

(Article)

Phytochemical profile, GC-MS profiling and *In vitro* evaluation of some biological applications of the extracts of *Origanum syriacum* L. and *Cousinia libanotica* D.C.

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Supplementary materials

Table S1. Identification of the volatile compounds of *Origanum syriacum* and *Cousinia libanotica* extracts by Gas Chromatography-Mass spectrometry “GC-MS” before and after derivatization.

18	1417	<i>trans</i> -caryophyllene	+	+					
19	1434	cuminal acetate						+	
20	1524	phenol, 2,5-bis(1,1-di-methylethyl)-	+		++				
21	1574	<i>p</i> -cymene-2,5-diol		+	+	+			
22	1585	(+) spathulenol	+						
23	1588	caryophyllene oxide	+++	+					
24	1613	humulene oxide II	+						
25	1646	Cadinol T	+						
26	1670	14-hydroxycaryophyllene	+	+					
27	1785	loliolide		+					
28	1883	3,7,11,15-tetramethyl-2-hexadecen-1-ol		++	++				
29	1930	methyl palmitate						+++	
30	1937	7,9-di-tert-butyl-1-oxo-aspiro(4,5)deca-6,9-diene-2,8-dione	+	+++	+		+	++	+
31	1978	palmitic acid					++	++	
32	2005	Ethyl palmitate		+++	+			++	
33	2115	phytol	+	+	+	+++			
34	2144	pregna-4,16-diene-3,20-dione	+						
35	2154	linoleic acid	+	+	+		+++	+++	+
36	2156	stearic acid	+	+++	+			+	
37	2160	oleic acid		+			+	++	
38	2442	phenol, 2,2'-methylenebis[6-(1,1-di-methylethyl)-4-methyl-	++	+++	+++	++	+++	++	+++
39	2527	2-monopalmitin		+		++			
40	2713	heptacosane	+	+			+++	++	+

41	2725	β -monostearin			++				
42	2727	α -monostearin		+					
43	2921	octacosane	++	++					
44	2950	hexatriacontane	+++	+++	+				
45	2963	vitamin E	+	+	+		+	+	
46	3014	tetratetracontane	+++	+++	+				
47	3063	γ -sitosterol				+	+	++	
48	3070	β -sitosterol	+	+++	++		+	++	++
49	-	β -amyrin				+++	+	+	
50	-	stigmastan-6,22-dien, 3,5-dedihydro-						+	
51	-	lupeol	+			+++	+		
52	-	stigmasta-3,5-diene						++	
53	-	β -amyrin acetate				+		+	
54	-	epilupeol				+	++	+	
55	-	3-epilupeol						+++	
56	-	lupeol acetate				+			
57	-	epilupeol acetate				+	+	+	

After derivatization

N°	tR (min)	Compound	<i>Origanum syriacum</i>				<i>Cousinia libanotica</i>			
			CHX	DCM	EtOAc	MeCN	CHX	DCM	EtOAc	MeCN
1'	8.1	propylene glycol					+	+		
2'	8.2	cyclohexanol	+							
3'	9.1	2,3-butane diol		+			+			
4'	9.7	carbamic acid					+			
5'	10.0	hexanoic acid	+				+	++		
6'	10.3	glycolic acid						+		
7'	10.46	oct-1-en-3-ol	++	+				+		
8'	10.48	1-butoxy-2-propanol				+				
9'	11.2	octan-3-ol	+	+						

10'	12.4	levulinic acid			+	+
11'	13.1	benzyl alcohol			+	
12'	15.2	acetin, bis-1,3-tri-methylether	+			+
13'	19.3	benzoic acid			+	+
14'	21.7	octanoic acid			+	
15'	24.2	4-isopropylphenol		+		
16'	25.1	glycerol	+	+	+	+
17'	31.2	diacetin, 2-trimethylether	+			+
18'	31.8	2-butenedioic acid, (E),			+	+++
19'	32.1	nonanoic acid	+		+	+
20'	32.2	cuminol	+	+	+	++
21'	35.1	decanoic acid			+	+
22'	35.2	4'-hydroxyacetophenone			++	+++
23'	36.0	isopropyl catechol	+			
24'	36.1	2-tert-Butyl-4-methylphenol			+	
25'	36.2	malic acid			+++	+++
26'	36.3	propyl gallate			+++	++
27'	36.6	vanillin			+	+
28'	36.8	2,6-di-tert-butylphenol	+			
29'	36.83	2,4-di-tert-butylphenol			+	
30'	36.9	myrtenoic acid			+	+
31'	37.0	β -thujaplicin	+			
32'	37.3	tert-Butylhydroquinone	+			
33'	37.4	allyl carbamate				+
34'	37.6	4-hydroxy- α -methylene-benzenemethanol			+	
35'	37.9	3,4-dihydroxybenzaldehyde	+			
36'	38.1	4-hydroxybenzoic acid	+		+	+++

		5-(7a-isopropenyl-4,5-dimethyl-octahydroinden-4-yl)-3-methyl-pent-2-en-1-ol	+	+		+
37'	38.2	4-(acetoxy)-3-methoxybenzoic acid				+
38'	38.3	dodecanoic acid			+	+
40'	38.9	L-(+)-lactic acid	+			
41'	39.1	syringaldehyde			+	
42'	39.2	homovanillyl alcohol			+	
43'	39.3	9-hydroxynonanoic acid			+	
44'	39.7	L-(-)-arabitol				+++
45'	39.9	vanillic acid	+		++	+
46'	40.2	azealic acid			++	++
47'	40.7	myristic acid	+++	+	+++	+++
48'	41.1	3-phenyllactic acid				+
49'	41.2	quininic acid		+		
50'	41.3	glyoxylic acid monohydrate				+
51'	41.4	syringic acid		+	+	+
52'	41.47	D-(-)-fructopyranose				+
53'	41.6	β -D-(+)-talopyranose				+
54'	41.7	4-coumaric acid		+		
55'	41.78	pentadecanoic acid	+	+	+	++
56'	42.0	mannitol				+++
57'	42.2	myo-inositol				+++
58'	42.4	talose				+++
59'	42.5	palmitelaidic acid	+	+	+	+
60'	43.3	tuberonic acid	+	+		
61'	43.6	heptadecanoic acid			+	

62'	43.68	methyl α -D-glucofuranoside						+ +
63'	43.7	caffein acid		+				
64'	43.8	methyl galactoside (1S,2R,3S,4S,5R)-						+ +
65'	44.3	α -linolenic acid	+	+	+		+	
66'	45.3	moracin M		+				
67'	45.9	D-(+)-galacturonic acid						+ +
68'	46.0	thymol-B-D-glucopyranoside						+ +
69'	46.13	andrographolide		+				
70'	46.16	retinol		+				
71'	46.18	arachidic acid		+		++	++	+ +
72'	46.3	prostaglandin E2	+					
73'	46.37	triptophenolide		+				
74'	46.93	heneicosanoic acid				+	+	
75'	47.13	2-palmitoylglycerol			+	+		++ +
76'	47.17	1,3-dipalmitin						+ +
77'	47.3	1-monopalmitin	+	+	+++		++	++ ++ +
78'	47.5	β -arabinopyranose						+ +
79'	47.6	aucubin						+ +
80'	47.67	behenic acid	+++	+		+	+++	+ +
		(10E,15Z)-9,12,13-trihydroxyoctadeca-10,15-dienoic acid						
81'	47.8		+	+			+	
82'	47.9	D-(+)-turanose						+ +
83'	48.1	sucrose						+++ +++
84'	48.2	maltose (isomer 2)						++ ++
85'	48.29	lactulose						+ +
86'	48.3	tricosanoic acid				+		
87'	48.4	tetracosanol				+	+	+ +

88'	48.5	2-monostearin		+				
89'	48.58	1-monooleoylglycerol			+			+
90'	48.6	1-monolinolein				++		
91'	48.63	1,5-anhydroglucitol						+
92'	48.69	D-arabinose						++
93'	48.7	glycerol monostearate	++	+++	+++		++	++
94'	48.79	monostearin						+++
95'	48.92	lactose						+++
96'	48.93	15-tetracosenoic acid, (Z)-				+		
97'	49.0	(±)-naringenin		+	+++			
98'	49.1	lignoceric acid	+			+	++	+
99'	49.76	pentacosanoic acid				+		
100'	49.8	1-hexacosanol	++			+		
101'	50.4	hexacosanoic acid				+	++	
102'	50.6	nonacosan-10-ol	+					
103'	50.7	5,7,4'-trihydroxy-8-c- prenyldihydro-flavonol		+				
104'	50.8	genistein					+	
105'	50.9	5-hydroxy-7-methoxy-2- methylisoflavone		+++				
106'	51.1	1-octacosanol				+		
107'	51.3	chlorogenic acid						+
108'	51.36	cholesterol				+		
109'	51.8	octacosanoic acid				+	++	
110'	52.2	campesterol	+	+		+	+	
111'	52.4	homoeriodictyol chal- cone		+				
112'	52.5	stigmasterol	+++	+		+	+	
113'	52.7	1-triacontanol				+	+	
114'	53.6	α - amyrin				+++	+	

115'	54.8	erythrodiol	+			
116'	55.2	uvaol	+	+		
117'	55.4	betulinic alcohol	+			
118'	55.7	oleanolic acid	+++	++	+	
119'	55.9	betulinic acid	+++	+		
120'	56.0	lup-20(29)-en-3-ol, acetate, (3 β)-			+	+
121'	56.3	ursolic acid	+	+	+	
122'	59.9	pomolic acid		+		

Note: +++: high amount; ++: moderate amount; + : low amount; RI is the retention index determined in regards to a series of n-alkanes (C7–C35) on the apolar DB-5 MS. The RI values are identified as following: $RI = 100x n + 100x ((\text{Apex } Rt_{(\text{lower alkane})} - Rt_{(\text{lower alkane})}/Rt_{(\text{follower alkane})} - Rt_{(\text{lower alkane})}))$ where n is the number of carbon of lower alkane. The tR is the retention time in minute. Cyclohexane = CHX, Dichloromethane = DCM, Ethyl acetate = EtOAc, acetonitrile = MeCN