

Novel formula of antiprotozoal mixtures

Hubert Iwiński ^{1,3*}, Jacek Łyczko¹, Henryk Różański ^{2,3} and Antoni Szumny ¹

Table of content

Figure S1. GC-MS chromatogram of tea tree essential oil	1
Table S1. Composition of tea tree essential oil	1
Figure S2. GC-MS chromatogram of cedar essential oil	3
Table S2 Composition of Cedar essential oil	3
Figure S3. GC-MS chromatogram of eucalyptus essential oil.....	4
Table S3 Composition of eucalyptus essential oil.....	4
Figure S4. GC-MS chromatogram of lavender oil	5
Table S4. Composition of lavender essential oil	5

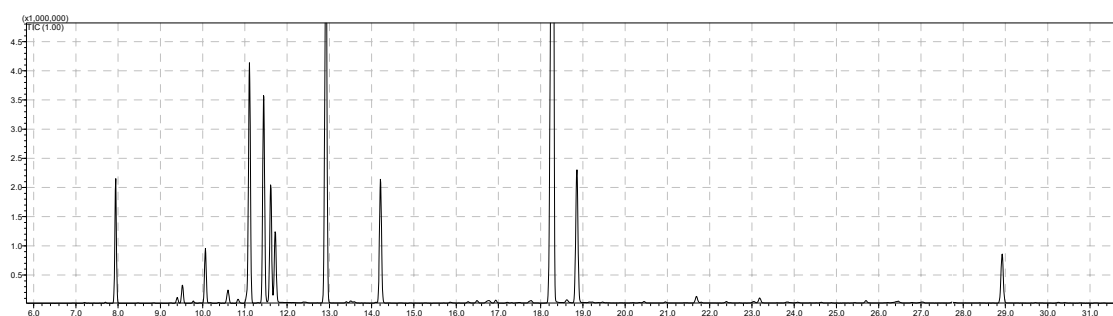


Figure S1. GC-MS chromatogram of tea tree essential oil

Table S1. Composition of tea tree essential oil

No.	Peak Name	tR (min)	KI exp.	KI Adams	KI NIST	CAS	Area (%)
1	Hexadienol	7.208	915		916	17102-64-6	0.032
2	α -Thujene	7.700	931		929	2867-05-2	0.03
3	α -Pinene	7.950	938	939	938	80-56-8	3.835
4	Sabinene	9.400	977		974	3387-41-5	0.189
5	b-Pinene	9.533	980	979	979	127-91-3	0.606
6	p-Menth-2-ene	9.775	986		984	5256-65-5	0.084
7	β -Myrcene	10.058	992		991	123-35-3	1.77
8	Carene < δ -2->	10.383	999		1001	554-61-0	0.035
9	α -Phellandrene	10.600	1005		1005	99-83-2	0.518
10	3-Carene	10.842	1012		1010	498-15-7	0.159
11	α -Terpinene	11.108	1019		1017	99-86-5	8.994
12	p-Cymene	11.442	1028		1024	99-87-6	7.624
13	Limonene	11.608	1032		1031	5989-27-5	3.966
14	Eucalyptol	11.725	1035		1032	470-82-6	2.263

15	Ocimene	12.392	1051	1050	3779-61-1	0.062	
16	γ -Terpinene	12.917	1063	1060	99-85-4	15.384	
17	p-Mentha-3,8-diene	13.400	1073	1075	586-67-4	0.033	
18	cis-Linalool oxide	13.508	1075	1069	5989 - 33 - 3	0.053	
19	Cresol <para->	13.583	1077	1073	106 - 44 - 5	0.02	
20	p-Mentha-2,4(8)-diene	14.100	1088	1085	586-63-0	0.013	
21	Terpinolene	14.208	1090	1086	586 - 62 - 9	4.827	
22	Dihydrocitronellal	15.858	1128	1125	5988 - 91 - 0	0.053	
23	Terpin-3-en-1-ol	16.283	1138	1136	586 - 82 - 3	0.067	
24	cis-b-Terpineol	16.492	1142	1140	7299-41-4	0.112	
25	Camphor	16.775	1149	1144	464-49-3	0.186	
26	Isopulegol	16.942	1152	1150	7786-67-6	0.121	
27	unknown	17.208	1158			0.036	
28	Isoborneol	17.500	1164	1165	10385 - 78 - 1	0.046	
29	Thujol	17.775	1170	1169	21653 - 20 - 3	0.157	
30	1-Terpinen-4-ol	18.250	1180	1177	562-74-3	39.239	
31	Cymen-8-ol	18.625	1188	1189	1197 - 01 - 9	0.134	
32	γ -Terpineol	18.858	1192	1197	586-81-2	5.576	
33	trans-Dihydro carvone	19.167	1198	1201	1200	147-86-02	0.054
34	unknown	19.467	1205			0.038	
35	neoiso-Dihydro carveol	20.450	1229	1230	18675 - 34 - 8	0.089	
36	Isobornyl formate	20.958	1240	1240	1200 - 67 - 5	0.054	
37	Cinnamyl alcohol<Z->	21.683	1257	1261	4510 - 34 - 3	0.253	
38	Carvone oxide<cis->	21.800	1259	1262	18383 - 49 - 8	0.014	
39	Isopulegyl acetate	22.400	1272	1273	89 - 49 - 6	0.094	
40	neo-Isopulegyl acetate	23.042	1286	1278	109010 - 10 - 8	0.061	
41	Isobornyl acetate	23.183	1289	1287	125 - 12 - 2	0.214	
42	Terpinyl acetate <trans-dihydro- α ->	23.833	1302	1300	20777-41-7	0.068	
43	a-Terpinyl formate	24.083	1308	1306	2153 - 26 - 6	0.04	
44	Dihydrocarvyl acetate	24.642	1322	1325	20405 - 60 - 1	0.03	
45	a-Terpinyl acetate	25.700	1347	1349	80 - 26 - 2	0.13	
46	Cyclosativene	26.467	1365	1367	30541 - 92 - 5	0.205	
47	Longicyclene	27.033	1377	1372	1137 - 12 - 8	0.076	
48	7-Epi-Sesquithujene	27.742	1393	1389	159407 - 35 - 9	0.081	
49	Caryophyllene	28.933	1422	1419	87-44-5	2.235	
50	Humulene	30.258	1455	1454	6753-98-6	0.039	

tR – retention time; KI exp.– Kovats index experimental, KI Adams– Kovats index according to Adams library, KI NIST – Kovats index according to NIST library

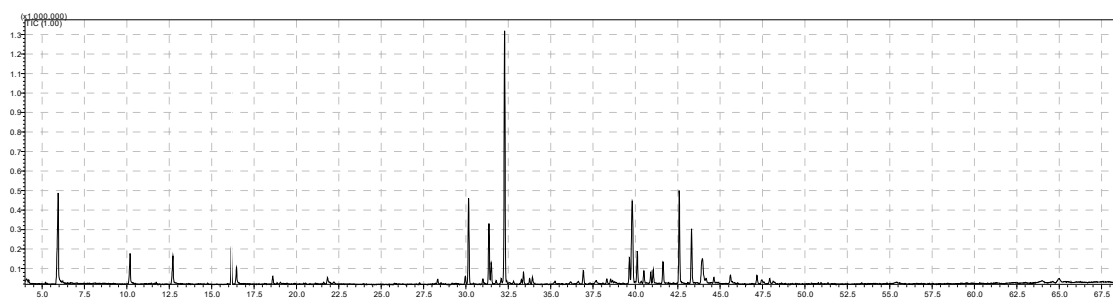


Figure S2. GC-MS chromatogram of cedar essential oil

Table S2 Composition of Cedar essential oil

No.	Peak Name	tR (min)	KI exp.	KI Adams	KI NIST	CAS	Area (%)
1	Limona ketone	16.167	1135	1131	1137	6090-09-1	3.656
2	cia-b-terpineol	16.467	1142	1144	1144	7299-41-4	2.072
3	Melilotal	18.608	1187	1188	1183	122 - 00 - 9	0.887
4	<i>trans</i> -Myrtanol	21.833	1260		1262	15358-91-5	0.687
5	Vestitenone	29.967	1448		1448	69401-36-1	0.859
6	α -Himachalene	30.158	1452		1499	3853-83-6	9.072
7	Thujopsadiene <cis->	31.000	1473		1467	51446 - 91 - 4	0.456
8	Himachalene <gamma-	31.492	1484		1484	53111 - 25 - 4	1.859
9	b-Himachalene	32.283	1502		1500	1461-03-6	27.350
10	Himachalene <alpha-dehydro-ar->	32.808	1517		1517	78204 - 62 - 3	0.354
11	Himachalene <gamma-dehydro-ar->	33.400	1532		1530	51766 - 65 - 5	1.148
12	g-Vetivenene	33.758	1541		1532	28908 - 26 - 1	0.638
13	Bisabolene <(E)-, alpha->	33.925	1546		1541	25532 - 79 - 0	0.936
14	Himachalene epoxide	35.258	1579		1579	64825 - 84 - 9	0.183
15	b-Himachalene oxide	36.925	1623		1619	57819 - 73 - 5	1.733
16	Cedren-13-ol<8->	39.642	1695		1689	18319 - 40 - 9	2.234
17	Atlantone<(Z)-gamma->	39.808	1699		1694	108549 - 48 - 0	12.261
18	Atlantone<(E)-gamma->	40.108	1708		1707	108549 - 47 - 9	3.222
19	Atlantone <(Z)-alpha->	40.500	1720		1716	56192 - 70 - 2	1.363
20	Eremophilone	40.908	1731		1733	562 - 23 - 2	1.126
21	Tumerone	41.050	1735		1734	180315-67-7	1.463
22	Cyclocolorenone	41.625	1752		1757	489 - 45 - 2	2.564
23	Atlantone <trans-, alpha->	42.583	1778		1775	32207 - 08 - 2	9.638
24	Acetoxyelemol<8-alpha->	43.308	1798		1793	256332 - 39 - 5	6.188
25	Longifolol acetate	43.950	1818		1820	205697 - 15 - 0	4.841
26	Khusinol acetate	44.433	1835		1828	78405 - 34 - 2	0.620
27	Flourensadiol	45.608	1867		1670	55812 - 89 - 0	0.796
28	Farnesyl acetone	47.167	1913		1913	1117-52-8	1.135
29	Acetoxyeudesman-4-alpha-ol <11->	47.925	1937		1940	67996 - 33 - 2	0.658

tR – retention time; KI exp.– Kovats index experimental, KI Adams– Kovats index according to Adams library, KI NIST – Kovats index according to NIST library

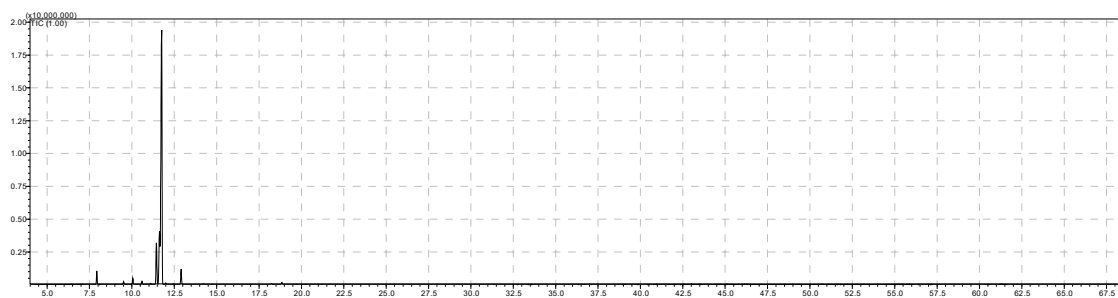


Figure S3. GC-MS chromatogram of eucalyptus essential oil

Table S3 Composition of eucalyptus essential oil

No.	Peak Name	tR (min)	KI exp.	KI Adams	KI NIST	CAS	Area (%)
1	α -Pinene	7.950	938	939	938	80-56-8	2.522
2	b-Pinene	9.533	980	979	979	127-91-3	0.576
3	β -Myrcene	10.058	992		991	123-35-3	1.203
4	α -Phellandrene	10.600	1005		1005	99-83-2	0.715
5	α -Terpinene	11.100	1019		1017	99-86-5	0.184
6	p-Cymene	11.450	1028		1025	99-87-6	9.831
7	Eucalyptol	11.725	1035		1032	470-82-6	80.665
8	trans- β -Ocimene	12.442	1052		1049	3779-61-1	0.091
9	γ -Terpinene	12.908	1062		1060	99-85-4	3.367
10	trans-Linalool oxide (furanoid)	14.225	1090		1086	34995-77-2	0.142
11	1-Terpinen-4-ol	18.250	1180		1177	562-74-3	0.218
12	γ -Terpineol	18.858	1192		1197	586-81-2	0.486

tR – retention time; KI exp.– Kovats index experimental, KI Adams– Kovats index according to Adams library, KI NIST – Kovats index according to NIST library

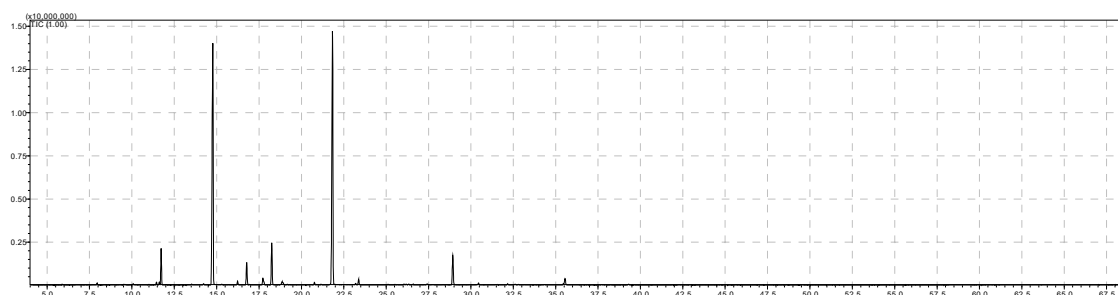


Figure S4. GC-MS chromatogram of lavender oil

Table S4. Composition of lavender essential oil

No.	Peak Name	tR (min)	KI exp.	KI Adams	KI NIST	CAS	Area (%)
1	α -Pinene	7.95	938	939	938	80-56-8	0.196
2	b-Pinene	9.533	980	979	979	127-91-3	0.063
3	p-Cymene	11.45	1028		1025	99-87-6	0.312
4	Limonene	11.617	1032		1030	138-86-3	0.249
5	Eucalyptol	11.725	1035		1032	470-82-6	4.029
6	cis-Linalool oxide	13.525	1076		1074	5989-33-3	0.166
7	trans-Linalool oxide (furanoid)	14.225	1090		1086	34995-77-2	0.156
8	Linalool	14.775	1101		1099	78-70-6	37.262
9	1-Octen-3-yl-acetate	15.292	1114		1111	2442-10-6	0.098
10	1,2-Dihydrolinalool	16.233	1136	1135	1120	18479-51-1	0.498
11	Camphor	16.775	1149		1144	464-49-3	2.955
12	Borneol	17.725	1169		1166	464-45-9	1.271
13	1-Terpinen-4-ol	18.25	1180		1177	562-74-3	5.461
14	γ -Terpineol	18.858	1192		1197	586-81-2	0.531
15	trans-Dihydro carvone	19.167	1198	1201	1200	09.04.5948	0.09
16	Fenchyl acetate	20.767	1236	1234	1234	13851-11-1	0.312
17	Butanoic acid, 3-methyl-, hexyl ester	21.158	1245	1244	1244	10032-13-0	0.096
18	Linalyl acetate	21.833	1260		1257	115-95-7	38.875
19	Isopulegol acetate	23.2	1289		1285	57576-09-7	0.206
20	Lavandulol acetate	23.375	1292		1290	25905-14-0	0.728
21	Hexyl tiglate	25.117	1334		1330	16930-96-4	0.101
22	8-Hydroxylinalool*	25.508	1343		1361	64142-78-5	0.089
23	unknown	26.05	1355				0.104
24	Neryl acetate	26.583	1367		1364	141-12-8	0.087
25	Geranyl acetate	27.417	1386		1382	105-87-3	0.178
26	Caryophyllene	28.933	1422		1419	87-44-5	4.244
27	(E)- β -Farnesene	30.45	1459		1457	18794-84-8	0.227
28	Bicyclogermacrene	32.158	1499		1500	24703-35-3	0.164
29	Lavandulyl isovalerate	32.608	1511		1508	51117-21-6	0.138
30	γ -Cadinene	32.808	1517		1514	39029-41-9	0.084
31	Germacrene B	34.35	1557		1559	15423-57-1	0.094
32	Caryophyllene oxide	35.55	1586		1581	1139-30-6	0.729
33	tau-Cadinol	37.733	1645		1642	147-47-90	0.071
34	α -Bisabolol	39.3	1686		1684	515-69-5	0.136

tR – retention time; KI exp.– Kovats index experimental, KI Adams– Kovats index according to Adams library, KI NIST – Kovats index according to NIST library