

Table 1. Chemical composition of *Atractylodes lancea* volatile oils

Compound name	t/R min	Area%
Humulene alpha-Caryophyllene	10.195	4.31%
Chloracetic acid, tridecyl ester tride	10.575	1.85%
Panaginsene	10.735	4.29%
Naphthalene,1,2,3,4,4a,7-hexahydro-1	10.9	2.66%
7-(6-Methyl-pyridin-2yl)-heptane-1,6-dio	11.005	1.65%
2,4,7,14-Tetramethyl	11.21	1.50%
Naphthalene, decahydro-4a-methyl-1m	11.33	3.77%
Cyclohexene, 3-(1,5-dimethyl-4-hexenyl)	12.455	6.02%
1H-Cyclopropa[a]naphthalene,decahyd	13.04	15.02%
Cyclohexanemethanol,4-ethenyl-alpha	13.385	2.24%
1,5-Cyclodecadiene,1,5-dimethyl-8-(1-	13.86	3.68%
(8R,8aS)-8,8a-Dimethyl-2-(propan-2-yl)	14.15	4.18%
Epicubenol(1S,4R,4aS,8aR)-1-Isopr	16.105	10.40%
2-Naphthalenemethanol, decahydro-al	17.93	0.79%
(4aS,8aR)-3,8a-Dimethyl-5-methylene-4	18.025	2.13%
2-(4a,8-Dimethyl-2,3,4,5,6,8a-hexahydro	18.295	3.04%
1H-Benzocyclohepten-9-ol,2,4a-beta,5	19.13	2.12%
[1,1'-Biphenyl]-4-carboxaldehyde	19.84	4.39%
1,1,4,7-Tetramethyldecahydro-1H-cyclo	20.265	4.74%
(3aR,4R,7R)-1,4,9,9-Tetramethyl-3,4,5,6	21.1	4.26%
3-(1,1-Dimethylallyl)-6-hydroxycoumarin	30.13	4.59%
9,12-Octadecadienoic acid (Z, Z)-, methy	32.525	4.00%
2-(3,7-Dimethyl-octa-2,6-dienyl)-1,4-dim	33.93	1.94%
Tetracosamethyl-cyclododecasiloxane	35.945	1.00%
Total		94.57%

Table 2. The binding energy for different moleculars from Atractylodes lancea volatile oils with ADAR2 enzyme.

Mol ID	Molecule name	Molecular weight	Receptor	Mean binding energy
MOL000024	alpha-humulene	204.39	ADAR2	-5.81
MOL000032	beta-Eudesmol	222.41		-5.42
MOL000043	atractylenolide i	230.33		-6.53
MOL000060	selina-4(14),7(11)-dien-8-one	218.37		-5.90
MOL000084	beta-daucosterol	576.95		-5.27
MOL000085	beta-daucosterol_qt	414.79		-6.92
MOL000086	(24S)-5beta-Stigmastan-3beta-ol	416.81		-6.83
MOL000087	beta-sitosterol 3-O-glucoside	576.95		-4.65
MOL000088	beta-sitosterol 3-O-glucoside_qt	414.79		-6.91
MOL000091	daucosterin	576.95		-5.78
MOL000092	daucosterin_qt	414.79		-7.19
MOL000093	daucosterol	576.95		-5.81
MOL000094	daucosterol_qt	414.79		-6.95
MOL000114	vanillic acid	168.16		-3.72
MOL000162	beta-Chamigrene	204.39		-5.82
MOL000163	Atractylodin	182.23		-4.77
MOL000164	atractylone	216.35		-5.60
MOL000165	2-[(2S,5S,6S)-6,10-dimethylspiro[4.5]dec-9-en-2-yl]propan-2-ol	222.41		-5.12
MOL000166	ZINC01609418	222.41		-4.39
MOL000167	3β-hydroxyatractylone	232.35		-5.49
MOL000168	()-2-Carene	136.26		-4.47
MOL000169	alpha-Guaiene	204.39		-5.43
MOL000170	guaiene	204.39		-5.53
MOL000171	Guaiol	222.41		-5.35
MOL000172	Furol	96.09		-2.66
MOL000173	wogonin	284.28		-4.78
MOL000174	(2E,8E)-9-(2-furyl)nona-2,8-dien-4,6-diyn-1-ol	198.23		-3.07
MOL000175	cyperene	204.39		-5.79
MOL000178	atractylenolide iii	248.35		-6.33
MOL000179	2-Hydroxyisoxyparyl-3-hydroxy-7-isopentene-2,3-dihydrobenzofuran-5-carboxylic	306.39		-4.20
MOL000180	Aractylenolide II	232.35		-6.68
MOL000181	atractylenolide III	248.35		-6.34
MOL000182	Atractylayne	314.46		-3.24
MOL000183	Beta- Eudesmol	222.41		-5.28
MOL000184	NSC63551	412.77		-7.33
MOL000185	Stigmasterol 3-O-beta-D-glucopyranoside	574.93		-6.13
MOL000186	Stigmasterol 3-O-beta-D-glucopyranoside_qt	412.77		-7.15
MOL000187	butenolide B	234.32		-5.78
MOL000188	3β-acetoxyatractylone	274.39		-5.57
MOL000189	acetyl atractylodinol	240.27		-3.89
MOL000190	3,5-dimethoxy-4-glucosyloxyphenylallyl alcohol	372.41		-2.27
MOL000191	3,5-dimethoxy-4-glucosyloxyphenylallyl alcohol_qt	210.25		-3.18
MOL000192	2-(1,4a-dimethyl-2,3-dihydroxydecahydronaphthalen-7-yl)isopropyl glucoside	418.59		-3.32
MOL000193	(Z)-caryophyllene	204.39		-5.59
MOL000194	patchoulene	204.39		-5.61
MOL013068	Oroxindin	459.41		-4.25