

Supporting Information

Preparation of nanoemulsions from *Elsholtzia kachinensis* and *Elsholtzia ciliata* essential oils using ultrasonic homogenization and their application for antibacterial and anticancer activities

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Table S1. Chemical compositions of essential oils of *E. kachinensis* and *E. ciliata*

No.	Compounds	RT	Contents (%)	
			<i>E. kachinensis</i>	<i>E. ciliata</i>
1	α -Pinene	7.314	0.215	-
2	Camphene	7.631	0.074	-
3	Sabinene	8.16	1.498	-
4	β -Pinene	8.226	0.388	0.07
5	1-Octen-3-ol	8.292	0.086	1.98
6	6-Methylhept-5-en-2-one	8.438	-	1.07
7	β -Myrcene	8.519	0.089	0.16
8	α -Terpinene	9.056	0.147	-
9	D-Limonene	9.307	6.748	1.08
10	<i>trans</i> - β -Ocimene	9.699	-	29.21
11	γ -Terpinene	9.92	0.342	-
12	Acetophenone	10.086	-	0.19
13	α -Terpinolene	10.516	0.075	-
14	p-Cymene	10.665	-	0.11
15	Durenol	10.669	1.013	-
16	β -Linalool	10.735	0.516	0.15
17	1-Octen-3-yl acetate	10.947	4.821	0.27
18	β -Citronellal	11.753	-	0.10
19	2-Methyl pyrazine	11.967	-	0.39
20	4-Terpineol	12.267	0.124	-
21	Vinylcyclohexane	12.303	-	0.63
22	4-Octynoic acid, 7-(t-butyldimethylsilyloxy)-, t-butyldimethylsilyl ester	12.52	0.083	-
23	2-Formyl-1-methylpyrrole	12.984	2.273	-

24	Neral	13.157	-	0.96
25	3-tert-Butylphenol	13.222	-	0.21
26	β -Citral	13.395	-	8.99
27	Geraniol	13.611	-	0.95
28	2-Ethyl-1,4-Benzodioxine	13.824	0.147	-
29	α -Citral	13.915	-	11.15
30	1-Cyclohexene-1-carboxaldehyde	14.032	-	0.42
31	Methyl nerate	14.079	-	0.12
32	Anethol	14.207	-	3.96
33	Bornyl acetate	14.224	0.202	-
34	Dehydroelsholtzia ketone	14.536	62.858	0.26
35	Methyl geranate	14.815	-	0.43
36	Isovaleric acid	15.3	-	0.1
37	3-Carene	15.482	-	0.87
38	Terpilene	15.723	-	0.14
39	Copaene	15.792	0.45	-
40	Car-3-ene-2,5-dione	15.796	-	0.41
41	β -Bourbonene	15.96	0.528	-
42	β -Elemene	16.04	0.22	-
43	Cedr-8-ene	16.436	0.161	-
44	β-Caryophyllene	16.538	5.42	6.24
45	α -Bergamotene	16.72	-	0.35
46	β -Farnesene	16.992	0.968	24.25
47	β -Selinene	17.08	-	0.73
48	α-Humulene	17.083	4.401	-
49	α -Gurjunene	17.402	0.269	-
50	α -Curcumene	17.447	0.408	-
51	Germacrene D	17.507	-	1.85
52	β -Cubebene	17.508	0.479	-
53	(-)-Zingiberene	17.639	0.155	-
54	Germacrene B	17.746	-	0.62
55	β -Bisabolene	17.847	0.207	-

56	α -Cedrene	17.896	1.089	-
57	β -Patchoulene	18.104	1.824	-
58	Cadinene	18.108	-	0.14
59	Nerolidol	18.65	-	0.2
60	Caryophyllene oxide	19.089	0.08	-
61	<i>trans</i> -3-Octene	24.511	0.847	-
62	Bis(2-ethylhexyl)-1,2-Cyclohexanedicarboxylate	26.579	0.699	-

Note: RT: relative time; (-): undetected

Table S2. Mulliken atomic charge of tween 80, dehydroelsholtzia ketone, *trans*- β -ocimene and β -farnesene

Tweens			
Atoms	Charges	Atoms	Charges
O1	-0.52527	H52	0.154194
O2	-0.50308	H53	0.138717
O3	-0.48553	H54	0.121677
O4	-0.50598	H55	0.186049
O5	-0.48092	H56	0.128362
O6	-0.60662	H57	0.130823
O7	-0.60842	H58	0.115923
O8	-0.60776	H59	0.134787
O9	-0.46074	H60	0.120895
O10	-0.48466	H61	0.131471
C11	0.139508	H62	0.123256
C12	0.08626	H63	0.12756
C13	0.126974	H64	0.118517
C14	0.105097	H65	0.168879
C15	-0.02203	H66	0.154364
C16	-0.00993	H67	0.391456
C17	-0.04245	H68	0.394601
C18	-0.01688	H69	0.129434
C19	-0.04088	H70	0.130858
C20	-0.05234	H71	0.390958
C21	-0.04601	H72	0.126436
C22	-0.01733	H73	0.126053

C23	-0.04859	H74	0.126691
C24	-0.04886	H75	0.126384
C25	-0.2533	H76	0.151157
C26	-0.25649	H77	0.143914
C27	-0.25254	H78	0.127711
C28	-0.24873	H79	0.126377
C29	-0.25274	H80	0.127356
C30	-0.25223	H81	0.126254
C31	-0.25234	H82	0.128521
C32	-0.364	H83	0.135574
C33	-0.25216	H84	0.126043
C34	-0.25232	H85	0.126494
C35	-0.30151	H86	0.167062
C36	0.62954	H87	0.172445
C37	-0.24545	H88	0.127414
C38	-0.3017	H89	0.135094
C39	-0.09431	H90	0.133511
C40	-0.24642	H91	0.135986
C41	-0.09369	H92	0.126275
C42	-0.4413	H939	0.12577
H43	0.126034	H94	0.134089
H44	0.157274	H95	0.136132
H45	0.119863	H6	0.129363
H46	0.16251	H97	0.129635
H47	0.130983	H98	0.112346
H48	0.145299	H99	0.111717
H48	0.115946	H100	0.140874
H50	0.143062	H101	0.141021
H51	0.169928	H102	0.140733

Table S3. Mulliken atomic charge of dehydroelsholtzia ketone

Atom	Charge
O1	-0.45101
O2	-0.52453
C3	0.112705
C4	0.223567

C5	0.388054
C6	0.211375
C7	-0.21761
C8	-0.24746
C9	-0.50462
C10	0.09926
C11	-0.51198
C12	-0.53255
H13	0.140685
H14	0.14384
H15	0.141891
H16	0.18142
H17	0.181269
H18	0.161629
H19	0.161233
H20	0.159525
H21	0.161232
H22	0.152837
H23	0.216397
H24	0.152834

Table S4. Mulliken atomic charge of *trans*- β -ocimene

C1	-0.34889
C2	0.191543
C3	-0.15773
C4	-0.17426
C5	0.198649
C6	-0.50575
C7	-0.51196
C8	-0.53615
C9	-0.09973
C10	-0.3633
H11	0.145624
H12	0.15408
H13	0.112247
H14	0.120896
H15	0.14867
H16	0.150205
H17	0.151168
H18	0.152449
H19	0.151358
H20	0.153632
H21	0.150808
H22	0.160368
H23	0.160526
H24	0.120948
H25	0.138398
H26	0.136198

Table S4. Mulliken atomic charge of β -farnesene

C1	-0.33505
C2	0.213973
C3	-0.30652
C4	-0.30187
C5	-0.17134
C6	-0.34974
C7	-0.1414
C8	-0.52647
C9	0.181708
C10	0.233834
C11	-0.50499
C12	-0.51304
C13	-0.10221
C14	-0.41613
C15	-0.35531
H16	0.136186
H17	0.132954
H18	0.138368
H19	0.142655
H20	0.142439
H21	0.148714
H22	0.107625
H23	0.147694
H24	0.141361
H25	0.106825
H26	0.155124
H27	0.148223
H28	0.158897
H29	0.150775
H30	0.147782
H31	0.147367
H32	0.151908
H33	0.14982
H34	0.151775
H35	0.12441
H36	0.139034
H37	0.139497
H38	0.143032
H39	0.142084