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SUPPLEMENTARY MATERIAL TO

Achillea clypeolata Sibth. & Sm. essential oil composition and QSRR model for predicting retention indices

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Table S-I. Predicted retention indices and molecular descriptors of essential oil compounds in *A. clypeolata* obtained by hydrodistillation

No	$Ri_{pred.}$	AATS0v	AATSC4c $\times 10^{-4}$	VR2 Dzi	VP-0	ETA Epsilon 3	IC0	BIC2
1	902.5058	182.020	-5.8	8.005	7.146	0.454	0.961	0.577
2	974.3304	182.020	-1.3	10.363	7.146	0.443	0.961	0.768
3	985.0507	182.020	-1.6	14.594	7.146	0.443	0.961	0.768
4	1001.993	182.020	-6.4	5.539	6.983	0.443	0.961	0.698
5	1006.013	194.598	-3.7	8.125	6.724	0.443	0.980	0.776
6	1015.869	182.020	-2.5	9.047	6.983	0.443	0.961	0.742
7	1017.944	182.020	-2.0	15.842	6.983	0.443	0.961	0.742
8	1047.053	183.293	-2.5	5.604	7.555	0.442	1.154	0.670
9	1062.964	182.020	-2.2	13.626	7.146	0.433	0.961	0.688
10	1068.251	194.598	-4.0	6.353	6.887	0.433	0.980	0.629
11	1071.717	172.795	-1.7	6.508	7.814	0.442	1.124	0.545
12	1077.483	182.020	-2.2	5.817	7.146	0.433	0.961	0.688
13	1097.757	182.020	-3.0	7.158	7.146	0.433	0.961	0.768
14	1123.312	172.795	-2.5	4.167	7.723	0.426	1.124	0.777
15	1132.768	172.795	-4.5	9.049	7.671	0.433	1.124	0.705
16	1135.335	183.293	-8.1	6.108	7.555	0.433	1.154	0.748
17	1155.812	183.293	-1.4	6.472	7.607	0.442	1.154	0.670
18	1160.327	183.293	8.8	13.688	7.464	0.442	1.154	0.794
19	1161.855	172.795	-5.0	9.560	7.723	0.442	1.124	0.647
20	1164.145	172.795	-0.6	5.917	7.560	0.433	1.124	0.712
21	1175.352	172.795	-9.4	6.941	7.723	0.433	1.124	0.763
22	1205.055	172.795	2.5	5.780	7.723	0.433	1.124	0.749
23	1214.242	195.469	-0.9	7.911	7.132	0.442	1.183	0.787

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Table S-I. Continued

No	$RI_{pred.}$	AATS0v	AATSC4c $\times 10^{-4}$	VR2 Dzi	VP-0	ETA Epsilon 3	IC0	BIC2
24	1220.251	195.469	8.5	7.064	7.257	0.433	1.183	0.725
25	1233.067	195.469	-10.0	7.675	7.257	0.433	1.183	0.725
26	1423.17	182.020	0.4	10.610	10.475	0.440	0.961	0.753
27	1469.839	182.020	-0.4	7.947	10.422	0.446	0.961	0.695
28	1491.72	182.020	-0,9	6.628	10.422	0.433	0.961	0.772
30	1493.986	182.020	-0.03	6.969	10.422	0.440	0.961	0.751
31	1502.399	182.020	0.5	7.513	10.638	0.440	0.961	0.711
33	1543.659	182.879	-0.3	6.024	10.792	0.445	1.106	0.719
34	1555.02	182.879	-1.2	7.221	10.883	0.445	1.106	0.711
35	1556.701	182.879	-1.7	22.398	10.831	0.439	1.106	0.735
36	1572.945	182.879	-6.2	7.221	10.792	0.439	1.106	0.777
37	1597.633	182.879	-4.6	7.351	10.629	0.439	1.106	0.736
38	1601.932	175.651	0.9	16.877	11.162	0.439	1.087	0.737
39	1646.202	173.568	0.9	15.457	10.619	0.418	1.067	0.737

$RI_{pred.}$ – predicted retention time, AATS0v - Average Broto-Moreau autocorrelation - lag 0 / weighted by van der Waals volumes; AATSC4c - Average centered Broto-Moreau autocorrelation - lag 4 / weighted by charges; VR2 Dzi - Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by first ionization potential; VP-0 - Valence path, order 0; ETA Epsilon 3 - Extended topochemical atom descriptor; IC0 - Information content index, neighborhood symmetry of 0-orderand; BIC2 - Bond information content index (neighborhood symmetry of 2-order.

1) Tricyclene; 2) α-Thujene; 3) α-Pinene; 4) Camphene; 5) Thuja-2,4(10)-diene; 6) Sabinene; 7) β-Pinene; 8) dehydro-1,8-Cineole; 9) α-Terpinene; 10) p-Cymene; 11) 1,8-Cineole; 12) γ-Terpinene; 13) p-Mentha-2,4(8)-diene; 14) Linalool; 15) Z-p-Menth-2-en-1-ol; 16) α-Campholenal; 17) Camphor; 18) Z-Chrysanthenol; 19) Borneol; 20) δ-Terpineol; 21) Terpinen-4-ol; 22) α-Terpineol; 23) Myrtenal; 24) Thymol; 25) Carvacrol; 26) E-Caryophyllene; 27) allo-Aromadendrene; 28) Germacrene D; 30) γ-Cadinene; 31) δ-Cadinene; 33) Spathulenol; 34) Caryophyllene oxide; 35) β-Oplopenone; 36) Muurola-4,10(14)-dien-1-β-ol; 37) Caryophylla-4(12),8(13)-dien-5-α-ol; 38) epi-α-Cadinol; 39) α-Cadinol

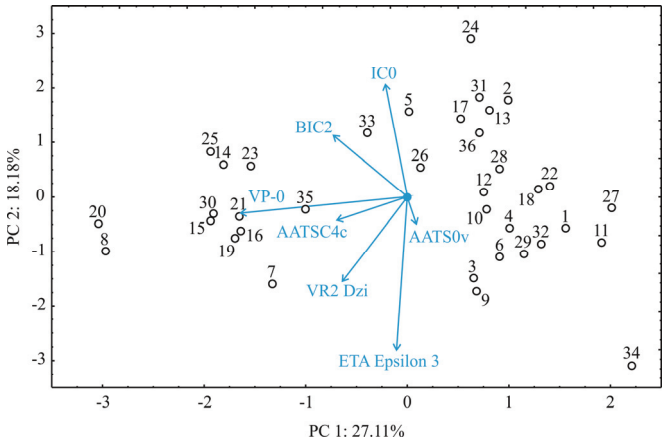

Fig. S-1. PCA ordination of molecular descriptors based on component correlations