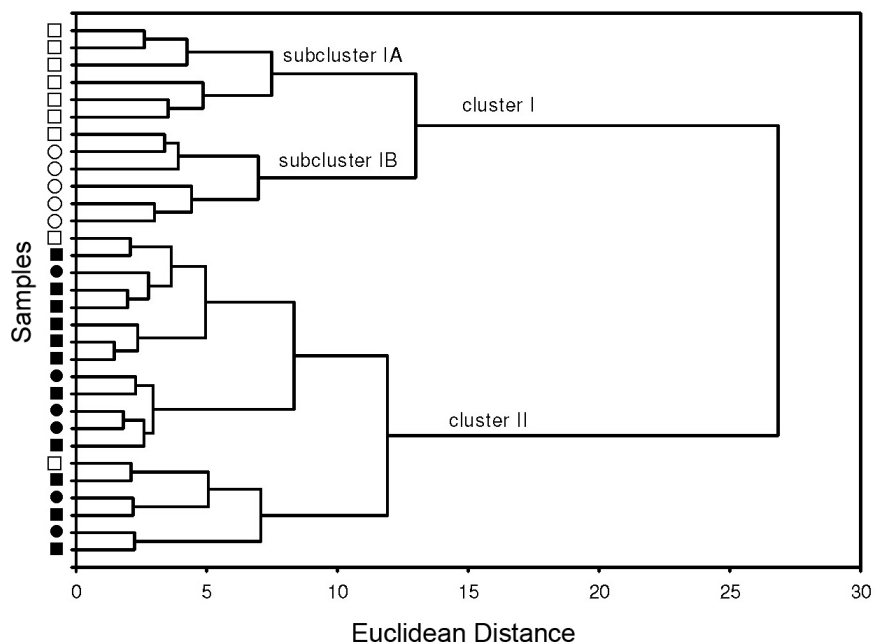


Figure S3. Dendrogram representing chemical composition similarity relationships among 31 *E. dysenterica* samples to which cluster it belongs: I, Senador Canedo (unshaded symbols); II, Campo Alegre de Goiás (shaded symbols), collected from wild (circle symbols) and adjacently-cultivated (square symbols) populations.

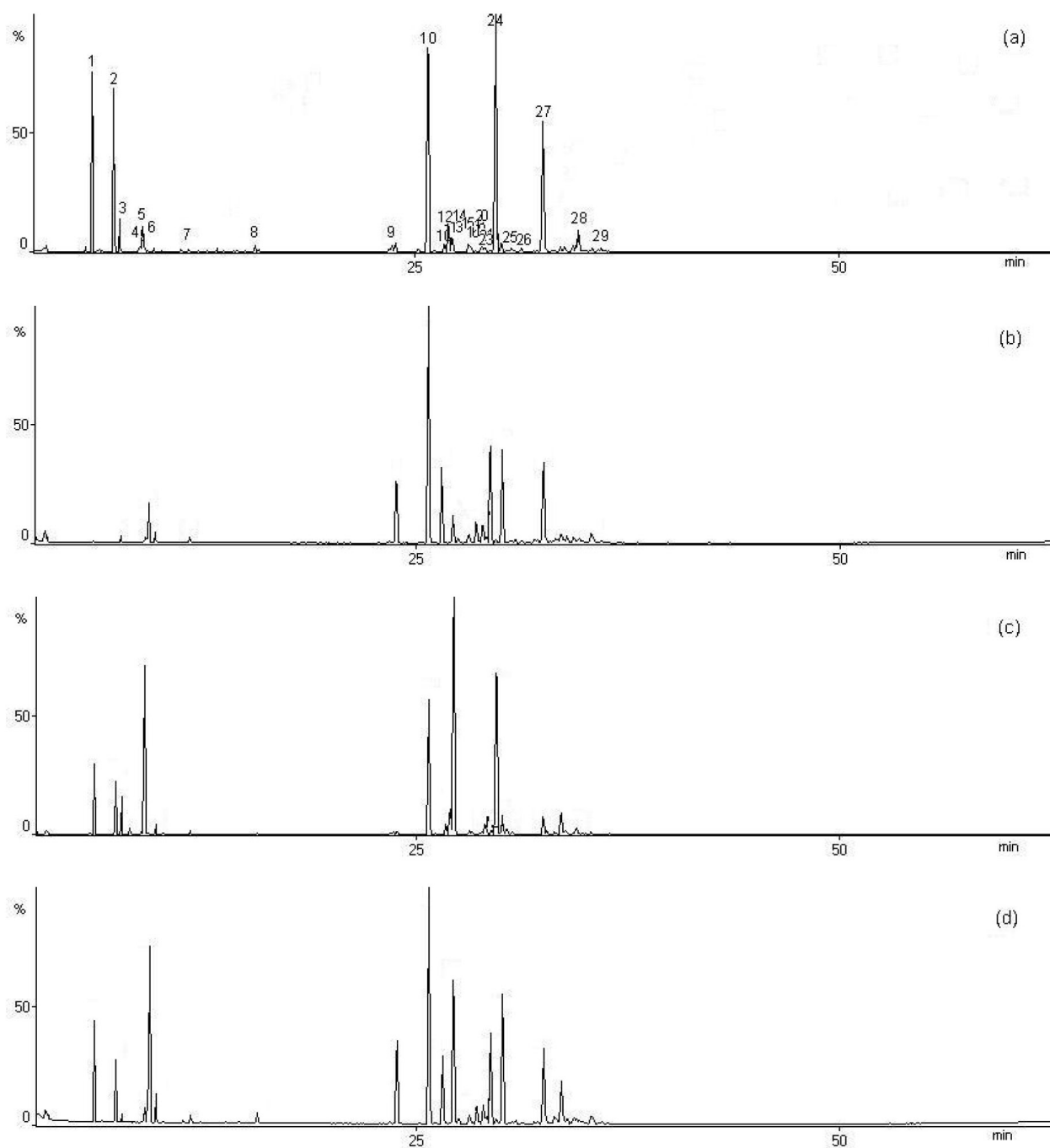
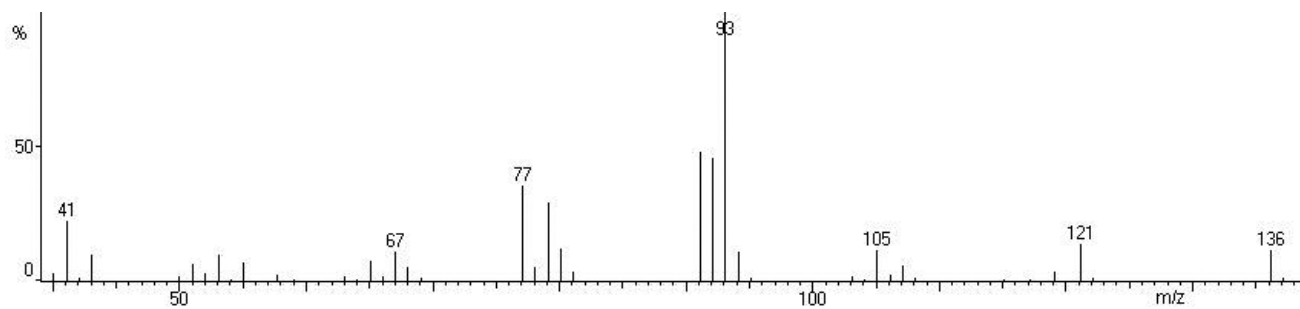
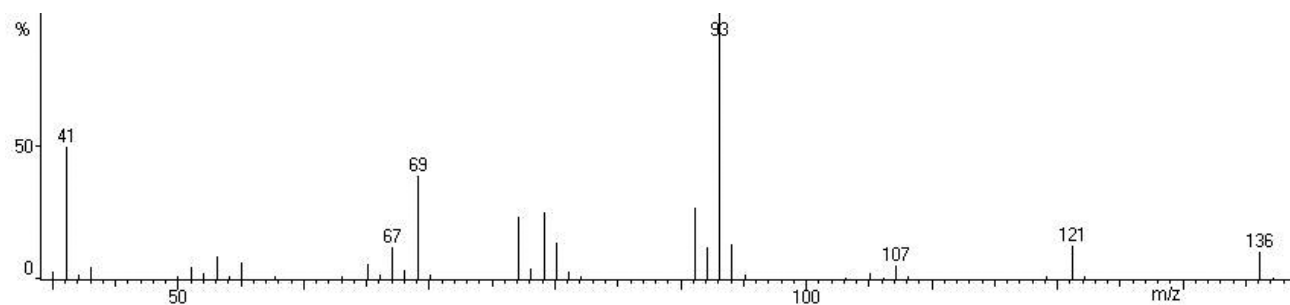
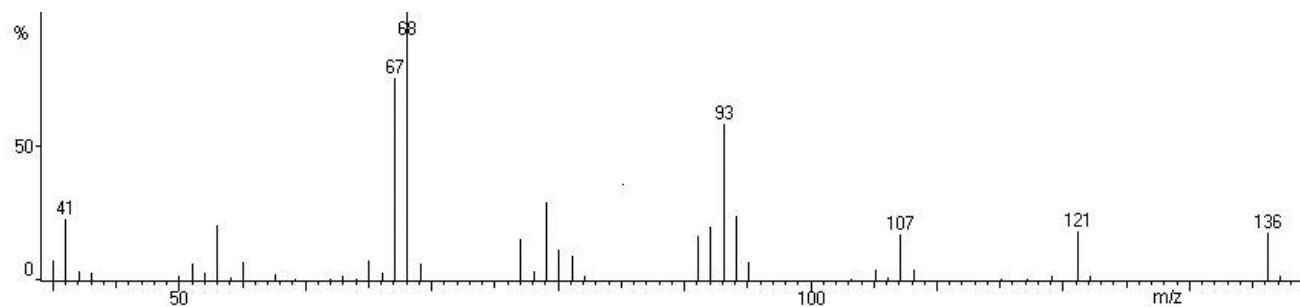
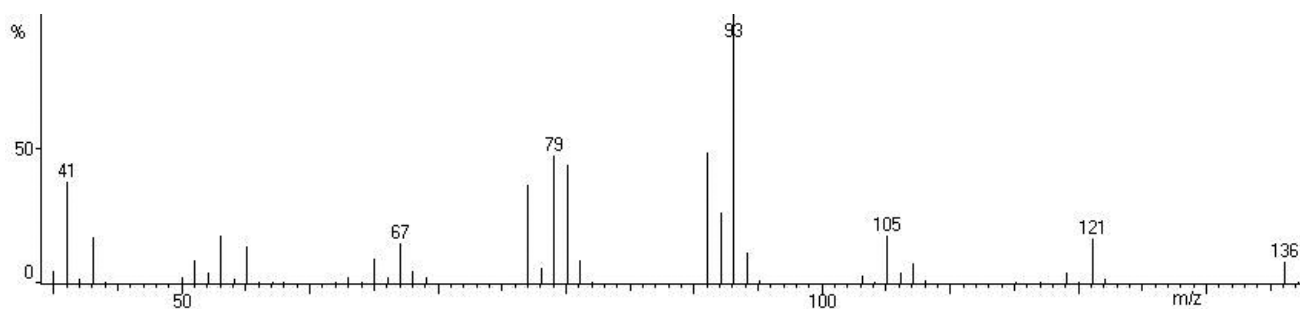


Figure S4. Total ion chromatograms (TIC) of leaf essential oils from *E. dysenterica* : wild samples collected in (a) Senador Canedo (SC) and (b) Campo Alegre de Goiás (CA); cultivated samples collected in SC (c) and CA (d).

**Figure S5.** Mass spectrum of α -pinene (1).**Figure S6.** Mass spectrum of β -pinene (2).**Figure S7.** Mass spectrum of limonene (4).**Figure S8.** Mass spectrum of (*Z*)- β -ocimene (5).

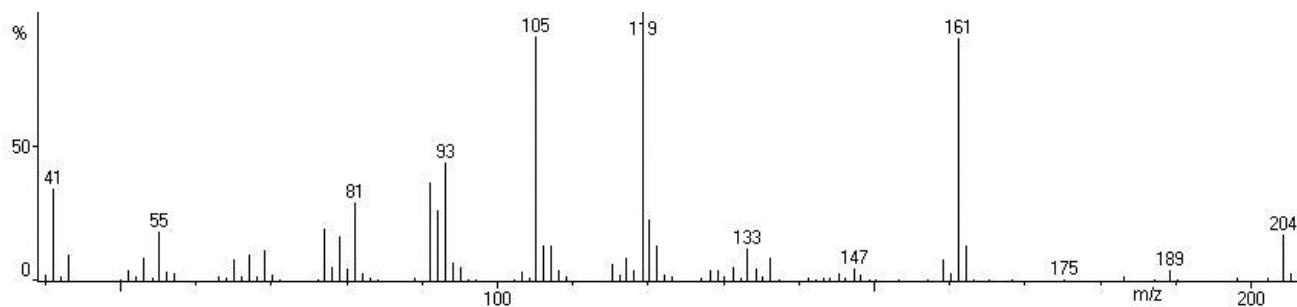


Figure S9. Mass spectrum of α -copaene (9).

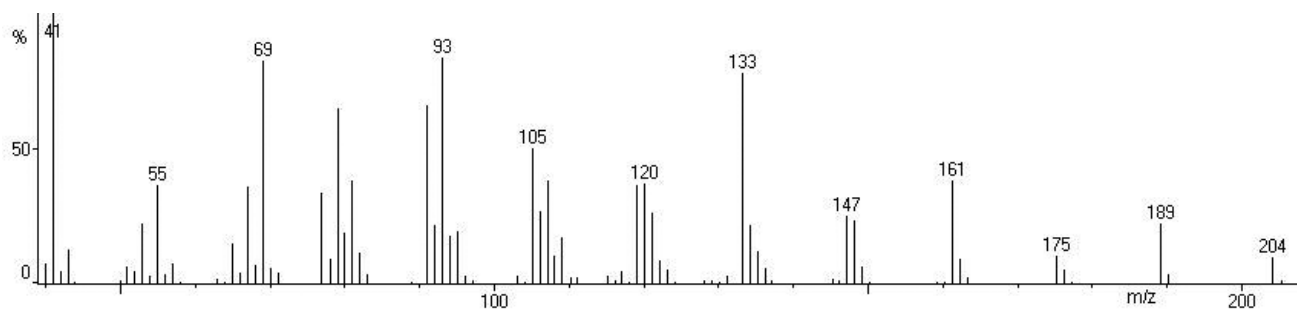


Figure S10. Mass spectrum of β -caryophyllene (10).

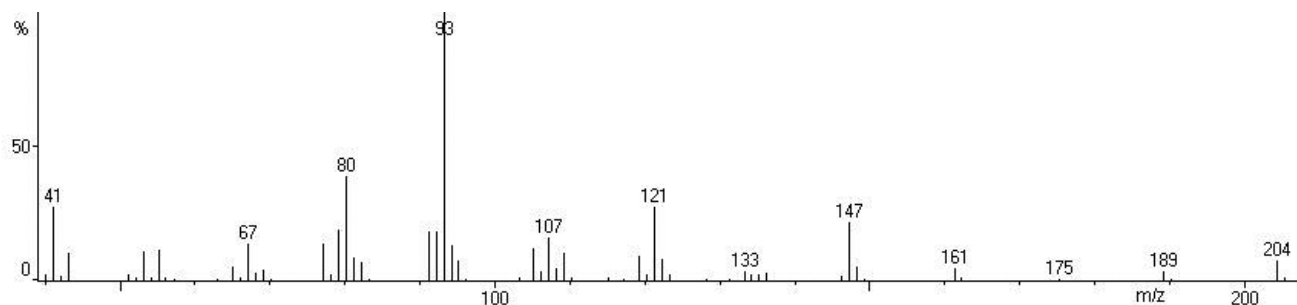


Figure S11. Mass spectrum of α -humulene (14).

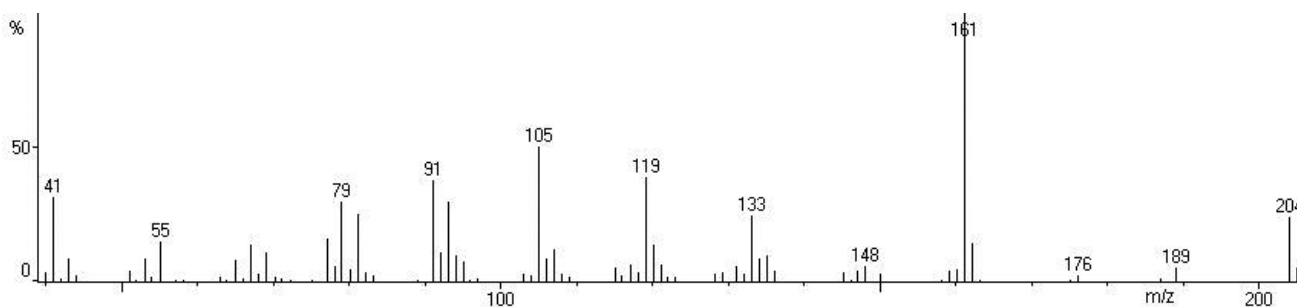
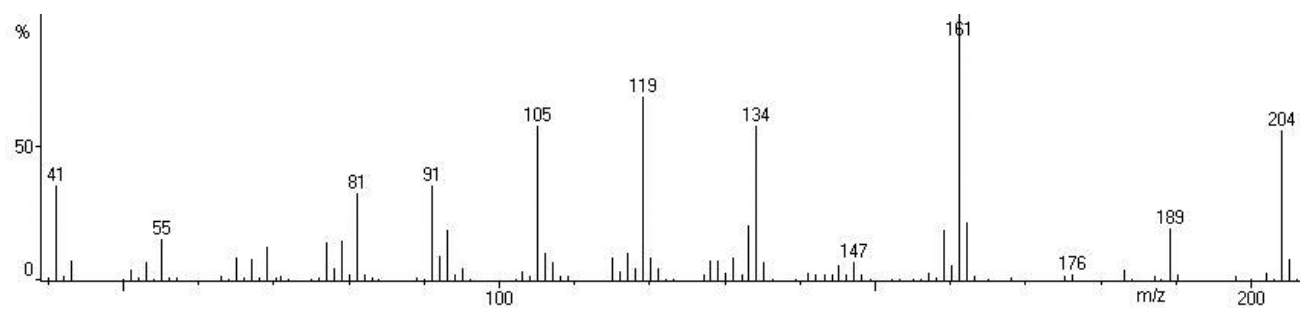
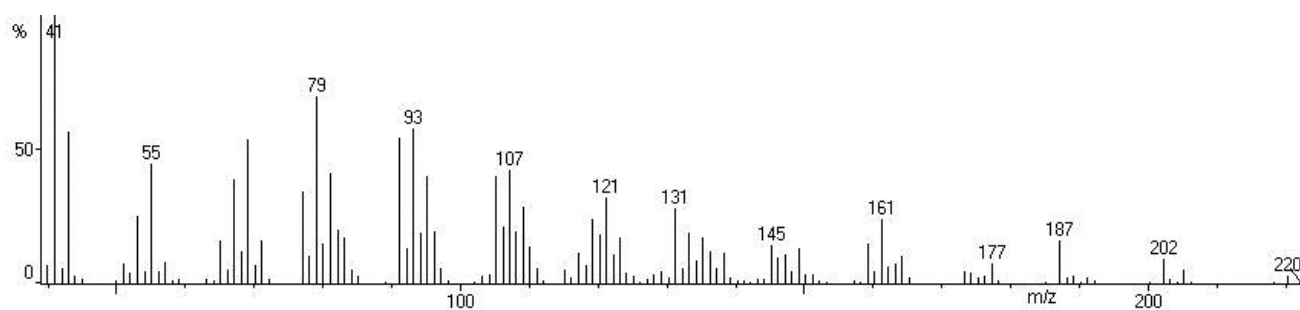


Figure S12. Mass spectrum of γ -cadinene (24).

**Figure S13.** Mass spectrum of δ -cadinene (26).**Figure S14.** Mass spectrum of caryophyllene oxide (27).