

Essential Oils from Colombian Plants: Antiviral Potential against Dengue Virus Based on Chemical Composition, In Vitro and In Silico Analyses

Lina Silva-Trujillo ¹, Elizabeth Quintero-Rueda ¹, Elena E. Stashenko ¹, Sergio Conde-Ocazonez ², Paola Rondón-Villarreal ², and Raquel E. Ocazonez ^{1,*}

¹ Centro de Cromatografía y Espectrometría de Masas, CROM-MASS, Universidad Industrial de Santander, Bucaramanga 680002, Santander, Colombia. (LST); (EQR); (EES); (REO)

² Instituto de Investigación Masira, Facultad de Ciencias de la Salud, Universidad de Santander, Bucaramanga 680003, Santander, Colombia. (SCO); (PRV)

* Correspondence: Raquel E Ocazonez. relocaz@uis.edu.co

Table S1. Chemical composition of essential oils studied in this work

Compound	LRIs (DB-5MS		LaCi	LaCif	LaCaf1	LaCaf2	LoP	LoC	LoT	LoTf	LoTC	TdS1	TdS2	PaS1	ObS1	VcS1
	column)															
	Exp.	Lit.														
<i>cis</i> -3-Hex-3-en-1-ol	853	850 ^a	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-
α -Thujene	927	930 ^a	-	-	-	-	-	1.6	-	-	0.7	-	-	-	-	-
α -Pinene*	935	932 ^a	0.3	0.2	0.2	-	1.7	0.4	-	-	0.4	-	-	4.6	0.5	9.4
Camphene*	951	954 ^a	-	-	0.2	-	-	0.2	-	-	-	-	-	-	-	-
Sabinene	976	975 ^a	-	-	-	-	-	-	-	-	-	-	-	-	0.5	0.6
Oct-1-en-3-ol	978	980 ^b	0.2	-	0.004	-	-	-	-	-	-	-	-	-	-	-
β -Pinene*	982	974 ^a	-	-	-	-	-	-	-	-	-	-	-	1.2	1.0	4.1
6-Methyl-hept-5-en-2-one*	985	985 ^a	1.3	3.3	-	-	-	-	-	-	-	-	-	-	-	-
β -Myrcene*	990	990 ^a	-	-	1.4	-	1.3	2.4	0.4	-	5.2	0.2	0.2	1.5	0.6	0.7
Octan-3-ol	994	991 ^a	-	-	0.02	-	-	-	-	-	-	-	-	-	-	-
α -Phellandrene	1005	1002 ^a	0.1	-	-	-	7.1	-	-	-	0.5	-	-	4.4	-	-
β -Phellandrene	1009	1002 ^a	-	-	-	-	1.4	-	-	-	-	-	-	-	-	-
Δ^3 -Carene	1012	1011 ^a	-	-	-	-	0.7	0.1	-	-	0.3	0.2	-	0.6	-	-
α -Terpinene	1020	1017 ^a	-	-	-	-	0.5	1.7	-	-	2.9	1.3	1.6	0.8	-	-
<i>p</i> -Cymene*	1027	1024 ^a	-	-	-	-	12.6	14.4	2.3	2.0	19.1	3.0	3.6	3.0	-	-
Limonene*	1034	1029 ^a	2.4	5.9	82.2	0.9	2.1	0.3	-	-	0.9	-	-	6.0	-	0.8
1,8-Cineol*	1036	1031 ^a	-	-	-	-	13.0	1.3	-	-	-	-	-	3.6	8.1	0.8
<i>cis</i> - β -Ocimene	1046	1050 ^a	-	-	-	-	-	-	-	-	1.2	-	-	-	-	-
<i>trans</i> - β -Ocimene	1047	1050 ^a	-	0.4	1.0	-	-	-	-	-	0.4	-	-	0.4	0.3	-
γ -Terpinene	1061	1059 ^a	-	-	-	-	2.4	5.3	0.9	6.9	9.2	0.6	0.7	0.8	-	-
<i>cis</i> -Sabinene hydrate	1072	1070 ^a	-	-	-	-	-	0.3	-	-	-	-	-	-	-	-
Terpinolene	1088	1088 ^a	-	-	-	-	-	-	-	-	0.3	-	-	0.8	-	-
α -Terpineol	1098	1088 ^a	-	-	-	-	0.5	-	-	-	-	-	0.2	-	-	-
Linalool*	1099	1096 ^a	1.1	2.5	0.4	0.5	0.7	1.0	-	-	0.3	-	-	0.4	42.7	-
<i>trans-p</i> -Mentha-2,8-dien-1-ol	1123	1122 ^a	-	-	0.1	0.4	-	-	-	-	-	-	-	-	-	-
<i>cis</i> -p-Menth-2-en-1-ol	1129	1123 ^b	-	-	-	-	-	-	-	-	-	-	-	0.5	-	-
<i>cis</i> -Limonene oxide	1141	1136 ^a	-	-	0.3	0.1	-	-	-	-	-	-	-	-	-	-

Table S1. Cont.

Compound	LRIs (DB-5MS column)		LaCi	LaCif	LaCaf1	LaCaf2	LoP	LoC	LoT	LoTf	LoTC	TdS1	TdS2	PaS1	ObS1	VcS1
	Exp.	Lit.														
<i>trans</i> - <i>p</i> -Menth-2-en-1-ol*	1146	1137 ^b	-	-	-	-	-	-	-	-	-	-	-	0.5	-	-
Citronellal*	1152	1153 ^a	0.7	1.1	-	-	-	-	-	-	-	-	-	-	-	-
<i>cis</i> -Isocitral	1164	1164 ^a	1.6	2.1	-	-	-	-	-	-	-	-	-	-	-	-
Borneol*	1172	1169 ^a	-	-	-	1.3	-	-	-	-	-	-	-	-	-	-
Isogeranial	1180	1185 ^a	2.1	2.8	-	-	-	-	-	-	-	-	-	-	-	-
Terpinen-4-ol*	1186	1177 ^a	-	-	-	-	0.9	0.5	0.8	-	0.8	-	0.1	0.3	-	-
<i>cis</i> -Dihydrocarvone	1200	1192 ^a	-	-	0.4	2.0	-	-	-	-	-	-	-	-	-	-
Estragole*	1203	1196 ^a	-	-	-	-	-	-	-	-	-	-	-	-	18.6	-
<i>trans</i> -Dihydrocarvone	1208	1200 ^a	-	-	0.5	3.4	-	-	-	-	-	-	-	-	-	-
Nerol*	1229	1229 ^a	2.5	2.2	-	-	-	-	-	-	-	-	-	-	-	-
Thymol-methyl-ether	1230	1235 ^a	-	-	-	-	0.8	1.9	1.3	-	1.8	-	-	-	-	-
<i>cis</i> -Carveol	1231	1229 ^a	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-
<i>neo-iso</i> -Dihydrocarveol	1242	1228 ^a	-	-	0.1	0.8	-	-	-	-	-	-	-	-	-	-
Ascaridole	1246	1237 ^c	-	-	-	-	-	-	-	-	-	0.4	0.4	-	-	-
Neral*	1246	1252 ^b	11.9	18.1	-	-	-	-	-	-	-	-	-	-	-	-
Carvone*	1259	1258 ^c	-	-	12.2	78.2	-	-	-	-	-	-	-	-	-	-
Geraniol*	1260	1240 ^b	19	8.1	-	-	-	-	-	-	-	-	-	-	-	-
Piperitone*	1265	1264 ^c	-	-	-	4.8	-	-	-	-	-	-	-	14.8	-	-
Geranial*	1272	1270 ^b	24.5	24.8	-	-	-	-	-	-	-	-	-	-	-	-
Bornyl acetate	1289	1285 ^a	-	-	-	-	-	-	-	-	-	-	-	-	-	0.9
Thymol*	1290	1290 ^a	-	-	-	-	14.0	8.0	75.3	82.9	49.4	-	0.2	-	-	-
Carvacrol*	1300	1298 ^a	-	-	-	-	0.9	35	4.9	1.2	2.7	-	0.4	-	-	-
<i>iso</i> -Ascaridole	1310	1307 ^c	-	-	-	-	-	-	-	-	-	0.3	-	-	-	-
<i>trans</i> -Carvyl acetate	1346	1342 ^a	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-
Thymyl acetate*	1346	1352 ^a	-	-	-	-	-	-	1.6	-	0.5	-	-	-	-	-

Table S1. Cont.

Compound	LRIs (DB-5MS column)		LaCi	LaCif	LaCaf1	LaCaf2	LoP	LoC	LoT	LoTf	LoTC	TdS1	TdS2	PaS1	ObS1	VcS1
	Exp.	Lit.														
Piperitenone	1347	1343 ^a	-	-	0.3	0.3	-	-	-	-	-	-	-	14.8	-	-
α -Cubebene	1355	1351 ^a	-	-	-	-	-	-	-	-	-	-	-	0.8	-	-
Carvacryl acetate	1366	1372 ^a	-	-	-	-	-	2.0	-	-	-	-	-	-	-	-
Neryl acetate	1376	1361 ^a	0.4	0.6	-	-	-	-	-	-	-	-	-	-	-	-
α -Ylangene	1380	1375 ^a	-	-	-	-	-	-	-	-	-	-	-	-	-	0.6
Cyclosativene	1382	1374 ^c	-	-	-	-	-	-	-	-	-	-	-	1.6	-	-
Isoledene	1382	1376 ^a	-	-	-	-	-	-	-	-	-	-	-	-	-	0.5
Geranyl acetate*	1383	1381 ^a	2.8	4.8	-	-	-	-	-	-	-	-	-	-	-	-
α -Copaene	1385	1376 ^a	-	-	-	0.3	0.6	0.7	-	-	-	-	-	2.9	-	7.0
β -Bourbonene	1396	1387 ^a	-	-	0.3	3.8	-	-	-	-	-	-	-	-	0.6	1.1
β -Elemene	1398	1390 ^a	2.6	1.2	0.1	1.5	-	-	-	-	-	4.0	5.0	0.7	2.2	2.8
α -Gurjunene	1419	1409 ^b	-	-	-	-	-	-	-	-	-	-	-	1.3	-	-
α -Santalene	1428	1420 ^c	-	-	-	-	-	-	-	-	-	-	-	0.8	-	-
β -Copaene	1433	1432 ^a	-	-	-	0.6	-	-	-	-	-	-	-	-	-	-
<i>trans</i> - β - Caryophyllene*	1433	1427 ^c	9.1	13.3	-	0.1	15.1	4.4	5.4	7.0	1.6	4.0	4.9	7.4	0.9	19.2
β -Gurjunene	1437	1432 ^a	-	-	-	0.4	-	0.4	-	-	-	-	-	-	-	-
<i>trans</i> - α -Bergamotene	1440	1434 ^a	-	-	-	-	0.5	0.3	1.0	-	-	-	-	-	1.1	-
α -Guaiene	1443	1437 ^a	-	2.9	-	-	-	-	-	-	-	-	-	-	1.0	-
6,9-Guaiadiene	1451	1444 ^a	-	-	-	-	-	-	-	-	-	1.3	1.8	-	-	1.6
Aromadendrene	1452	1441 ^b	-	-	-	-	-	-	-	-	-	-	-	1.4	-	-
<i>trans</i> - β -Farnesene	1460	1456 ^a	0.5	0.1	-	0.2	-	-	-	-	-	-	-	0.6	-	-
N.I. M ⁺ • <i>m/z</i> 204	1462	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.0
α -Humulene*	1467	1468 ^c	2.8	2.8	-	-	8.1	1.1	3.2	-	0.9	-	0.4	1.5	2.5	2.7
γ -Muurolene	1473	1479 ^a	-	-	-	-	0.6	-	-	-	-	-	-	1.5	-	0.6
<i>trans</i> -Muurola- 4(14),5-diene	1475	1493 ^a	-	-	-	-	-	-	-	-	-	-	-	-	0.7	-

Table S1. Cont.

Compound	LRIs (DB-5MS column)		LaCi	LaCif	LaCaf1	LaCaf2	LoP	LoC	LoT	LoTf	LoTC	TdS1	TdS2	PaS1	ObS1	VcS1
----------	-------------------------	--	------	-------	--------	--------	-----	-----	-----	------	------	------	------	------	------	------

	Exp.	Lit.														
<i>trans</i> -9- <i>epi</i> -Caryophyllene	1477	1466 ^a	-	-	-	0.3	-	-	-	-	-	-	-	-	-	-
N.I. M ⁺ • <i>m/z</i> 180	1477	-	-	-	-	-	-	0.4	-	-	-	-	-	-	-	-
<i>trans</i> -Cadina-1(6),4-diene	1482	1476 ^a	-	-	-	-	-	-	-	-	-	-	-	1.1	-	-
Aristolochene	1483	1488 ^a	-	-	-	-	-	-	-	-	-	17.9	20.9	-	-	-
N.I. M ⁺ • <i>m/z</i> 180	1484	-	-	-	-	-	-	6.1	-	-	-	-	-	-	-	-
Germacrene D*	1492	1481 ^a	4.3	1.5	0.1	-	0.9	-	-	-	-	-	-	1.7	4.9	12.3
Premnaspirodienene	1499	1505 ^a	-	-	-	-	-	-	-	-	-	3.7	4.7	-	-	-
β-Selinene	1502	1490 ^a	-	-	-	-	0.5	0.3	-	-	-	5.2	5.8	-	-	-
Valencene	1503	1496 ^a	-	-	-	-	-	-	-	-	-	7.4	6.5	1.2	-	-
Viridiflorene	1503	1496 ^a	-	-	-	-	-	-	-	-	-	-	-	-	-	2.4
Viridiflorol	1503	1496 ^a	-	-	-	-	-	-	-	-	-	-	-	6.5	-	1.6
α-Muurolene	1506	1500 ^a	-	-	-	-	0.9	-	-	-	-	-	-	-	-	0.6
Geranyl isobutyrate	1506	1515 ^a	1.2	0.3	-	-	-	-	-	-	-	-	-	-	-	-
Bicyclogermacrene	1509	1500 ^a	-	-	-	-	-	-	-	-	-	-	-	2.8	2.2	3.9
α-Selinene	1509	1498 ^a	-	-	-	-	-	0.8	-	-	-	1.6	1.7	-	-	-
α-Bulnesene	1510	1509 ^a	-	0.6	-	-	-	-	-	-	-	-	-	-	1.1	-
δ-Amorphene	1515	1511 ^c	-	-	-	-	-	-	-	-	-	-	-	1.0	-	-
<i>trans</i> -β-Guaiene	1517	1502 ^a	2.2	-	-	-	-	-	-	-	-	-	-	-	-	11.8
β-Bisabolene	1517	1505 ^a	-	-	-	-	0.8	0.8	0.8	-	-	-	-	-	-	-
γ-Cadinene	1523	1513 ^a	-	-	-	-	0.5	0.3	-	-	-	-	-	0.7	3.7	-
δ-Cadinene	1528	1523 ^a	-	-	-	-	1.2	1.1	-	-	-	-	0.3	5.5	-	2.8
<i>cis</i> -Calamenene	1530	1529 ^a	-	-	-	-	0.5	-	-	-	-	-	-	-	0.4	-
<i>trans</i> -γ-Bisabolene	1533	1531 ^a	-	-	-	-	-	0.4	-	-	-	-	-	-	-	-
7- <i>epi</i> -α-Selinene	1533	1534 ^c	-	-	-	-	-	-	-	-	-	0.5	0.6	-	-	-
Zonarene	1534	1529 ^a	-	-	-	-	-	-	-	-	-	-	-	1.2	-	-
α-Cadinene	1535	1538 ^a	-	-	-	-	-	-	-	-	-	-	-	0.6	-	0.6

Table S1. Cont.

Compound	LRIs (DB-5MS															
	column)		LaCi	LaCif	LaCaf1	LaCaf2	LoP	LoC	LoT	LoTf	LoTC	TdS1	TdS2	PaS1	ObS1	VcS1
	Exp.	Lit.														
N.I. M ⁺ • <i>m/z</i> 222	1539	-	-	-	-	-	-	0.2	-	-	-	-	-	-	-	-
N.I. M ⁺ • <i>m/z</i> 204	1544	-	-	-	-	-	-	0.4	-	-	-	-	-	-	-	-

<i>trans</i> - α -Bisabolene	1545	1544 ^c	2.0	0.3	-	-	-	-	-	-	-	-	-	-	-	-
Selina-3,7(11)-diene	1552	1546 ^a	-	-	-	-	-	-	-	-	-	-	-	-	-	1.0
N.I. M ⁺ • <i>m/z</i> 222	1554	-	-	-	-	-	-	1.7	-	-	-	-	-	-	-	-
Elemol	1556	1548 ^a	-	-	-	-	-	-	-	-	-	0.2	0.3	-	-	-
N.I. M ⁺ • <i>m/z</i> 204	1557	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.8
<i>trans</i> -Nerolidol	1562	1563 ^a	-	-	-	-	0.9	0.7	-	-	-	-	-	-	0.5	1.3
Zierone	1564	1574 ^c	-	-	-	-	-	-	-	-	-	-	0.3	-	-	-
Germacren D-4-ol	1585	1575 ^c	-	-	-	-	-	-	-	-	-	-	-	0.4	-	-
Spathulenol	1591	1578 ^a	-	-	-	-	-	-	-	-	-	-	-	1.9	0.8	-
Caryophyllene oxide*	1595	1583 ^a	1.8	0.1	-	-	2.5	0.9	1.3	-	0.4	3.3	3.2	3.8	-	0.6
Guaiol	1606	1600 ^a	-	-	-	-	0.6	-	-	-	-	3.5	3.3	-	-	0.7
Humulene epoxide II	1625	1608 ^a	-	-	-	-	1.0	-	0.5	-	-	-	-	-	-	-
1,10-di- <i>epi</i> -Cubenol	1629	1619 ^a	-	-	-	-	-	-	-	-	-	-	-	-	0.9	-
<i>neo</i> -Intermedeol	1632	1631 ^c	-	-	-	-	-	-	-	-	-	1.3	1.2	-	-	-
<i>epi</i> - α -Cadinol	1640	1640 ^c	-	-	-	-	-	0.9	-	-	-	-	-	0.8	4.2	-
Intermedeol	1640	1658 ^a	-	-	-	-	-	-	-	-	-	-	-	-	-	0.6
γ -Eudesmol	1644	1632 ^a	-	-	-	-	1.0	0.2	-	-	-	-	-	-	-	-
N.I. M ⁺ • <i>m/z</i> 220 + <i>m/z</i> 204	1647	-	-	-	-	-	0.5	-	-	-	-	-	-	-	-	-
<i>epi</i> - α -Muurolol	1655	1642 ^c	-	-	-	-	-	-	-	-	-	-	-	0.2	-	-
Eudesm-7(11)-en-4-ol	1696	1700 ^a	-	-	-	-	-	-	-	-	-	1.2	1.0	-	-	-
α -Eudesmol	1670	1653 ^a	-	-	-	-	2.6	0.3	-	-	-	-	-	0.8	-	-
Pogostol	1671	1660 ^c	-	-	-	-	-	-	-	-	-	2.8	3.3	-	-	-
α -Selin-11-en-4-ol	1674	1659 ^a	-	-	-	-	-	-	-	-	-	-	-	-	-	0.5

Table S1. Cont.

Compound	LRIs (DB-5MS		LaCi	LaCif	LaCaf1	LaCaf2	LoP	LoC	LoT	LoTf	LoTC	TdS1	TdS2	PaS1	ObS1	VcS1
	column)															
	Exp.	Lit.														
Germacra-4,5,10-trien-1- α -ol	1680	1686 ^a	-	-	-	-	-	-	-	-	-	3.5	3.6	-	-	-
Valerenal	1720	1716 ^c	-	-	-	-	-	-	-	-	-	0.6	0.6	-	-	-
Vetiselinenol	1740	1730 ^a	-	-	-	-	-	-	-	-	-	2.1	1.7	-	-	-

Dehydrofukinone	1827	1820 ^c	-	-	-	-	-	-	-	-	-	25.4	19.3	-	-	-
<i>trans,trans</i> -Geranil linalool	2028	2026 ^a	-	-	-	-	-	-	-	-	-	-	-	-	-	1.6

LRIs, linear retention indices calculated using *n*-alkanes C₈-C₂₅ mixture on the DB-5MS (non-polar) column. *L. alba*: neat EO (LaCif) and light fraction (LaCif) of citral chemotype EO; limonene-rich fraction (LaCaf1) and carvone-rich fraction (LaCaf2) of carvone chemotype. *L. origanoides*: neat EO of phellandrene chemotype (LoP), carvacrol (LoC), thymol-carvacrol (LoTC), and thymol (LoT) chemotype; and thymol-rich fraction (LoTf) of thymol chemotype. Neat EOs of *T. diffusa* collected in 2019 (TdS1) and in 2016 (TdS2). Neat EOs of *O. basilicum* (ObS1), *P. auduncum* (PaS1) and *V. curassavica* (VcS1). Exp. Experimental. Lit. Literature ^aAdams, 2007; ^bBabushok et al., 2011; ^cNIST 2017. * Standard compounds were used for confirmatory identification.

Table S2. Docking energies (kcal/mol) of essential oil terpenes with dengue virus serotype 2 proteins

Compound	Structural DENV-2 proteins		
	E	C	prM
Epigallocatechin gallate: positive control	-7.85 ± 0.3	-7.67 ± 0.4	-7.37 ± 0.1
1,10-di- <i>epi</i> -Cubenol	-6.02 ± 0.7	-6.46 ± 0.4	-5.12 ± 0.2
1,8-Cineol	-4.76 ± 0.2	-5.07 ± 0.2	-4.24 ± 0.2
6,9-Guaiadiene	-7.30 ± 1.3	-6.69 ± 0.1	-5.15 ± 0.3
7- <i>epi</i> - α -Selinene	-6.74 ± 1.0	-6.52 ± 0.3	-5.33 ± 0.1
Eudesm-7(11)-en-4-ol	-6.91 ± 0.4	-6.40 ± 0.3	-5.38 ± 0.2
Aristolochene	-6.60 ± 0.5	-6.66 ± 0.3	-5.41 ± 0.3
Aromadendrene	-6.32 ± 0.9	-6.53 ± 0.3	-5.26 ± 0.1
Ascaridole	-6.12 ± 0.4	-5.67 ± 0.1	-4.88 ± 0.1
Bicyclogermacrene	-6.29 ± 0.5	-6.60 ± 0.3	-5.14 ± 0.1
Borneol	-4.77 ± 0.2	-4.54 ± 0.3	-4.17 ± 0.1
Bornyl acetate	-5.04 ± 0.2	-5.29 ± 0.3	-4.56 ± 0.1
Camphene	-5.55 ± 0.3	-5.41 ± 0.2	-4.14 ± 0.1
Carvacrol	-7.31 ± 0.4	-6.08 ± 0.5	-5.29 ± 0.4
Carvacryl acetate	-7.52 ± 0.8	-5.90 ± 0.2	-5.29 ± 0.3
Carvone	-7.29 ± 0.9	-5.99 ± 0.5	-4.90 ± 0.3
Caryophyllene oxide	-5.62 ± 0.3	-6.46 ± 0.4	-5.26 ± 0.1
<i>cis</i> -Calamenene	-8.73 ± 0.8	-6.91 ± 0.2	-5.33 ± 0.1
<i>cis</i> -Carveol	-6.98 ± 0.4	-5.78 ± 0.4	-4.77 ± 0.3
<i>cis</i> -Dihydrocarvone	-6.48 ± 0.8	-5.64 ± 0.3	-4.51 ± 0.1
<i>cis</i> -Isocitral	-6.08 ± 0.6	-5.37 ± 0.1	-4.78 ± 0.2
<i>cis</i> -Limonene oxide	-6.71 ± 0.5	-5.65 ± 0.5	-4.74 ± 0.3
<i>cis</i> -p-Menth-2-en-1-ol	-6.17 ± 0.5	-5.64 ± 0.2	-4.64 ± 0.1
<i>cis</i> -Sabinene hydrate	-5.93 ± 0.5	-5.81 ± 0.5	-4.21 ± 0.3
<i>cis</i> - β -Ocimene	-6.29 ± 0.5	-5.50 ± 0.2	-4.41 ± 0.1
Citronellal	-5.94 ± 0.3	-5.08 ± 0.3	-4.03 ± 0.3
Cyclosativene	-5.98 ± 0.4	-6.39 ± 0.3	-5.22 ± 0.1
Dehydrofukinone	-6.39 ± 0.8	-6.60 ± 0.5	-5.52 ± 0.3
Elemol	-5.92 ± 0.5	-6.04 ± 0.2	-5.01 ± 0.1
<i>epi</i> - α -Cadinol	-6.38 ± 0.7	-6.50 ± 0.3	-5.29 ± 0.2
<i>epi</i> - α -Muurolol	-6.10 ± 0.6	-6.22 ± 0.4	-5.04 ± 0.1
Estragole	-6.69 ± 0.6	-5.28 ± 0.1	-4.79 ± 0.3
Geranial	-6.32 ± 0.3	-5.22 ± 0.2	-4.29 ± 0.3
Geraniol	-6.14 ± 0.4	-5.24 ± 0.2	-4.24 ± 0.3
Geranyl acetate	-5.97 ± 0.7	-5.69 ± 0.2	-4.87 ± 0.2

Table S2. Cont.

Compound	E	C	prM
Geranyl isobutyrate	-6.07 ± 0.6	-6.15 ± 0.1	-5.10 ± 0.1
Germacra-4,5,10-trien-1- α -ol	-5.90 ± 0.6	-6.34 ± 0.2	-5.35 ± 0.2
Germacren D-4-ol	-6.01 ± 0.7	-6.37 ± 0.3	-5.23 ± 0.2
Germacrene D	-6.79 ± 1.1	-6.49 ± 0.2	-5.36 ± 0.1
Guaiol	-6.30 ± 0.7	-6.85 ± 0.4	-5.41 ± 0.1
Humulene epoxide II	-5.64 ± 0.3	-6.20 ± 0.4	-5.29 ± 0.1
<i>iso</i> -Ascaridole	-6.31 ± 0.5	-5.52 ± 0.4	-4.64 ± 0.2
Isogeranial	-6.13 ± 0.5	-5.34 ± 0.1	-4.74 ± 0.2
Limonene	-7.24 ± 0.1	-5.76 ± 0.6	-4.60 ± 0.4
Linalool	-6.06 ± 0.4	-4.87 ± 0.2	-4.31 ± 0.2
Intermedeol	-5.77 ± 0.4	-6.59 ± 0.3	-5.25 ± 0.0
Isoledene	-6.72 ± 0.7	-6.74 ± 0.3	-5.29 ± 0.1
<i>neo</i> -Intermedeol	-6.34 ± 1.0	-6.41 ± 0.3	-5.19 ± 0.1
<i>neo-iso</i> -Dihydrocarveol	-5.04 ± 0.5	-4.94 ± 0.3	-4.15 ± 0.1
Neral	-6.16 ± 0.5	-5.04 ± 0.2	-4.21 ± 0.2
Nerol	-6.13 ± 0.4	-5.27 ± 0.3	-4.42 ± 0.2
Neryl acetate	-6.32 ± 0.5	-5.91 ± 0.1	-5.16 ± 0.2
<i>p</i> -Cymene	-7.27 ± 0.3	-5.81 ± 0.5	-4.89 ± 0.4
Piperitenone	-6.81 ± 0.7	-6.01 ± 0.3	-5.07 ± 0.4
Piperitone	-6.82 ± 0.5	-6.02 ± 0.4	-4.65 ± 0.2
Pogostol	-5.90 ± 0.4	-6.40 ± 0.2	-5.30 ± 0.3
Premnaspirodiene	-5.75 ± 0.4	-6.44 ± 0.4	-5.07 ± 0.2
Sabinene	-6.59 ± 0.3	-5.86 ± 0.6	-4.62 ± 0.3
Selina-3,7(11)-diene	-6.61 ± 1.0	-6.81 ± 0.3	-5.18 ± 0.1
Spathulenol	-6.17 ± 0.6	-6.29 ± 0.3	-5.49 ± 0.2
Terpinen-4-ol	-6.38 ± 0.4	-5.72 ± 0.6	-4.81 ± 0.4
Terpinolene	-7.03 ± 0.6	-5.74 ± 0.5	-4.89 ± 0.4
Thymol	-6.98 ± 0.5	-5.98 ± 0.5	-5.31 ± 0.3
Thymol-methyl-ether	-7.11 ± 0.4	-5.64 ± 0.2	-4.99 ± 0.3
Thymyl acetate	-7.01 ± 0.8	-5.88 ± 0.2	-5.19 ± 0.1
<i>trans, trans</i> -Geranyl linalool	-6.37 ± 0.3	-6.61 ± 0.1	-5.31 ± 0.2
<i>trans</i> -9- <i>epi</i> -Caryophyllene	-5.60 ± 0.6	-6.08 ± 0.3	-5.32 ± 0.2
<i>trans</i> -Cadina-1(6),4-diene	-7.23 ± 1.2	-6.74 ± 0.4	-5.11 ± 0.0
<i>trans</i> -Carvyl acetate	-6.84 ± 1.0	-6.03 ± 0.1	-4.92 ± 0.2
<i>trans</i> -Dihydrocarvone	-7.23 ± 0.3	-5.85 ± 0.3	-4.84 ± 0.2
<i>trans</i> -Muurola-4(14),5-diene	-6.93 ± 1.4	-6.81 ± 0.4	-5.12 ± 0.4
<i>trans</i> -Nerolidol	-5.87 ± 0.4	-5.80 ± 0.2	-4.63 ± 0.2

Table S2. Cont.

Compound	E	C	prM
----------	---	---	-----

<i>trans-p</i> -Menth-2-en-1-ol	-6.53 ± 0.5	-5.58 ± 0.1	-4.60 ± 0.1
<i>trans-p</i> -Mentha-2,8-dien-1-ol	-6.14 ± 0.4	-5.59 ± 0.2	-4.50 ± 0.2
<i>trans-α</i> -Bergamotene	-6.07 ± 0.3	-6.32 ± 0.3	-4.97 ± 0.1
<i>trans-α</i> -Bisabolene	-6.91 ± 0.6	-6.65 ± 0.1	-5.50 ± 0.0
<i>trans-β</i> -Caryophyllene	-6.02 ± 0.4	-6.63 ± 0.4	-5.36 ± 0.2
<i>trans-β</i> -Farnesene	-6.43 ± 0.7	-6.04 ± 0.1	-5.01 ± 0.4
<i>trans-β</i> -Guaiene	-6.18 ± 1.0	-6.70 ± 0.3	-5.36 ± 0.3
<i>trans-β</i> -Ocimene	-6.49 ± 0.2	-5.86 ± 0.3	-4.45 ± 0.2
<i>trans-γ</i> -Bisabolene	-6.97 ± 0.7	-6.28 ± 0.1	-5.01 ± 0.2
Valencene	-6.84 ± 0.9	-6.50 ± 0.3	-5.34 ± 0.2
Valerenal	-6.01 ± 0.6	-6.58 ± 0.2	-5.26 ± 0.2
Vetiselinol	-7.07 ± 0.8	-6.59 ± 0.3	-5.45 ± 0.1
Viridiflorene	-8.13 ± 0.9	-6.61 ± 0.2	-5.42 ± 0.1
Viridiflorol	-6.24 ± 0.5	-6.09 ± 0.2	-5.40 ± 0.2
Zierone	-5.95 ± 0.5	-6.53 ± 0.3	-5.20 ± 0.3
Zonarene	-7.46 ± 0.9	-6.54 ± 0.3	-5.10 ± 0.1
α -Bulnesene	-7.42 ± 1.0	-6.87 ± 0.4	-5.42 ± 0.3
α -Cadinene	-8.28 ± 1.1	-6.72 ± 0.4	-5.26 ± 0.1
α -Copaene	-6.29 ± 0.5	-6.60 ± 0.3	-5.14 ± 0.1
α -Cubebene	-7.62 ± 1.0	-6.74 ± 0.3	-5.40 ± 0.2
α -Eudesmol	-6.37 ± 0.8	-6.43 ± 0.4	-5.47 ± 0.3
α -Guaiene	-8.26 ± 1.1	-6.73 ± 0.3	-5.29 ± 0.2
α -Gurjunene	-7.83 ± 1.0	-5.72 ± 0.2	-5.42 ± 0.2
α -Humulene	-5.74 ± 0.7	-6.50 ± 0.4	-5.29 ± 0.3
α -Muurolene	-5.87 ± 0.5	-6.78 ± 0.4	-5.27 ± 0.3
α -Phellandrene	-7.60 ± 0.2	-7.38 ± 0.5	-5.84 ± 0.2
α -Pinene	-5.09 ± 0.3	-5.48 ± 0.3	-4.24 ± 0.1
α -Santalene	-6.11 ± 0.5	-6.34 ± 0.2	-4.75 ± 0.1
α -Selin-11-en-4-ol	-6.75 ± 0.9	-4.53 ± 0.3	-5.26 ± 0.2
α -Selinene	-7.98 ± 1.1	-6.63 ± 0.2	-5.19 ± 0.3
α -Terpinene	-7.10 ± 0.6	-5.78 ± 0.6	-4.96 ± 0.4
α -Terpineol	-6.67 ± 0.4	-5.90 ± 0.5	-4.70 ± 0.3
α -Tujene	-6.16 ± 0.7	-6.06 ± 0.3	-4.69 ± 0.2
α -Ylangene	-6.11 ± 0.3	-6.63 ± 0.3	-5.16 ± 0.3
β -Bisabolene	-7.83 ± 0.5	-6.44 ± 0.2	-5.55 ± 0.2
β -Bourbonene	-7.95 ± 0.9	-6.76 ± 0.6	-5.17 ± 0.2
β -Copaene	-6.22 ± 0.7	-6.57 ± 0.3	-5.18 ± 0.2
β -Elemene	-6.07 ± 1.0	-6.04 ± 0.3	-4.85 ± 0.0

Table S2. Cont.

Compound	E	C	prM
----------	---	---	-----

β -Gurjunene	-7.83 ± 1.0	-6.72 ± 0.2	-5.42 ± 0.2
β -Myrcene	-6.12 ± 0.3	-5.08 ± 0.4	-4.08 ± 0.2
β -Phellandrene	-6.99 ± 0.5	-6.03 ± 0.6	-4.92 ± 0.3
β -Pinene	-5.11 ± 0.4	-5.36 ± 0.3	-4.21 ± 0.1
β -Selinene	-7.71 ± 1.2	-6.53 ± 0.3	-5.38 ± 0.1
γ -Cadinene	-8.19 ± 1.0	-6.77 ± 0.2	-5.27 ± 0.3
γ -Eudesmol	-6.30 ± 0.4	-6.70 ± 0.1	-5.43 ± 0.2
γ -Muurolene	-5.87 ± 0.5	-6.79 ± 0.4	-5.27 ± 0.3
γ -Terpinene	-7.28 ± 0.3	-5.79 ± 0.5	-4.96 ± 0.4
Δ^3 -Carene	-5.86 ± 0.4	-5.86 ± 0.4	-4.27 ± 0.1
δ -Amorphene	-7.96 ± 1.0	-6.80 ± 0.3	-5.25 ± 0.2
δ -Cadinene	-8.41 ± 0.9	-6.67 ± 0.3	-5.47 ± 0.3

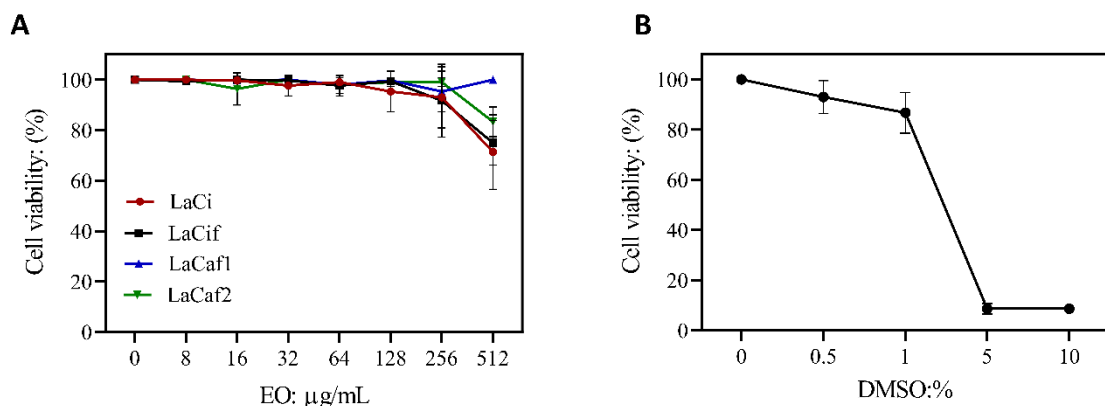


Figure S1. Representative results of the cytotoxicity assay. Essential oils and fractions of *L. alba* citral (LaCi and LaCif) and carvone (LaCaf1 and LaCaf2) chemotypes. Vero cells were cultured for 72 h in the presence of essential oil. Relative cell viability was measured by crystal violet quantification. Data represent averages and \pm SD of six independent measurements. Dimethyl sulfoxide (DMSO) is a positive control. The remaining ten essential oils studied (Table 1) showed similar results.