

Supplementary Material

A Comparative Study of Chamomile Essential Oils and Lipophilic Extracts Obtained by Conventional and Greener Extraction Techniques: Chemometric Approach to Chemical Composition and Biological Activity

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Table S1. Composition of chamomile essential oils and extracts determined by GC-FID/MS analysis

% ^a												
#	Constituent	<i>R</i> _{exp} ^b	HD-1	HD-2	MWHD-1	MWHD-2	Sox-MeCl	Sox-Hex	SFE-1	SFE-2	SFE-3	SFE-4
1	Yomogi alcohol	996.4	tr. ^c	n.d. ^d	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
2	Artemisia ketone	1058.3	0.24	n.d.	0.19	0.27	n.d.	n.d.	0.15	0.19	0.19	0.26
3	Artemisia alcohol	1081.6	tr.	n.d.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
4	Borneol	1167.8	tr.	n.d.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
5	Artemisia acetate	1171.0	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
6	Menthol	1172.3	tr.	n.d.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
7	4,8-Dimethyl-nona-3,8-dien-2-one	1273.4	tr.	tr.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
8	Decanoic acid	1375.1	1.87	1.52	1.48	1.50	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
9	(<i>E</i>)-Caryophyllene	1419.6	tr.	n.d.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
10	(<i>E</i>)-β-Farnesene	1456.2	4.12	3.23	3.48	3.49	0.78	n.d.	1.04	1.45	1.32	1.22
11	dehydro-Sesquicineole	1468.7	0.55	0.47	0.48	0.49	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

% ^a												
#	Constituent	<i>RI</i> _{exp} ^b	HD-1	HD-2	MWHD-1	MWHD-2	Sox-MeCl	Sox-Hex	SFE-1	SFE-2	SFE-3	SFE-4
12	Germacrene D	1482.1	0.17	tr.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
13	<i>β</i> -Selinene	1487.2	0.31	0.25	0.28	0.28	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
14	Bicyclogermacrene	1497.4	tr.	tr.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
15	<i>β</i> -Bisabolene	1508.4	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
16	(<i>E</i>)-Nerolidol	1563.0	0.67	0.50	0.58	0.61	n.d.	n.d.	0.19	0.22	0.20	n.d.
17	Dodecanoic acid	1567.0	tr.	n.d.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
18	Dendrolasin	1572.7	tr.	tr.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
19	Spathulenol	1578.6	1.58	1.20	1.25	1.26	n.d.	0.39	0.30	0.35	0.34	0.34
20	Caryophyllene oxide	1583.9	0.23	tr.	0.17	0.18	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
21	Viridiflorol	1592.3	n.d.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
22	Salvial-4(14)-en-1-one	1594.6	0.23	n.d.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
23	Nerolidol oxide	1631.7	0.60	0.60	0.60	0.71	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
24	Gossonorol	1640.3	0.14	0.12	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
25	<i>epi-α</i> -Cadinol	1641.5	0.14	0.12	0.24	0.26	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
26	<i>α</i>-Bisabolol oxide B	1657.9	25.83	21.06	21.88	21.99	8.38	5.53	9.26	9.21	9.47	9.69
27	<i>seco</i> -Bisabolol oxide B	1664.0	1.21	1.47	1.58	1.73	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
28	Xanthoxylin (brevifolin)	1672.7	0.16	0.23	0.19	0.21	0.58	0.93	0.30	0.27	0.28	0.26
29	<i>α</i>-Bisabolone oxide A	1684.8	8.20	6.26	6.74	6.83	2.21	0.61	2.34	2.78	2.58	2.59
30	<i>α</i> -Bisabolol	1685.5	0.43	0.33	0.35	0.36	tr.	tr.	0.26	0.40	0.52	0.29
31	Germacra-4(15),5,10(14)-trien-1- <i>α</i> -ol	1689.0	0.38	tr.	0.32	0.33	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
32	Chamazulene	1732.6	4.95	4.59	4.96	5.21	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
33	<i>α</i>-Bisabolol oxide A	1750.7	29.71	34.41	33.62	33.22	18.39	11.84	16.41	20.47	21.04	21.14
34	Benzyl benzoate	1765.8	n.d.	n.d.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
35	Hexahydrofarnesyl acetone	1843.2	0.20	0.20	0.22	0.25	n.d.	0.32	0.17	n.d.	n.d.	n.d.
36	(<i>Z</i>)-Spiroether (<i>cis</i>-en-yn-dicycloether)	1883.8	9.19	11.72	10.86	9.44	12.81	5.15	8.66	9.31	8.07	7.47

% ^a												
#	Constituent	<i>RI</i> _{exp} ^b	HD-1	HD-2	MWHD-1	MWHD-2	Sox-MeCl	Sox-Hex	SFE-1	SFE-2	SFE-3	SFE-4
37	(<i>E</i>)-Spiroether (<i>trans</i> -en-yn-dicycloether)	1895.5	0.48	0.61	0.52	0.80	5.32	6.61	1.21	1.19	1.02	0.92
38	(<i>Z</i>)-Tibetin spiroether	1919.4	tr.	tr.	tr.	tr.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
39	(<i>E</i>)-Tibetin spiroether	1952.8	0.48	0.57	0.49	0.45	n.d.	n.d.	0.26	0.34	0.26	0.80
40	Hexadecanoic acid	1963.4	1.28	2.17	1.67	1.72	n.d.	1.75	0.76	0.81	0.64	n.d.
41	Linoleic acid	2133.7	0.30	0.69	0.39	0.42	1.16	0.58	0.70	0.62	0.45	0.64
42	Linolenic acid	2139.7	0.33	0.67	0.37	0.41	1.32	0.79	0.80	0.72	0.56	0.73
43	Leucodin	2171.2	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.19	0.22	n.d.	n.d.
44	Achillin	2215.4	n.d.	n.d.	n.d.	n.d.	1.24	1.15	1.24	1.33	1.14	1.56
45	Matricin/Achillicin	2293.8	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	1.25	1.40	1.31	1.26
46	Tricosane	2298.4	0.24	0.26	0.32	0.30	1.04	0.98	0.89	0.82	0.82	0.82
47	Matricarin/Acetoxyachillin	2394.3	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.22	0.28	0.24	0.33
48	Tetracosane	2397.6	tr.	tr.	tr.	tr.	0.65	0.66	0.62	0.56	0.57	0.57
49	Matricarin/Acetoxyachillin	2411.7	n.d.	n.d.	n.d.	n.d.	1.57	1.63	1.56	1.74	1.93	2.11
50	Pentacosane	2499.1	1.89	2.61	2.60	2.59	13.79	15.35	13.87	12.54	12.75	12.79
51	3-ethyl-Tetracosane	2570.7	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.30	0.22	0.21	n.d.
52	Hexacosane	2597.3	n.d.	tr.	tr.	tr.	0.71	0.84	0.88	0.74	0.73	0.76
53	Heptacosane	2698.7	0.50	0.81	0.66	0.72	9.22	11.71	10.45	9.25	9.46	9.85
54	13-Methyl + 11-Methyl heptacosane	2730.6	n.d.	n.d.	n.d.	tr.	0.63	0.53	0.26	0.26	0.31	n.d.
55	7-Methyl heptacosane	2739.7	n.d.	n.d.	n.d.	n.d.	0.85	0.73	0.58	0.54	0.51	0.54
56	3-Methyl heptacosane	2771.7	n.d.	n.d.	n.d.	n.d.	0.81	0.92	0.79	0.71	0.70	0.73
57	Octacosane	2798.0	n.d.	n.d.	n.d.	n.d.	n.d.	0.77	0.71	0.61	0.62	0.59
58	12-Methyl octacosane	2836.3	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.14	n.d.	n.d.	n.d.
59	4,12-Dimethyl octacosane	2880.0	n.d.	n.d.	n.d.	n.d.	0.57	n.d.	n.d.	n.d.	n.d.	n.d.
60	Nonacosane	2900.5	0.15	0.25	0.18	0.21	7.72	10.27	8.61	7.50	7.77	8.35

% ^a												
#	Constituent	<i>RI</i> _{exp} ^b	HD-1	HD-2	MWHD-1	MWHD-2	Sox-MeCl	Sox-Hex	SFE-1	SFE-2	SFE-3	SFE-4
	11-Methyl+13-Methyl+15-Methyl											
61	nonacosane	2932.2	n.d.	n.d.	n.d.	n.d.	n.d.	0.75	0.59	0.51	0.47	0.56
62	7-Methyl nonacosane	2941.7	n.d.	n.d.	n.d.	n.d.	0.64	0.61	0.52	0.45	0.43	0.49
	13,17-Dimethyl+11,15-Dimethyl+9,13-											
63	Dimethyl nonacosane	2962.0	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.17	0.27	n.d.	0.27
64	3-Methyl nonacosane	2974.1	n.d.	n.d.	n.d.	n.d.	0.65	0.47	0.42	0.35	0.44	0.40
65	Triacontane	2999.9	n.d.	n.d.	n.d.	n.d.	n.d.	0.90	0.73	0.61	0.43	0.48
66	Untriacontane	3100.9	n.d.	n.d.	n.d.	n.d.	3.34	4.81	3.66	3.32	3.39	3.73
	9-Methyl+11-Methyl+13-Methyl+15-											
67	Methyl untriacontane	3128.3	n.d.	n.d.	n.d.	n.d.	0.79	0.76	0.63	0.50	0.52	0.65
	13,17-Dimethyl+11,15-Dimethyl+9,13-											
68	Dimethyl untriacontane	3138.7	n.d.	n.d.	n.d.	n.d.	0.80	0.94	0.80	0.70	0.73	0.79
Identified %			96.35	96.58	96.30	95.86	95.96	89.27	92.63	93.37	91.88	93.67
Oxygenated monoterpenes			0.24	n.d.	0.19	0.27	n.d.	n.d.	0.15	0.19	0.19	0.26
Sesquiterpenes			5.16	3.94	4.24	4.26	0.78	n.d.	1.04	1.45	1.32	1.22
Oxygenated sesquiterpenes			68.92	65.74	66.98	67.11	31.79	21.15	32.96	37.99	38.25	39.01
Sum of bisabolol oxides A and B			55.54	55.47	55.50	55.21	26.77	17.38	25.67	29.67	30.51	30.83
Sesquiterpene lactones			n.d.	n.d.	n.d.	n.d.	2.81	2.77	4.46	4.97	4.62	5.26
Azulenes ^e			4.95	4.59	4.96	5.21	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Other compounds			17.08	22.31	19.94	19.01	63.40	68.12	58.49	53.74	52.12	53.18
Spiroethers			10.16	12.90	11.86	10.69	18.13	11.76	10.12	10.84	9.35	9.19
Hydrocarbons			2.79	3.92	3.75	3.82	42.21	51.99	45.62	40.47	40.85	42.36

^aCalculated by peak normalization procedure. Major constituents (>4.00%) are marked in bold. ^bExperimentally obtained linear retention indices, relative to C8–C40 *n*-alkanes on HP5-MS column. ^cTrace, <0.005%. ^dNot detected compound. ^eArtefacts of sesquiterpene lactones formed during distillation.

Table S2. Pearson's correlation values between compounds and tested enzymes (red color indicates high correlation)

Correlation	AChE	BChE	Tyrosinase	Amylase	Glucosidase
AChE	1.00	0.94	0.94	-0.99	1.00
BChE	0.94	1.00	0.89	-0.97	0.99
Tyrosinase	0.94	0.89	1.00	-0.95	0.94
Amylase	-0.99	-0.97	-0.95	1.00	-0.99
Glucosidase	1.00	0.99	0.94	-0.99	1.00
C2	-0.24	-0.07	-0.21	0.20	-0.06
C8	-0.97	-0.97	-0.96	0.98	-0.99
C10	-0.93	-0.91	-0.92	0.94	-0.94
C11	-0.98	-0.97	-0.96	0.99	-1.00
C12	-0.32	-0.38	-0.50	0.39	-0.50
C13	-0.98	-0.96	-0.95	0.99	-0.99
C16	-0.93	-0.89	-0.91	0.92	-0.93
C19	-0.94	-0.93	-0.94	0.94	-0.96
C20	-0.80	-0.71	-0.75	0.78	-0.75
C22	-0.32	-0.38	-0.50	0.39	-0.50
C23	-1.00	-0.95	-0.96	0.99	-1.00
C24	-0.51	-0.64	-0.71	0.60	-0.75
C25	-0.96	-0.86	-0.83	0.92	-0.93
C26	-0.95	-0.94	-0.95	0.97	-0.97
C27	-1.00	-0.95	-0.92	0.99	-0.99
C28	0.51	0.47	0.50	-0.53	0.50
C29	-0.93	-0.92	-0.93	0.95	-0.95
C30	-0.35	-0.31	-0.37	0.36	-0.35
C31	-0.81	-0.72	-0.74	0.79	-0.75
C32	-0.99	-0.96	-0.95	0.99	-1.00
C33	-0.93	-0.90	-0.87	0.94	-0.92
C35	-0.58	-0.56	-0.54	0.53	-0.50
C36	-0.40	-0.47	-0.35	0.45	-0.44
C37	0.48	0.45	0.48	-0.49	0.48
C39	-0.43	-0.42	-0.44	0.46	-0.46
C40	-0.71	-0.73	-0.68	0.67	-0.68
C41	0.51	0.44	0.47	-0.47	0.47
C42	0.66	0.60	0.62	-0.64	0.63
C43	0.40	0.40	0.37	-0.45	0.37
C44	0.97	0.97	0.94	-0.98	0.98
C45	0.66	0.69	0.63	-0.67	0.62
C46	0.95	0.94	0.94	-0.96	0.97

C47	0.65	0.68	0.62	-0.66	0.61
C48	0.98	0.96	0.95	-0.99	0.99
C49	0.97	0.97	0.94	-0.98	0.98
C50	0.97	0.96	0.95	-0.99	0.99
C51	0.52	0.52	0.49	-0.54	0.48
C52	0.98	0.97	0.94	-0.99	0.99
C53	0.98	0.96	0.94	-0.99	0.99
C54	0.70	0.66	0.69	-0.71	0.69
C55	0.94	0.92	0.91	-0.94	0.95
C56	0.98	0.96	0.94	-0.99	0.99
C57	0.80	0.81	0.77	-0.84	0.78
C58	0.26	0.25	0.24	-0.27	0.24
C59	0.26	0.22	0.26	-0.21	0.25
C60	0.97	0.96	0.94	-0.99	0.98
C61	0.79	0.79	0.76	-0.83	0.77
C62	0.96	0.94	0.93	-0.96	0.97
C63	0.52	0.54	0.48	-0.54	0.48
C64	0.94	0.91	0.91	-0.93	0.94
C65	0.76	0.75	0.72	-0.81	0.73
C66	0.97	0.95	0.93	-0.98	0.97
C67	0.95	0.93	0.92	-0.95	0.96
C68	0.98	0.96	0.94	-0.99	0.99