Supporting information

Table S1.
Identification of volatile compounds in MEO and BEO.

NO.	compounds	CAS	rt	MEO-1	MEO-2	MEO-3	MEO-4	MEO(relative content %)	BEO-1	BEO-2	BEO-3	BEO-4	BEO(relative content %)
		29050-33-		0.1472	10.288	7.0071	117.63		189.17	270.06	280.71	320.32	
1	(+)-4-Carene	7	28.5	23799	13041	29632	68689	0.084±0.049	7981	62432	12211	75622	13.941±2.519
		59341-22-		7021.8	5189.5	5534.3	1.5043		20.936	23.742	33.592	23.208	
2	(3H)Indazole, 3,3-dimethyl-	9	47.1667	35941	06946	04819	769	37.02±3.376	40468	97927	09292	2248	0.278±0.040
				1184.9	1329.6	1238.6	14.246		0.1472	47.720	0.1472	0.1472	
3	Ethanol, 2-(ethenyloxy)-	764-48-7	47.1667	53113	44498	96759	50239	0.067±0.078	23799	09607	23799	23799	0.171±0.019
		92418-72-		0.1472	23.129	17.559	48.106		0.1472	309.94	0.1472	1254.0	
4	(3-Methyl-oxiran-2-yl)-methanol	9	41.5	23799	4614	64585	8453	31.820±6.350	23799	01905	23799	84353	15.173±3.722
				4507.0	4365.1	6293.0	0.1472		10.734	13.815	17.239	13.309	
5	α-Phellandrene	99-83-2	16	30823	35458	68021	23799	5.525±0.393	67916	01973	65961	27889	25.567±0.193
				0.1472	792.51	0.1472	66.390		165.20	183.47	342.71	179.51	
6	α-Pinene	80-56-8	19.6667	23799	04271	23799	02594	0.975±0.005	59228	4399	58872	38514	8.696±1.990
				166.72	133.02	151.09	106.85		288.96	344.12	397.30	346.90	67.807±19.99
7	α-Terpineol	98-55-5	30.4167	73503	7837	89398	49365	56.220±11.634	72662	83433	53884	1256	5
				8363.3	7353.7	11289.	18.556		24.035	15.847	23.307	30.627	
8	β-Myrcene	123-35-3	16	63771	7643	25187	5441	7.618±0.444	27571	45423	58609	67254	0±0

		13877-91-		1406.9	1082.1	1138.6	1.7214		7.8148	7.3683	10.499	9.6058	48.478±16.23
9	β-Ocimene	3	18.6667	87418	11405	43461	16388	86.215±3.214	39999	57394	16787	79132	6
				14281.	8929.9	13292.	4.6536		8.9940	9.9480	9.3779	11.126	
10	β-Phellandrene	555-10-2	17.5833	25636	14589	54585	79664	5.590±0.271	64067	17696	72826	71637	35.583±3.335
				1006.5	847.30	818.87	2.1827		6.6543	7.2485	8.8481	6.1950	
11	β-Pinene	127-91-3	14	57358	84093	55164	32065	0.244±0.279	4751	36282	49569	99736	0.314±0.249
		91216-95-		35.798	0.1472	19.180	10792.		12660.	18553.	15713.	13954.	
12	γ-Glutamyl-(S)-allyl-L-cysteine	4	45.1667	80714	23799	75315	71505	6.859±3.837	37914	37838	44023	16135	38.933±8.181
				1593.5	507.75	590.84	11.597		26.507	34.539	36.451	23.839	
13	γ-Terpinene	99-85-4	25.0833	94621	33004	69883	14017	0.001±0.000	22609	69842	73891	81754	0.071±0.042
		211321-		35.910	0.1472	0.1472	18.114		35.412	43.104	50.669	40.651	
14	1-(2-Methoxyethoxy)-2-methyl-2-propanol	90-3	47	60447	23799	23799	35106	0.006±0.008	20697	23094	53421	38945	5.452±4.729
				2.6665	0.1472	0.1472	12.943		1406.2	1516.5	1699.1	1409.3	
15	1,1,1-Tris(hydroxymethyl)propane	77-99-6	39.3333	91405	23799	23799	9333	0.001±0.000	91746	76335	35934	62498	12.845±1.330
		20521-44-		15.525	0.1472	810.91	8.9573		36.105	76.692	176.58	147.23	
16	1,11-Dodecadiyne	2	31.25	77835	23799	7766	62986	0.001±0.000	21362	07166	51002	28329	0.252±0.203
				0.1472	4.7015	0.1472	1.4355		2.8382	2.3060	5.6545	5.0955	
17	1,2-Propanediol	57-55-6	38.5833	23799	45597	23799	25938	0.720±0.471	36237	09696	39554	97131	0.3578±0.216
		18368-95-		79.769	65.542	194.89	36.010		4476.7	5801.2	5032.2	9103.8	
18	1,3,8-p-Menthatriene	1	22.9167	1598	43218	37868	95086	0.010±0.001	28175	98366	64162	36556	0.075±0.11
				1.8636	1.3392	1.8111	0.1472		1072.0	1220.6	1451.4	1184.1	
19	1,5-Diacetoxypentane	6963-44-6	16.8333	33532	49182	93216	23799	0.570±0.185	53836	67204	26446	16093	0±0
				142.63	59.924	86.399	27.331		10.797	18.613	24.101	0.1472	
20	1,6-Octadiene, 3,7-dimethyl-	2436-90-0	24.6667	1315	77562	70932	64896	9.075±0.720	36504	82131	89941	23799	5.280±0.815
		22460-59-		1641.7	1245.4	58.807	0.1472		0.1472	50.603	225.99	0.1472	
21	1,7-Octadien-3-ol, 2,6-dimethyl-	9	27.25	08592	42496	76225	23799	0.001±0.000	23799	72044	5166	23799	11.092±1.549

				0.1472	0.1472	9.7534	10.909		232.46	432.99	447.24	421.83	
22	1,8-Nonadiyne	2396-65-8	19.25	23799	23799	57573	57956	0.117±0.010	0827	77538	7048	78121	0.092±0.032
				21.169	13.416	16.269	120.99		116.34	135.90	170.75	126.67	
23	1-Butanamine, 3-methyl-	107-85-7	37.3333	39644	48782	67135	89928	0.544±0.269	9696	5267	86464	73125	0.145±0.127
				42.946	117.20	93.418	35.587		91.374	108.19	120.84	105.78	
24	1-Butanol, 3-methoxy-	2517-43-3	45.9167	29397	96838	88362	31104	0.045±0.014	25567	48441	51473	78046	0.055±0.012
				11.114	4.7952	6.2109	739.55		9233.6	5.4828	10776.	3647.7	
25	1-Butanol, 3-methyl-	123-51-3	17.3333	28485	88206	38768	19496	0.001±0.000	56557	9039	06932	80092	0.020±0.010
				0.1472	0.1472	0.1472	12.141		293.64	335.35	383.17	331.89	
26	1-Butene, 3-methyl-	563-45-1	28.6667	23799	23799	23799	77927	0.176±0.015	17536	47082	48571	22791	3.569±0.529
	1H-Cyclopenta[1,3]cyclopropa[1,2]benzene, octahydro-7-methyl-3-	13744-15-		26.454	27.214	28.210	0.1472		49.892	36.904	44.089	56.751	
27	methylene-4-(1-methylethyl)-, (3aS,3bR,4S,7R,7aR)-	5	26.8333	78862	88997	52686	23799	0.690±0.097	15123	75149	9961	23839	0.492±0.176
				127.65	87.280	1119.4	2.9305		42.032	42.930	6.3276	45.606	
28	1-Heptanol	111-70-6	26.0833	51562	43332	72554	55051	0.145±0.020	55326	11707	9501	6657	0.111±0.023
				28.309	21.759	23.982	10.692		5.2421	6.8488	10.329	4.2242	
29	1-Hexanol	111-27-3	21.75	54163	79971	32225	68243	0.263±0.019	84186	81222	86725	83354	1.111±0.023
				48.822	37.501	37.796	13.947		6.7466	13.240	11.475	13.908	
30	1-Octanol	111-87-5	27.25	22302	70191	50618	8477	0.001±0.000	45363	34592	68171	50707	0.056±0.007
				9.9974	7.0778	0.1472	391.71		17.198	0.1472	20.379	14.386	
31	1-Pentanol	71-41-0	18.6667	06399	96548	23799	92175	0.020±0.004	61985	23799	64652	90751	0.046±0.005
				2.8300	2.6569	3.6848	3.7078		10.169	15.146	14.194	14.552	
32	1-Penten-3-ol	616-25-1	15.6667	29615	63494	08408	44919	0.006±0.005	26981	70055	69352	30163	0±0
				2.0733	21.937	0.6203	302.38		9.4266	0.1472	0.1472	0.1472	
33	1-Propanol, 2-chloro-	78-89-7	11.75	59973	74805	96051	82031	0.238±0.045	83204	23799	23799	23799	0.366±0.017
				52.197	30.205	34.800	0.8306		0.9627	2.6193	1.9720	1.1431	
34	1-Propanol, 2-methyl-	78-83-1	13.5	1886	07261	77711	24452	0.296±0.082	9086	99588	82429	01774	0±0

				68.894	30.446	43.181	1852.6		0.1472	1879.7	1995.7	0.1472		
35	1-Propen-2-ol, acetate	108-22-5	5.75	83168	79054	52478	225	3.914±1.252	23799	42812	11416	23799	0±0	
				862.03	385.14	0.1472	5029.9		2812.0	5212.6	6058.9	3857.5		
36	1-Propene, 2-methyl-	115-11-7	45.6667	26044	03858	23799	1458	0.053±0.016	23029	90767	59616	78254	0±0	
				9.2847	5.6748	11.424	8716.7		31301.	18026.	16557.	27992.		
37	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	30.6667	74444	33832	36863	38841	0.507±0.160	96853	89136	19937	31248	1.958±0.618	
				65.278	103.67	70.345	0.1472		112.32	123.62	125.60	128.56		
38	2,4,6-Octatriene, 2,6-dimethyl-, (E,Z)-	7216-56-0	22.75	63204	85338	93389	23799	0.050±0.004	77846	73357	6643	02609	0.649±0.157	
				8.6142	7.1601	8.6186	0.1472		10.935	14.200	15.196	11.760		
39	2,4-Heptadienal, (E,E)-	4313-03-5	25.5	94584	24593	77678	23799	0.985±0.158	22453	49835	58559	68996	11.220±3.359	
				145.88	128.47	176.11	33.996		10.808	11.432	11.693	10.524		
40	2,4-Hexadienal, (E,E)-	142-83-6	23	23182	4926	19894	76367	1.187±0.164	80181	62313	2094	58655	0.046±0.049	
		22410-74-		188.63	164.34	212.38	3.9652		23.716	6.1139	6.4695	48.548		
41	2,6-Octadien-1-ol, 2,7-dimethyl-	8	27.25	93839	85917	12124	64951	0.001±0.000	34428	68352	09574	19602	2.459±0.761	
				91.256	0.1472	0.1472	14.697		1.6342	0.1472	3.8760	0.1472		
42	2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	106-25-2	33.75	18352	23799	23799	47381	0.192±0.238	22189	23799	39907	23799	0±0	
		14898-79-		12.799	5.4523	71.769	1.6193		4.7711	4.0887	8.3685	75.266		
43	2-Butanol, (R)-	4	37.75	7604	2149	40347	02488	0.080±0.092	12763	7289	76894	15396	4.228±0.302	
				0.1472	21.732	26.903	11.049		21.932	23.861	37.546	21.140		
44	2-Butenal	4170-30-3	11.6667	23799	6394	29789	32187	0.081±0.093	39309	06603	03809	3891	0.061±0.015	
		15798-64-		26.144	0.1472	0.1472	0.1472		30050.	37735.	43986.	27676.		
45	2-Butenal, (Z)-	8	11.6667	70005	23799	23799	23799	0.077±0.006	28786	11617	11389	94027	0.089±0.020	
				13.401	11.425	12.991	907.14		42.910	34.797	42.770	34.414		
46	2-Butenal, 3-methyl-	107-86-8	16.9167	81153	3034	41832	31141	0.226±0.007	21743	28741	74968	84818	34.540±7.498	
				38.526	35.418	34.075	6.8885		12.922	15.730	23.341	13.134		
47	2-Butene, 1-bromo-3-methyl-	870-63-3	20.25	58903	1373	80274	60045	0.008±0.005	62664	72479	14269	95662	0.006±0.002	

				1.8814	0.3571	1.9733	14337.		16082.	9835.0	0.1472	14094.		
48	2-Butenoic acid, ethyl ester, (E)-	623-70-1	15.8333	55414	93178	66082	15039	0.123±0.018	18799	80153	23799	98764	1.006±0.002	
				20.128	15.076	21.485	19.189		49.659	61.419	62.934	63.031		
49	2-Caren-10-al	6909-19-9	32.75	4465	07918	10865	06189	0.525±0.063	83018	29124	47046	45323	2.006±0.002	
				92.875	66.239	90.949	61.779		216.50	127.70	380.72	128.37		
50	2-Cyclohexen-1-one, 4-(1-methylethyl)-	500-02-7	30.0833	60254	1951	53527	81111	0.089±0.043	98664	87187	29491	44809	1.015±0.029	
				17.896	5.6047	11.666	3.2159		1.2197	0.1472	0.1472	0.1472	52.449±17.57	
51	2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, cis-	5989-33-3	27.0833	51436	79581	12235	23543	1.23±0.198	78249	23799	23799	23799	6	
				0.1472	219.39	165.26	14.747		0.7531	1.0432	1.1896	1.1178		
52	2-Heptanone, 6-methyl-5-methylene-	498-51-1	28.3333	23799	82243	91584	01234	0.001±0.000	57894	5052	5725	79729	0.045±0.005	
		154264-		37.077	27.299	0.1472	38.680		7.0477	0.1472	0.1472	4.4913		
53	2-Heptanone, 7,7,7-trichloro-	40-1	16.4167	17738	53519	23799	19492	0.031±0.005	72515	23799	23799	09666	0.029±0.002	
		18829-55-		4.8535	3.9715	4.8007	0.1472		15.593	0.1472	16.699	16.550		
54	2-Heptenal, (E)-	5	20.8333	1265	13498	08762	23799	0.135±0.014	08232	23799	8031	5721	0.203±0.008	
				25.879	21.502	19.978	1241.4		0.1472	30.524	4103.4	0.1472		
55	2-Hexenal	505-57-7	17.6667	50072	96342	13893	92873	0.126±0.038	23799	22076	57097	23799	0.572±0.067	
		75697-98-		21.945	11.169	21.253	0.8133		0.1472	4.9222	0.1472	0.1472		
56	2-Isopropenyl-5-methylhex-4-enal	2	30.1667	48767	21424	87013	99849	0.001±0.000	23799	42207	23799	23799	1.875±0.575	
				8.1117	3.2689	0.1472	370.27		34.172	39.581	38.979	34.636		
57	2-Isopropylmalic acid	3237-44-3	38.5	54023	05397	23799	8193	0.438±0.039	02799	98795	69733	7129	0.063±0.008	
		134225-		78.646	59.346	71.429	337.48		895.46	1137.4	1308.8	1138.7		
58	2-Nonen-4-yn-1-ol, (Z)-	90-4	27.0833	13797	71818	90631	44943	0.516±0.054	43055	1634	54414	64624	0.316±0.197	
				83.001	83.758	70.698	7.3157		2555.9	3706.9	3218.9	667.37		
59	2-Octanone	111-13-7	28	79362	55912	09707	58671	0.001±0.000	9639	62655	98278	73232	0.015±0.009	
				22.164	22.285	0.1472	23.314		0.1472	14.662	3.4772	14.183		
60	2-Octenal, (E)-	2548-87-0	23.75	64207	99767	23799	04589	0.018±0.012	23799	7409	39142	19672	0±0	

				1.5342	1.0232	3.7435	930.24		953.39	7336.2	2443.8	8004.9	
61	2-Pentanol	6032-29-7	32.3333	02441	44739	50068	24455	0.394±0.570	00791	42621	50665	79829	0.605±0.363
		19872-52-		15.573	0.1472	190.61	2.4444		25.994	16.221	21.673	47.429	
62	2-Pentanone, 4-mercapto-4-methyl-	7	21	16144	23799	41056	7011	0.176±0.045	30226	92348	93628	86988	0±0
				19.684	30.095	26.753	35.021		10.390	0.1472	0.1472	17.523	
63	2-Pentanone, 5-bromo-	3884-71-7	19.6667	60258	33267	98223	46148	0.057±0.027	46319	23799	23799	66687	0.060±0.007
				3.5778	8.4780	10.423	403.69		66.617	81.139	88.871	68.959	
64	2-Penten-1-ol, (Z)-	1576-95-0	24.0833	18728	14699	22721	45872	0.025±0.006	7214	78004	35927	67546	0.156±0.015
				5.0157	4.0498	0.1472	89.284		33.799	41.091	47.467	36.458	
65	2-Pentenal, (E)-	1576-87-0	14.6667	34349	30107	23799	93982	0.132±0.061	00371	7792	15564	87546	0.423±0.031
				32.322	21.367	10.234	31.004		0.8986	0.1472	0.9237	0.1472	
66	2-Pentenal, 2-ethyl-	3491-57-4	16	38458	16189	86197	99722	0.001±0.000	83108	23799	33864	23799	0.724±0.548
				0.1472	0.1472	9.0778	99.845		7733.5	12412.	6174.5	8973.6	
67	2-Propanol, 1-(1-methylethoxy)-	3944-36-3	43.5	23799	23799	56789	28226	0.001±0.000	45188	56128	0164	79494	0.410±0.301
		19686-73-		0.1472	71.049	0.1472	6.1294		7.6970	8.1599	8.8670	8.3879	
68	2-Propanol, 1-bromo-	8	46.75	23799	42587	23799	91244	0.101±0.088	72143	76039	35694	29637	0.001±0.000
				32.315	1.8975	16.015	52.190		0.1472	13.956	0.1472	0.1472	
69	2-Propanol, 1-propoxy-	1569-01-3	47.25	32881	29704	53839	49974	0.001±0.000	23799	55795	23799	23799	0.047±0.005
				36.936	0.2944	0.1472	40.164		196.23	237.55	60.462	26.737	
70	2-Propanone, 1-hydroxy-	116-09-6	5.91667	54875	47598	23799	87978	0.001±0.000	77837	58725	32728	59989	0.983±0.983
				0.1472	1262.6	0.1472	18.818		29.759	33.468	41.071	24.002	
71	2-Propenal	107-02-8	44.5	23799	70524	23799	2347	0.376±0.012	72081	92448	75724	68202	0±0
		58175-57-		67.147	54.608	58.438	0.1472		128.15	15.672	177.88	28.217	
72	2-Propyl-1-pentanol	8	25.6667	31409	7391	63138	23799	0.041±0.010	88136	36007	95076	59081	0±0
				7.4091	8.2119	4.9039	0.1472		11.366	13.572	22.873	14.744	
73	2-Undecanone	112-12-9	32.8333	58282	9313	48783	23799	0.027±0.010	05087	05962	03659	55462	0±0

		30086-02-		2.7819	4.5134	5.5785	760.14		116.58	280.51	160.16	139.97	
74	3,5-Octadien-2-one, (E,E)-	3	26.1667	77443	45098	93641	29898	32.914±15.423	25116	56244	69871	57288	0±0
		56805-23-		5176.1	6203.8	1938.8	945.54		15.209	16.287	29.648	29.260	
75	3,6-Nonadien-1-ol, (E,Z)-	3	25.4167	15285	71978	35832	80475	0.095±0.058	23948	90427	43394	25081	0.036±0.022
		59906-54-		7.9354	6.5783	22.246	0.1472		311.60	607.44	807.23	252.41	
76	3-Hexanone, 2,5-dimethyl-4-nitro-	6	19.5	81626	31508	26483	23799	5.464±0.614	47827	54531	14298	27788	0.076±0.019
				0.1472	3.8399	775.79	209.45		44.194	29.272	0.1472	11.144	
77	3-Hexen-1-ol, (Z)-	928-96-1	22.6667	23799	74995	15439	70093	5.231±0.372	9071	24473	23799	27508	0.181±0.017
				880.15	851.61	832.25	0.1472		129.24	122.88	0.1472	36.217	
78	3-Hexen-1-ol, acetate, (E)-	3681-82-1	26.0833	61805	26585	20773	23799	0.001±0.000	50598	96328	23799	7408	0.151±0.051
				0.1472	0.1472	148.49	176.18		3870.3	2466.4	3693.0	2815.3	
79	3-Hexen-1-ol, acetate, (Z)-	3681-71-8	26.6667	23799	23799	21293	14963	0.016±0.018	62319	56725	9912	44497	0.073±0.070
				4.3049	0.1472	5.7481	772.85		0.1472	0.1472	12.465	0.1472	
80	3-Hydroxy-2-butanone	513-86-0	35.25	2716	23799	27138	171	0.216±0.046	23799	23799	01113	23799	0.126±0.119
				29.546	27.776	41.333	38.015		228.85	190.36	222.87	210.81	
81	3-Isopropyl-4-methyl-1-pentyn-3-ol	5333-87-9	35.8333	06391	77428	14604	22085	0.470±0.885	97889	37736	5077	1731	0.161±0.180
				7.5027	0.1472	277.13	1.1408		30.191	46.590	3.4117	86.033	
82	3-Methyl-3-nitrobut-1-ene	1809-67-2	31.1667	68778	23799	24931	09659	0.001±0.000	96902	27876	27896	88399	0.305±0.269
				0.1472	14.223	0.1472	0.1472		2.3513	8.3580	3.8171	3.5613	
83	3-Nonanone	925-78-0	21.75	23799	69386	23799	23799	0.001±0.000	38792	69217	05079	67654	0.060±0.014
		20184-89-		22.057	0.1472	1.0517	20.030		16.809	17.104	21.053	19.855	
84	3-Nonyne	8	30.75	285	23799	57712	93216	0.582±0.650	46045	10547	30786	32962	0.774±0.181
				15.878	65.257	41.502	5.6872		6.3613	6.6178	8.8284	4.0989	
85	3-Penten-1-ol, 4-methyl-	763-89-3	41.1667	74892	16107	24937	03297	0.001±0.000	18829	35354	20313	91542	0.163±0.037
				3.2592	0.1472	2.5584	32.705		74.634	88.904	111.02	89.938	
86	3-Penten-2-one, (E)-	3102-33-8	14.5833	14582	23799	88459	86746	0.200±0.026	71409	62541	84937	1673	0.106±0.080

				0.1472	26.259	31.028	281.26		3721.6	5921.6	5519.7	4915.1		
87	3-Phenyl-1-propanol, acetate	122-72-5	35.6667	23799	40096	11909	95111	1.550±0.209	06124	89929	395	83098	9.748±0.463	
				275.93	268.88	196.81	13.614		14.633	18.549	21.002	15.779		
88	4-Carene, (1S,3S,6R)-(-)-	5208-50-4	25	62509	24993	27129	93361	0.339±0.022	38248	42406	88865	17928	0±0	
				63.761	48.728	52.270	79.041		0.1472	24.497	41.227	0.1472		
89	4-Hexen-1-ol, (E)-	928-92-7	20.9167	21744	57687	94827	23589	0.001±0.000	23799	9503	23052	23799	0.074±0.066	
				17.275	0.1472	0.1472	0.1472		219.16	367.88	365.48	384.87		
90	4-Penten-1-ol	821-09-0	16.5	42483	23799	23799	23799	0.114±0.018	5547	39908	90971	3975	0±0	
				23.350	15.842	15.856	0.1472		11.024	7685.9	0.1472	5.5489		
91	5-Hepten-1-ol, 2,6-dimethyl-	4234-93-9	43	37503	45687	37669	23799	0.001±0.000	06044	00079	23799	98733	0.025±0.004	
		609306-		17.109	0.1472	29.235	246.94		2256.6	2819.6	3307.4	640.26		
92	5-Octen-2-yn-4-ol	99-2	28.5833	18865	23799	51864	01181	0.082±0.015	11336	88456	93854	00534	0±0	
		41446-66-		11.512	14.097	15.019	1759.9		4173.1	8806.5	12780.	14596.		
93	5-Tetradecene, (E)-	6	28.5833	50962	5171	27219	28987	54.239±34.005	04962	2231	31617	41588	0±0	
				953.76	10289.	9164.0	28394.		881.53	1081.5	0.1472	843.88		
94	6-Octen-1-ol, 3,7-dimethyl-, acetate	150-84-5	29.4167	64509	34889	85961	01877	146.851±4.667	37591	41622	23799	90816	0±0	
				32609.	26299.	18761.	16361.		0.1472	0.1472	697.72	0.1472		
95	6-Octenal, 3,7-dimethyl-, (R)-	2385-77-5	25.3333	66254	68356	81265	28529	0.048±0.021	23799	23799	94241	23799	0.6060±0.293	
		31499-72-		11.756	8.0847	2.9943	5601.1		2849.7	1651.6	0.1472	6173.6		
96	7,8-Dihydro-α-ionone	6	36.9167	48084	61601	42973	57484	5.914±1.876	4058	12917	23799	1725	5.0300±1.507	
				19.314	25.272	27.410	7681.2		0.1472	15.559	0.1472	18.875		
97	Acetaldehyde	59-66-5	47.1667	66168	66442	51229	34616	0.125±0.044	23799	62718	23799	68753	0.304±0.128	
				28.081	16.860	10.522	5428.4		7.2975	0.1472	4.8594	9.9971		
98	Acetaldehyde, tetramer	108-62-3	44.8333	44588	35305	64352	99581	0.333±0.362	88739	23799	67416	55638	0.399±0.263	
				333.19	256.15	285.75	7.5236		101.69	221.52	224.36	223.74		
99	Acetic acid	64-19-7	24.0833	01095	39847	04539	40175	1.810±0.106	65928	33705	05044	53576	17.155±2.362	

				103.48	80.760	106.10	14.003		170.52	0.1472	0.1472	176.65	
100	Acetic acid, 2-phenylethyl ester	103-45-7	33	40623	77335	89462	64972	0.628±0.075	70516	23799	23799	59482	2.531±0.262
				756.60	634.53	695.62	1100.7		109.43	352.09	182.13	231.52	
101	Acetic acid, heptyl ester	112-06-1	22.1667	64437	55856	11271	9292	4.463±0.226	84847	86717	18034	95206	0.599±0.250
				75.760	61.763	78.566	59.520		0.1472	1801.8	0.1472	0.1472	
102	Acetic acid, hexyl ester	142-92-7	17.9167	20969	32615	03817	92068	0.436±0.054	23799	12488	23799	23799	0.730±0.368
				28.340	2.6221	25.888	99.285		198.09	792.45	575.48	234.43	
103	Acetic acid, hydroxy-, ethyl ester	623-50-7	41.3333	07605	12163	8213	98089	0.090±0.088	36939	777	37525	74215	0.017±0.003
				5.9195	3.9753	0.1472	120.18		0.1472	195.19	105.49	147.91	
104	Acetic acid, octyl ester	112-14-1	29.9167	40957	37036	23799	90569	0.046±0.052	23799	76392	04748	51673	0±0
				17.107	11.491	13.980	765.20		46.887	48.601	0.1472	0.1472	
105	Acetic acid, pentyl ester	628-63-7	14.5	66801	27042	56287	94431	0.085±0.012	80358	44859	23799	23799	1.154±0.062
				28.689	18.848	18.689	0.1472		36.364	0.1472	0.1472	97.312	
106	Acetonitrile	75-05-8	10.4167	82287	72474	69391	23799	0.131±0.024	17926	23799	23799	15584	0.145±0.011
				0.1472	3.4894	0.1472	47.175		35.761	50.036	71.875	47.137	
107	Acetophenone	98-86-2	29.4167	23799	83996	23799	34067	0.001±0.000	73949	13485	36439	84473	0.492±0.055
				9.7656	5.2094	66.649	12.474		25.386	36.265	46.220	0.1472	
108	Allyl acetate	591-87-7	33.1667	0029	60893	84555	97806	0.1471±0.190	4223	68043	50276	23799	0.561±0.363
		14289-96-		7736.7	4742.2	4319.5	3404.1		38315.	32294.	66718.	30706.	
109	Allyl methallyl ether	4	25.4167	90458	93131	11709	88549	34.561±7.346	71949	25003	43452	24479	0.026±0.009
				0.1472	0.1472	0.1472	4.7905		44.758	4223.3	2423.3	35.753	
110	Aromandendrene	489-39-4	29.5833	23799	23799	23799	74925	0.001±0.000	58548	29057	89741	1046	1.181±0.116
				0.1472	0.1472	0.1472	1.8023		28.301	39.592	39.971	70.650	
111	Azulene	275-51-4	31.5833	23799	23799	23799	67277	0.001±0.000	68675	09244	13458	22209	0.010±0.004
				63.929	53.808	51.129	29.858		739.31	1052.1	1384.4	1034.1	
112	Benzaldehyde	100-52-7	26.25	70417	5209	04673	82564	0.338±0.034	32162	0944	10718	79145	0.173±0.034

				8.6231	9.4280	8.4735	833.41		21262.	22293.	22324.	28427.	
113	Benzaldehyde, 4-(1-methylethyl)-	122-03-2	32.4167	75112	54064	20297	61664	0.064±0.018	91937	03071	01053	84713	0.551±0.034
				289.80	256.94	313.50	22.259		245.21	293.76	341.31	305.93	
114	Benzene, 1-methyl-3-(1-methylethyl)-	535-77-3	19.25	11881	07546	69636	35925	1.881±0.219	23966	796	11473	3661	3.828±0.189
				32.186	30.886	38.173	0.1472		15.990	20.260	17.609	0.1472	
115	Benzene, 1-methyl-4-(1-methylethenyl)-	1195-32-0	24	37868	58533	61903	23799	0.211±0.026	89658	77719	79394	23799	0.311±0.022
				0.1472	359.01	505.51	44.100		31.416	22.910	71.504	12.264	
116	Benzeneacetic acid, methyl ester	101-41-7	31.75	23799	98628	40447	86765	3.129±0.689	63108	49024	47125	46125	0.575±0.059
				28.882	28.590	28.900	1059.9		24.947	5.9668	21332.	4.6042	
117	Benzoic acid, 2-methylpropyl ester	120-50-3	32.5833	82229	04525	32315	89781	0.187±0.014	93023	50046	57008	5086	0±0
				34.241	43.274	45.352	1512.5		1165.7	1666.9	1429.3	1913.0	
118	Benzoic acid, methyl ester	93-58-3	28.6667	49099	76112	81536	72584	0.261±0.043	96184	48662	62984	24493	0.405±0.060
				32.150	23.658	23.167	133.63		35.171	38.366	55.980	18.751	
119	Benzyl alcohol	100-51-6	34.4167	85657	38418	25184	72487	0.165±0.016	0456	58413	24511	51174	0±0
				2651.2	860.13	0.1472	7389.8		170.81	0.1472	0.1472	0.1472	
120	Bicyclo[2.2.1]heptane-2-methanol	5240-72-2	15.8333	83382	86652	23799	60479	10.888±4.893	86585	23799	23799	23799	0±0
		17699-16-		43.447	162.84	55.384	91.413		104.38	108.99	140.46	7.1050	
121	Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, (1α,2α,5α)-	0	24.6667	49637	74355	9732	57809	0.563±0.449	31218	83769	32783	27795	0.032±0.019
				2.0555	1.5292	2.0241	187.52		2624.3	5016.5	3743.8	3040.7	
122	Butanal, 2-methyl-	96-17-3	7.83333	38092	39475	25759	6436	0.011±0.001	49224	83951	25143	49748	0.030±0.003
				5.3806	3.2435	3.4588	0.1472		3426.7	4111.8	5100.7	4601.3	
123	Butanal, 3-methyl-	590-86-3	7.91667	26727	46988	7527	23799	0.026±0.005	81189	64582	43987	97867	0.034±0.004
				0.1472	0.1472	0.1472	187.27		19.199	11545.	1903.6	20205.	
124	Butane, 2-bromo-2-methyl-	507-36-8	33.5	23799	23799	23799	44253	0.001±0.000	49881	27021	45604	07688	0.120±0.115
				7.9611	5.1267	5.9556	1.9288		708.47	457.93	1065.3	3158.1	
125	Butanoic acid	107-92-6	28.6667	50002	49412	10902	23385	0.042±0.006	39258	87934	72214	49663	0.108±0.047

				368.65	285.54	316.16	22.245		3549.8	4428.7	3314.5	4860.4	
126	Butanoic acid, 2-methylpropyl ester	539-90-2	15.75	74175	30176	66368	36129	1.992±0.126	93542	88406	34332	46499	0±0
				9.1074	6.5567	7.7140	11.334		0.1472	2.1776	0.1472	0.5396	
127	Butyrolactone	96-48-0	28.9167	68013	08741	84792	83271	0.045±0.008	23799	67637	23799	92245	0.028±0.004
				14.761	11.313	11.808	0.1472		5.8713	8.7709	8.4329	6.5735	
128	Camphene	79-92-5	12.5833	32304	05838	60313	23799	0.076±0.006	30364	20434	07758	04814	0.141±0.008
				1379.3	1200.0	0.1472	42.451		102.06	119.88	150.38	100.11	
129	Caryophyllene	87-44-5	28.3333	08698	17764	23799	48142	7.982±0.036	80097	59611	75998	44813	1.492±0.075
				15.898	39.934	0.1472	7.6210		20.494	21.968	57.746	28.790	
130	CHF2CH2OH	359-13-7	42.25	82135	21932	23799	56456	0.174±0.086	51248	88783	60368	70412	0.079±0.018
		157477-		0.1472	8.8111	0.1472	7.1553		3.1454	4.4481	10.087	0.8327	
131	cis-Muurola-4(15),5-diene	72-0	40.1667	23799	89905	23799	75315	0.001±0.000	21789	60818	97309	73897	0.044±0.022
				27157.	18395.	32889.	5.5966	167.513±38.15	7.8591	8.6391	8.1694	7.6439	
132	Citronellal	106-23-0	25.3333	88648	82093	86264	67367	4	65223	09671	29451	90907	3.360±0.567
				2936.6	2171.2	65.106	0.1472		106.72	140.99	153.40	177.04	
133	Citronellol	106-22-9	32	60668	75261	88521	23799	15.979±1.418	82785	70232	71033	32814	0±0
				105.41	95.133	105.50	13444.		713.75	0.1472	0.1472	0.1472	
134	Copaene	3856-25-5	25.75	94091	98073	80033	01843	0.637±0.032	87042	23799	23799	23799	1.522±0.941
				2.5402	1.6899	0.1472	11.587		277.91	222.68	425.35	339.12	
135	Cycloheptylamine	5452-35-7	11.0833	56771	15976	23799	50767	0.009±0.006	83539	31242	38977	18547	0.013±0.004
				3.9872	0.1472	0.9508	19.493		305.85	0.1472	0.1472	362.51	
136	Cyclooctylamine	5452-37-9	32.3333	96222	23799	11913	60047	0.010±0.009	53003	23799	23799	43715	0±0
				0.1472	37.407	55.455	85.566		399.74	455.82	488.24	542.96	
137	Cyclopentane, nitro-	2562-38-1	33.75	23799	56377	85512	56085	0.354±0.104	38534	91425	3345	47123	0±0
				1665.8	1683.1	1425.3	254.37		1830.1	2468.4	3174.2	2591.1	
138	Decanal	112-31-2	25.6667	98359	70552	67574	93909	9.234±1.775	41845	94061	09243	66793	0.585±0.148

				80.055	0.1472	62.402	26.162		133.82	154.91	217.82	165.11	
139	Diethylene glycol	111-46-6	44.75	58724	23799	61801	74849	0.218±0.252	89186	50484	21954	42957	0.216±0.039
				0.1472	9528.8	3393.9	156.51		2458.8	0.1472	0.1472	2270.0	
140	D-Limonene	5989-27-5	25.3333	23799	63011	5675	62192	40.013±21.006	67768	23799	23799	02886	12.419±7.076
				4.1043	2.4660	8.3460	7.1562		0.1472	0.1472	26.377	0.1472	
141	Dodecanoic acid, ethyl ester	106-33-2	41.4167	24549	06328	47549	29427	0.032±0.016	23799	23799	00297	23799	0.015±0.006
		54550-10-		62.136	11.351	0.1472	0.1472		11.710	15.013	25.771	19.052	
142	Estran-3-one, 17-(acetyloxy)-2-methyl-, (2α,5α,17β)-	6	27.5833	20248	24982	23799	23799	0.423±0.383	94687	00462	71953	83706	0.150±0.020
				588.17	711.73	308.49	234.94		3723.5	3275.3	4307.7	9643.1	20.049±13.63
143	Ethanamine, N,N-difluoro-	758-18-9	43.6667	83507	058	51864	04536	2.987±1.354	42338	09325	41482	93474	3
				11639.	9410.2	10363.	6.0389		19.137	5.3988	137.56	38.447	
144	Ethanol	64-17-5	8.58333	25465	27103	66546	07863	66.122±2.553	49295	87421	83895	02734	5.240±0.847
				1390.4	706.01	625.50	0.1472		3354.8	0.1472	3861.0	9063.1	
145	Ethanol, 2-(vinyloxy)-	75-07-0	47.1667	90743	09184	90127	23799	8.225±1.012	93403	23799	61776	72072	1.216±0.061
				694.43	252.19	418.95	3.3831		1.5078	3.2967	4.7054	2.7149	
146	Ethanol, 2-[2-(ethenyloxy)ethoxy]-	929-37-3	44.5833	03397	01622	80893	39799	2.877±0.978	61298	01805	27459	03915	3.015±0.450
				2.8192	1.6243	10.845	598.12		119.94	182.50	191.12	181.75	
147	Ethylmalonic acid	601-75-2	19.6667	63495	88443	60316	78992	0.028±0.028	3872	88173	37067	11733	0.010±0.004
				114.72	126.32	286.67	2643.2		0.1472	0.1472	0.1472	82.178	
148	Formaldehyde	50-00-0	47.0833	57766	46033	58859	30166	1.309±0.647	23799	23799	23799	92876	0.193±0.018
				23.305	12.176	16.510	169.89		0.1472	10.430	12.799	20.589	
149	Formic acid	64-18-6	25.6667	85074	60668	27795	66989	0.103±0.025	23799	243	64966	67058	0±0
				4.8397	3.9814	6.5952	134.92		120.98	0.1472	0.1472	140.18	
150	Furan, 2-pentyl-	3777-69-3	18	05254	01959	68864	68163	0.029±0.010	21456	23799	23799	24901	0±0
				66.514	50.004	34.183	1.4760		0.1472	6.4355	0.1472	1.7798	
151	Furan, 3-(4-methyl-3-pentenyl)-	539-52-6	23.4167	42441	49595	91799	01383	0.294±0.078	23799	02158	23799	28212	0.741±0.133

				1.5185	0.5075	1.4581	4.8982		0.1472	4.5499	0.1472	10.770	
152	Furfural	98-01-1	23.5833	09453	63706	69701	40557	0.007±0.003	23799	59748	23799	78049	0.187±0.079
		23986-74-		238.64	205.30	204.22	14.460		134.18	168.17	183.55	157.10	
153	Germacrene D	5	30.9167	55759	0004	10925	31523	1.384±0.060	43241	15313	55137	64823	13.312±1.973
				46.001	30.643	0.1472	32.361		96.241	0.1472	0.1472	0.1472	
154	Heptanal	111-71-7	16.5	86467	37314	23799	70755	0.227±0.035	99372	23799	23799	23799	0.038±0.005
		16630-91-		1496.5	1115.5	1257.4	21.693		14.195	16.685	14.301	12.131	
155	Heptanal, 2-methyl-	4	17.1667	63175	41962	84913	08263	8.079±0.660	57043	14631	43385	2829	0.135±0.029
		51209-78-		81.099	64.042	70.600	0.1472		58.943	76.538	125.01	100.45	
156	Heptanoic acid, 2-methyl-, methyl ester	0	19.75	1101	94598	21024	23799	0.478±0.057	09006	84542	0381	45697	0.136±0.013
				176.63	125.84	118.59	5.7546		0.1472	0.1472	0.1472	119.09	
157	Hexanal	66-25-1	13.0833	81411	12114	19074	78188	0.846±0.125	23799	23799	23799	20986	0.471±0.049
				242.37	180.93	28.629	110.51		539.34	749.67	922.35	767.31	
158	Hexane, 1-(ethenyloxy)-	5363-64-4	22.9167	73441	67264	74826	63272	1.305±0.106	32733	4168	64421	5027	0.142±0.057
				49.438	37.832	39.055	10.448		58.316	1390.1	158.85	297.14	
159	Hexanoic acid, 5-methyl-, methyl ester	2177-83-5	18.3333	99394	94338	26969	64349	0.248±0.020	78762	72603	63406	12114	0±0
				16.850	11.923	13.303	7.1083		45.309	6.2042	80.793	7.5328	
160	Hexanoic acid, ethyl ester	123-66-0	18.0833	68013	68183	91056	04223	0.089±0.008	40521	3007	24086	35346	0.003±0.000
				29.423	10.976	0.1472	2.9023		183.88	374.30	512.96	349.49	
161	Hexanoic acid, methyl ester	106-70-7	16.5833	25715	93862	23799	21886	0.112±0.052	95304	93885	9414	13145	0.006±0.006
				234.12	210.12	250.02	34.638		643.49	564.53	1120.3	554.09	
162	Humulene	6753-98-6	30.0833	81244	36831	75904	96141	1.490±0.133	7845	01911	17432	45535	8.546±0.939
		19411-65-		8.2564	0.1472	0.1472	73.027		9.4687	0.1472	3.8435	0.1472	
163	Hydroxylamine, O-(3-methylbutyl)-	5	41.5	57969	23799	23799	28709	0.028±0.032	21074	23799	79379	23799	0.614±0.486
				22.334	12.012	15.692	26.338		10.971	0.1472	13.493	0.1472	
164	Isobutyl acetate	110-19-0	10.8333	89274	67797	00519	55332	0.098±0.024	38946	23799	9677	23799	5.200±0.515

				0.1472	5.2509	0.1472	0.1472		36.531	15.095	0.1472	4.7651	
165	Isoprene	78-79-5	23.9167	23799	92428	23799	23799	0.018±0.020	58889	12243	23799	06498	0.022±0.006
				6731.9	4310.1	5924.2	42.681		33.047	43.773	56.472	48.450	
166	Isopulegol	89-79-2	27.75	28795	46958	6661	3326	38.046±7.226	08223	31384	04318	6559	0±0
		58461-27-		3474.8	0.1472	9.3267	36.073		0.1472	0.1472	52.606	15.439	
167	Lavandulol	1	26.5833	44262	23799	32154	77558	0.030±0.030	23799	23799	62672	83489	0.149±0.049
				7140.3	6825.6	5843.3	38.667		9.7671	75.626	24.306	0.1472	129.967±6.11
168	Limonene	138-86-3	17.0833	44032	48066	20698	33578	41.528±3.653	8995	57619	86446	23799	3
				41.345	0.1472	33.818	51.410		10.598	8.7121	0.1472	0.1472	
169	Limonene oxide, trans-	4959-35-7	24.6667	18344	23799	75421	55264	0.115±0.132	05608	78681	23799	23799	1.213±0.077
				3251.0	2772.1	2853.1	8.2060		145.97	271.93	212.03	71.313	158.365±46.8
170	Linalool	78-70-6	26.5833	68218	46658	16312	28649	19.247±1.347	29792	37484	61275	13779	88
		60047-17-		3.0514	0.1472	1.5087	19.746		30.965	30.730	27.222	16.007	
171	Linalool oxide	8	37.9167	95384	23799	38192	74045	0.011±0.008	96039	68407	15707	14491	0.037±0.034
				831.03	654.15	769.11	8.6813		0.1472	46.403	0.1472	0.1472	81.189±10.13
172	Linalyl acetate	115-95-7	26.9167	29927	53466	73155	42282	4.837±0.370	23799	34576	23799	23799	4
				27.896	15.710	31.367	0.1472		0.1472	6.4419	24.091	0.1472	
173	Methacrolein	78-85-3	7	77956	30308	61625	23799	0.157±0.050	23799	87127	02303	23799	0.630±0.051
				107.24	84.662	84.091	2.5781		5.8496	3.0580	28.510	8.2819	
174	Methyl Alcohol	67-56-1	7.5	14988	54023	57791	86174	0.599±0.056	93226	39868	96647	82167	1.180±0.047
				91.069	78.650	111.82	0.1472		506.07	669.00	4.1705	381.73	
175	Methyl salicylate	119-36-8	32.3333	08418	66371	08438	23799	0.654±0.157	85832	65842	45419	24539	0±0
				3.9258	1.1914	4.4886	1.8169		7.8314	84.503	0.1472	134.33	
176	Methylene chloride	75-09-2	8.25	62433	05706	94477	34641	0.018±0.009	07865	2921	23799	77461	0.025±0.004
		24406-05-		0.1472	3.5819	0.1472	1526.0		513.11	2537.4	0.9943	9832.5	
177	α-Cadinene	1	32.75	23799	08142	23799	96128	0.001±0.000	85046	11559	03894	18329	0.006±0.002

				9.4448	5.0000	6.2387	0.1472		57.195	199.79	87.396	111.94	
178	Nerolidol	142-50-7	37.4167	67249	89216	56218	23799	0.001±0.000	11834	93279	30232	04212	0.304±0.064
		80556-89-		7.1069	226.06	154.33	8.2760		0.1472	45.060	34.975	61.129	
179	N-Nitroso(2-hydroxyethyl)glycine	4	45.75	16204	4629	60402	65878	0.046±0.011	23799	65557	35824	53246	0±0
		36393-56-		140.05	158.28	83.022	76.237		207.82	92.163	0.1472	195.51	
180	Norpseudoephedrine	3	3.75	38939	44294	54709	94361	0.741±0.640	23697	09606	23799	17705	0.489±0.266
				455.33	287.79	103.76	26.361		2.1355	0.1472	0.1472	2.1505	
181	Octanal	124-13-0	19.75	73919	77624	77398	66181	0.784±0.211	23787	23799	23799	69955	0.902±0.107
				30.557	14.152	30.875	246.10		179.16	298.27	199.28	221.73	
182	Octanoic acid, 2-methyl-, methyl ester	2177-86-8	14.9167	83584	98038	3621	74532	2.357±0.396	88631	0866	91735	84566	0.263±0.028
				32.165	0.1472	25.337	1.6856		4.6435	4.3345	1500.8	0.1472	
183	Oxirane, 2,3-dimethyl-, cis-	1758-33-4	41.0833	4547	23799	72989	86013	0.140±0.058	77284	98455	50845	23799	0.038±0.009
				5.2031	45.323	12.479	5.3878		5.2602	0.1472	3.6622	3.8066	
184	Paraldehyde	123-63-7	46.6667	98645	14919	90225	843	0.172±0.013	35742	23799	21991	68783	0±0
		20902-45-		26.860	0.1472	0.1472	0.1472		0.1472	45.346	59.817	0.5026	
185	Penicillamine disulfide	8	44.75	61659	23799	23799	23799	0.214±0.194	23799	37124	75395	99912	0.299±0.063
				14.908	8.6318	11.237	10.078		296.79	56.781	257.02	76.487	
186	Pentanal	110-62-3	9.75	09505	79149	00711	0061	0.001±0.000	0761	03035	36361	15391	0.157±0.060
				18.102	10.452	12.420	26.317		49.712	11.398	213.53	284.44	
187	Pentanoic acid, 3-methyl-, methyl ester	2177-78-8	14.75	95622	01517	87381	34286	0.072±0.012	56297	53934	14196	45529	0.114±0.006
				419.98	283.93	318.71	1087.9		0.1472	15.485	0.1472	0.1472	
188	Pentanoic acid, 4-methyl-, methyl ester	2412-80-8	15.1667	15772	25609	3941	98219	0.080±0.018	23799	05004	23799	23799	0.023±0.008
				0.1472	18.261	24.716	35.129		16.092	0.4350	67.084	5.6645	
189	Pentanoic acid, 4-oxo-	123-76-2	20.0833	23799	48202	99927	03221	2.208±0.282	83841	96169	27486	43972	0.060±0.012
				33.634	27.788	31.325	208.15		0.1472	55.827	417.44	215.17	
190	Phenylethyl Alcohol	60-12-8	35.25	87795	20095	02974	63383	0.158±0.036	23799	06126	38996	90881	0±0

		21195-59-		18.844	11.491	26.663	291.39		2533.1	744.99	9629.0	0.1472		
191	p-Mentha-1,5,8-triene	5	23.75	41948	05068	50383	64864	0.212±0.037	63645	94103	48091	23799	0.154±0.016	
				58.902	87.988	147.24	0.1472		115.97	1624.1	5.6170	1320.3		
192	p-Mentha-1,5-dien-8-ol	1686-20-0	32.25	9604	05158	45979	23799	0.121±0.040	92682	39196	20243	06879	0.064±0.004	
				2.4627	2.0525	2.1152	494.23		704.73	132.50	1139.0	820.99		
193	Propanal	123-38-6	5.41667	65041	36821	73314	45505	0.735±0.332	34827	09599	44711	22263	0.047±0.016	
				15.436	12.181	12.150	0.1472		53.375	50.467	82.065	18.696		
194	Propanal, 2-methyl-	78-84-2	5.66667	12151	48499	44231	23799	0.013±0.002	88514	08366	81578	60357	0.087±0.012	
				154.07	0.1472	0.1472	11.968		33.978	27.090	76.756	49.333		
195	Propane	74-98-6	43.0833	83764	23799	23799	96383	0.085±0.006	28287	05269	24732	87388	0±0	
				13.621	10.908	10.679	24.978		76.297	136.08	85.621	51.457		
196	Propanoic acid	79-09-4	26.4167	02675	15888	98896	56889	0.001±0.000	50967	73739	09088	06416	0.073±0.093	
				0.1472	7.3346	0.1472	3.4278		37.854	29.028	14.956	0.1472		
197	Propanoic acid, 2-methylpropyl ester	540-42-1	22	23799	88887	23799	85807	0.075±0.005	85449	0027	96788	23799	0.124±0.019	
				0.1472	0.1472	0.1472	30.808		51.224	136.35	74.762	126.33		
198	Propanoic acid, 2-oxo-, ethyl ester	617-35-6	7.66667	23799	23799	23799	78859	0.001±0.000	68988	18249	83369	92329	0.053±0.012	
				3.8227	35.638	49.483	102.84		90.468	0.1472	13.561	164.66		
199	Propanoic acid, 2-phenylethyl ester	122-70-3	36.6667	63153	23246	22873	04177	0.001±0.000	0923	23799	24952	66974	0.081±0.021	
				0.1472	169.47	139.41	670.35		67.795	0.1472	915.63	0.1472		
200	Propylene Glycol	57-55-6	40.5833	23799	38908	5802	64961	0.225±0.141	8327	23799	06208	23799	0±0	
				0.1472	0.1472	47.718	68.327		129.47	243.98	107.53	77.317		
201	R-(-)-1,2-propanediol	4254-14-2	44.9167	23799	23799	11115	77006	0.834±0.329	701	8283	91135	62136	0.600±0.268	
				2.0652	1.8733	1.1949	0.1472		5.7931	38.518	32.696	100.84		
202	Styrene	100-42-5	18.8333	70177	57911	07648	23799	0.001±0.000	27562	67927	4353	18285	0.101±0.055	
				163.14	92.091	174.01	71.363		58.207	1997.1	118.40	91.627		
203	Terpinen-4-ol	562-74-3	28.25	53346	67491	26323	09625	0.009±0.004	48916	93743	13334	22591	0±0	

				72.419	0.1472	0.1472	0.1472		55.190	60.600	276.31	108.78	
204	Tetraethylene glycol	112-60-7	47.25	24559	23799	23799	23799	0.964±0.255	90108	82784	03324	84096	12.370±3.425
		30361-34-		90.715	77.760	121.11	0.1472		20.690	11.863	40.337	10.770	
205	trans, trans-Octa-2,4-dienyl acetate	3	28.4167	99196	96593	72253	23799	0.001±0.000	48314	79816	39051	78049	0.254±0.199
				0.1472	0.1472	0.1472	300.44		509.42	603.48	575.32	555.32	
206	trans-β-Ocimene	3779-61-1	11.25	23799	23799	23799	225	0.609±0.153	03466	79631	72675	20264	2.594±0.892
				3.1846	2.3552	3.6116	140.13		38.530	54.531	216.30	181.24	
207	trans-Carveol	1197-07-5	33.5	42477	55567	8006	65707	0.001±0.000	1805	65102	70897	6286	20.813±5.934
				885.82	736.21	779.10	1096.9		1751.3	1154.9	1595.2	1246.8	
208	Trichloroacetic acid, 3-tridecyl ester	0-00-0	23.25	54852	49363	03387	57006	0.019±0.003	7895	39028	26751	32159	1.334±0.232
				28.536	0.9060	0.1472	1471.3		2934.1	3465.8	4217.0	3595.7	
209	Trichloromethane	67-66-3	11	725	46701	23799	40586	0.076±0.082	17756	67422	7105	34364	0.358±0.183
				14.924	0.1472	0.1472	135.31		74.455	0.1472	80.832	6011.9	
210	Triethylene glycol	112-27-6	40.4167	6396	23799	23799	31599	0.001±0.000	43494	23799	2778	5086	0.153±0.044
				0.1472	29.457	201.40	38.330		88.034	108.20	7.8176	0.1472	
211	Triethylene glycol monomethyl ether	112-35-6	45.1667	23799	06549	31657	57819	0.564±0.642	16146	84172	75373	23799	0.330±0.129
				107.02	83.822	109.38	0.1472		0.1472	0.1472	141.66	16.183	
212	Undecanal, 2-methyl-	110-41-8	18.8333	97043	10896	63389	23799	0.629±0.077	23799	23799	58355	25281	0.127±0.014

Table S2 Regression equation and linearity range (μg/mL n=8)

	Regression equation	Linearity range (μg/mL)	Related Coefficientt
hydroxy-α-sanshool	y=7.8504x+19.582	20~1000	0.9993
hydroxy-β-sanshool	y=4.4179x+3.3323	20~1000	0.9998
hydroxy-γ-sanshool	y=3.917x+30.392	20~1000	0.9987

Table S3 Degree of precision (n=6)

	Peak area						RSD value(%)
hydroxy-α-sanshool	4054.5	4054.5	4232.1	4071.4	4091.7	4083.8	1.6448
hydroxy-β-sanshool	4590.8	4590.8	4593.2	4602.9	4623.4	4625.9	0.353
hydroxy-γ-sanshool	8150.2	8150.2	8131.5	8181.6	8201.8	8198	0.3543

Table S4 Research on the reproducibility

	Sample content (μg/mL)					RSD value(%)
hydroxy-α-sanshool	12.63926	13.60939	13.83916	13.25198	12.25632	5.0434
hydroxy-β-sanshool	26.09106	25.29883	29.03364	25.59308	24.52923	6.6261
hydroxy-γ-sanshool	729.5193	716.4499	801.9869	788.357	859.1305	7.4284

Table S5 Research on the stability

	Injection time/h						RSD/%
	0	2	4	6	8	10	
hydroxy-α-sanshool	75.6	87	78.7	75.1	88.1	85.7	7.24
hydroxy-β-sanshool	120.1	121.8	115.4	119	137.8	131.6	6.89
hydroxy-γ-sanshool	5588.5	6073	5561.5	6187.3	6223.6	5669.4	5.27

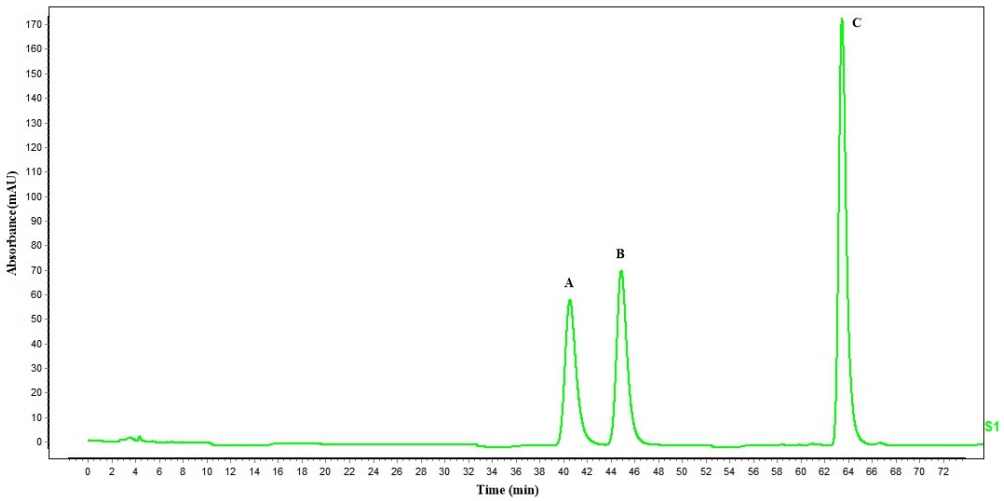

Figure S1 HPLC chromatogram of mixed standard of three compounds. A: hydroxy-α-sanshool; B: hydroxy-β-sanshool C: hydroxy-γ-sanshool

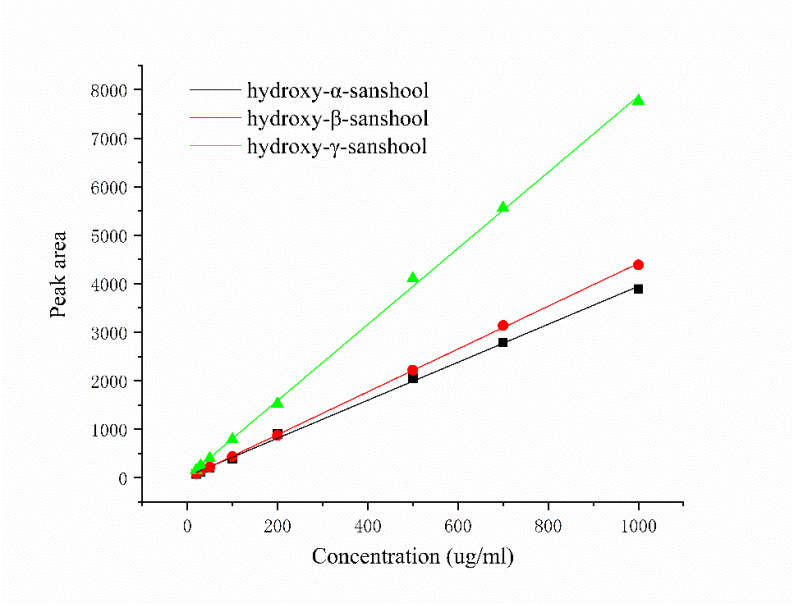

Figure S2 Standard curve of three sanshools