

Supporting Information

Rec. Nat. Prod. 15:4 (2021) 312-323

Metabolic Correlations of *Salvia dugesii* Fernald and *Salvia gesneriflora* Lindl. & Paxton with Native *Salvia* Plants from Four Continents Using Essential Oils Compositions

Mónica A. Calderón-Oropeza^{1,4}, Ernesto Ramírez-Briones¹,
Gabriela Rodríguez-García¹, José L. Salvador-Hernández¹,
Brenda Y. Bedolla-García², Sergio Zamudio³,
Luis D. Maldonado-Bonilla⁴, Rosa E. del Río^{1*} and
Mario A. Gómez-Hurtado¹

¹*Instituto de Investigaciones Químico-Biológicas, Universidad Michoacana de San Nicolás de Hidalgo, Ciudad Universitaria, Morelia, Michoacán 58030, Mexico*

²*Instituto de Ecología, A.C. Centro Regional del Bajío, Pátzcuaro, Michoacán 61600, Mexico*

³*Apartado Postal 392, Pátzcuaro, Michoacán 61608, Mexico*

⁴*Instituto de Genética, Universidad del Mar Campus Puerto Escondido, Carretera Vía Sola de Vega km 1.5, San Pedro Mixtepec, Juquila, Oaxaca 71980, Mexico*

Table of Contents	Page
Table S1: Chemical composition of essential oils of the twelve analyzed <i>Salvia</i> plants	1
Table S2: Chemical composition of essential oils of the twelve analyzed <i>Salvia</i> plants, according to their structural skeleton	10

Table S1. Chemical composition of essential oils of the twelve analyzed *Salvia* plants

Number	Compound	Structural Skeleton	Composition (%)										
			A	B	C	D	E	F	G	H	I	J	K
1	Spathulenol	IX	7.63	4.74									
2	β -Bourbonene	XVII	1.60	1.01	5.60		2.90		0.29				
3	δ -Cadinene	X	4.80		0.80				0.45	2.30	1.70		
4	9-Methoxy calamene	X	0.73										
5	Aromadendrene	IX	2.95	1.09			0.10		0.08				1.22
6	Bornyl acetate	XXII	3.35	5.80					1.05				0.50
7	Camphor	XXII		1.00				6.80	25.14				0.08
8	Caryophyllene	V	10.04	15.68	27.70	2.00			3.30		11.55	14.00	0.88
9	Caryophyllene oxide	V	5.84	2.54	4.20		2.00	1.10	0.06	3.00	0.20	3.38	15.54
10	<i>cis</i> -1-Methyl-4-(1-methylethyl)-2-cyclohexen-1-ol	XXIII		0.73									
11	<i>cis</i> - β -Farnesene	XV	1.47										
12	Diepicedrene-1-oxide	XVI	2.24										
13	Elixene	XIV		1.59									
14	<i>endo</i> -Borneol	XXII	1.06	1.40		0.90		7.60	2.81		1.66		0.55
15	Eugenol	XXIX		1.96					0.28				0.78
16	Geranyl- α -terpinene	XXV		5.49									

17	Germacrene D	XI	4.97	19.50	7.90	0.17	0.20	4.37	
18	Guaiol	IX		2.73	1.50				
19	Hedycaryol	XI		7.57					
20	Humulene	V	4.62	2.30	10.70	3.60	2.48	3.60	0.40
21	Isoalloaromadendrene epoxide	IX	2.23						
22	Isoaromadendrene epoxide	IX	3.38						
23	Ledol	IX		3.20					5.14
24	Phenyl ethyl alcohol	XXIX		2.06					
25	Podocarp-7-en-3-one,13 β -methyl-13-vinyl	XXVI	0.62						
26	Sandaracopimaradiene	XXVI	4.89						
27	Rimuene	XXVI	0.65						
28	Sclareol oxide	XXVII	0.84						
29	Terpinen-4-ol	XXIII		1.06		0.30		0.74	
30	Valeranone	XIII		6.26					
31	Viridiflorol	IX	0.81	0.50	32.40	0.10	7.98	2.20	33.00
32	α -Cedrene	XVI	1.13						
33	α -Copaen-11-ol	VI		3.66					
34	α -Copaene	VI	1.74	1.70		1.10		0.07	
35	α -Pinene	XXI		1.45	0.50	0.50	2.10	6.80	0.84
36	β -Bisabolene	IV	1.48					3.10	4.20

37	β -Cadinene	X	1.20								
38	β -Cubebene	XII	0.81	3.56		0.30					0.62
39	β -Eudesmane	VIII	0.95								
40	<i>7-epi-</i> α -Eudesmol	VIII		3.66	0.70			12.30	0.30		
41	γ -Cadinene	X	1.39		2.00		0.12				5.30
42	γ -Elemene	XIV		7.54							
43	γ -Murolene	X	8.31		0.80						1.84
44	γ -Terpinene	XXIII		1.03	0.20	5.40	0.61				
45	(<i>E</i>)-Nerolidol	XV		1.20				0.20	2.00		
46	(<i>E</i>)- β -Ocimene	XIX			3.00						
47	(<i>Z</i>)-Caryophyllene	V			0.10	3.30					0.91
48	(<i>Z</i>)- β -Ocimene	XIX			1.50						
49	1,8-Cineole	XXIII		0.80	3.10	40.10	14.14	1.80	4.80		0.18
50	14-Hydroxy- δ -Cadinene	X			0.20						
51	14-Hydroxy- δ -Murolene	X			0.10						
52	1- <i>epi</i> -Cubenol	X			0.70						
53	1-Hydroxy-1,7-dimethyl-4-isopropyl-2,7-cyclodecadiene	XI									0.98
54	2-Cyclohexen-1-one,5-methyl-2-(1-methylethyl)-	XXIII									0.14

55	3-Cyclohexen-1-carboxaldehyde, 3,4-dimethyl	XXIX					2.04
56	Acetophenone	XXIX					0.21
57	Allo-aromadendrene	IX		0.30		0.06	
58	Benzaldehyde	XXIX	0.60				
59	Benzene acetaldehyde	XXIX		0.20			
60	Bicyclogermacrene	XI	18.30	1.50	5.40	0.90	
61	Cadalene	X					5.28
62	Calarene	I			0.14		
63	Camphene	XX		0.20	3.00	0.78	1.63
64	Carvacrol	XXIII			0.18		1.20
65	Caryophylla-(14),8(15)-dien-5 α -ol	V	1.00				
66	Widdrol	XVIII					3.54
67	cis-Calamenene	X			0.08		0.73
68	cis-Linalool oxide	XIX					9.60
69	cis-Muurola-3,5-diene	X		0.20			0.19
70	cis-Sabinene hydrate	XXIV		0.10			
71	cis-Thujone	XXIV	7.30		18.83		
72	Cubenol	X		0.10			
73	Cyclohexene, 3-acetoxy-4-(1-	XXIII					0.47

	hydroxy-1-methylethyl) -1-methyl-							
74	Cyclosativene	IV						0.11
75	Dehydroabietan	XXVIII					0.56	
76	Elemol	XIV	0.70					1.16
77	<i>ent</i> -Pimara-8,15-diene	XXVI			0.13			
78	<i>epi</i> -13-Manoyl oxide	XXVI		0.20				
79	<i>epi</i> -Manool	XXVII			1.18			
80	<i>epi</i> -Zonarene	X	0.80					
81	Farnesyl acetone	XV		0.10				
82	Fenchone	XXII						0.16
83	Geranyl acetate	XXV					7.20	
84	Germacrene A	XI	1.20					
85	Germacrene B	XI	0.40	0.20				0.27
86	Hexahydrofarnesyl acetone	XV	3.50	0.10				
87	Humulene epoxide II	V	2.30	0.70				
88	Isophytol	XXV					1.64	
89	Limonene	XXIII	0.90	0.20	1.43	3.20	17.30	
90	Linalool	XIX		0.10	0.40	0.39		0.65 38.00 0.48
91	Linalyl acetate	XIX					3.60	
92	Longibornene	II		0.04				

93	Manool	XXVII		14.60				
94	Mintsulfide	XI		0.10				
95	Myrtenol	XXI			0.30			
96	Naphthalene	XXIX			0.20			
97	Neointermedol	VIII		1.60				
98	<i>o</i> -Xylene	XXIX					0.26	
99	<i>p</i> -Cymene	XXIII		0.10	0.10			
100	Phytol	XXV		1.20			1.57	
101	Pinocarvone	XXI		0.10				
102	<i>p</i> -Mentha-1(7),8-diene	XXIII		0.20				
103	Sabinene	XXIV			0.30			
104	Selina-3,7(11)-diene	VIII		0.10				
105	Sinularene	VII			0.17			
106	Spathulenol	IX	2.40	4.00		0.70	0.30	0.21
107	Terpinolene	XXIII		0.20		0.52		0.10
108	Thujyl alcohol	XXIV			0.17			
109	<i>τ</i> -Muurolol	X			0.09			
110	<i>trans</i> -Calamenen-10-ol	X		0.10				
111	<i>trans</i> -Muurola-4(14),5-diene	X		9.00				
112	<i>trans</i> -Pinocarveol	XXI		0.10				

113	<i>trans</i> -Thujone	XXIV	1.70	4.46		
114	Valencenne	III		0.05		
115	Valerianol	VIII			3.10	0.10
116	Ylangene	VI	0.20			0.24
117	Zonarene	X	3.80			
118	α -Amorphene	X		0.30		
119	α -Bisabolol	IV			0.20	0.50
120	α -Bourbonene	XVII		0.12		
121	α -Cadinene	X	0.20			
122	α -Cadinol	X	1.50	1.40		5.08
123	α -Calacorene	X		0.50	0.23	2.75
124	α -Cubebene	XII		0.50		3.76
125	α -Eudesmol	VIII			12.4	0.40
126	α -Gurjenene	IX		0.17		
127	α -Muurolene	X				5.19
128	α -Terpinene	XXIII		0.10	0.30	
129	α -Terpineol	XXIII			0.50	1.33
130	α -Thujene	XXIV		0.20	0.50	0.36
131	β -(<i>E</i>)-Ionone	XXIX	1.00			1.27
132	β -Calacorene	X		0.10		
133	β -Copaene	VI	13.30			

134	β -Cyclocitral	XXIII		0.30				
135	β -Elemene	XIV	0.50	0.50				
136	β -Himachalene	II			0.95			
137	β -Myrcene	XIX		0.40	1.93	3.00	1.50	0.11
138	β -Patchoulene	IX			0.42			
139	β -Phellandrene	XXIII		1.30		1.60	2.10	
140	β -Pinene	XXI	1.10	26.4	0.85			
141	γ -Eudesmol	VIII						14.04
142	γ -Terpineol	XXIII		0.20				
143	γ -Vanillin	XXIX					0.35	
144	δ -3-Carene	XXIV			1.20	6.50		
145	δ -Amorphene	X		0.20				
146	τ -Cadinol	X				7.60	2.20	10.21

A) *S. dugesii*, B) *S. gesneriflora*, C) *Salvia angulata*, D) *Salvia argentea*, E) *Salvia viridis*, F) *Salvia lavandulifolia*, G) *Salvia officinalis*, H) *Salvia africana-lutea*, I) *Salvia chamaeleagnea*, J) *Salvia miltiorrhiza*, K) *Salvia sclarea* and L) *Salvia plebeia*

Table S2. Chemical composition of essential oils of the twelve analyzed *Salvia* plants, according to their structural skeleton

Structural Skeleton	Composition (%)											
	A	B	C	D	E	F	G	H	I	J	K	L
I	8.3	1.2	1.5				0.5			0.7		
II							1.0					
III		6.3										
IV	1.5							0.2	0.5			
V	10.0	15.7	27.7	10.7	3.6	1.1	3.3	3.6	0.4	8.3	14.0	15.4
VI	1.7	3.7	0.1		13.3							5.7
VII							0.2					
VIII	1.0	3.7		0.7	1.6			12.4	0.4			14.0
IX	7.6	4.7	2.4	32.4	0.3		8.0	2.2	33.0			5.1
X					9.0			7.6	2.2			10.2
XI	5.0	7.6	19.5		7.9	5.4	0.2	0.9		4.4		0.3
XII	0.8	3.6			0.5							2.9
XIII												
XIV		7.5	0.7		0.5							1.2
XV	1.5		1.2	3.5	0.2							
XVI	2.2											
XVII	1.6	1.0	5.6		2.9		0.3					
XVIII									2.7			
XIX					0.4	0.4	1.9	3.0	1.5	0.7	38.0	0.5
XX					0.2	3.0	0.8			1.6		
XXI		1.5	0.5	0.5	26.4	6.8	0.9	3.1	42.0			
XXII	3.4	5.8		0.9		7.6	25.1			1.1		0.6
XXIII	1.1	1.0	0.9	3.1	1.3	40.1	14.1	10.1	17.3	0.8	1.2	0.2
XXIV				7.3	0.2	0.5	18.8	1.2	6.5			
XXV		5.5		1.2						1.6	7.2	
XXVI	4.9				0.2		0.1					
XXVII	0.8			14.6			1.2					
XXVIII										0.6		
XXIX		2.1		1			0.3			2.0		0.8