Supporting Information

Melissa officinalis Extract Induces Apoptosis and Inhibits Migration in Human Colorectal Cancer Cells

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Table S1. Compounds identified in the hot water extract of *Melissa officinalis* in MS^E-negative ionization mode.

RT (min)	m/z	Formula	Score	Mass Error (ppm)	Identified Compound
0.84	827.2680	$C_{30}H_{52}O_{26}$	43.5	0.68	Maltopentaose
0.91	195.0510	$C_6H_{12}O_7$	42.8	0.06	Gluconic acid
0.91	503.1615	$C_{18}H_{32}O_{16}$	43.1	-0.61	Raffinose
0.91	701.1903	$C_{24}H_{42}O_{21}$	41.1	-1.39	Maltotetraose
8.68	447.0925	$C_{21}H_{20}O_{11}$	45.9	-1.74	Chrysanthemin
10.09	197.0455	$C_9H_{10}O_5$	39.8	-0.37	2-Hydroxy-3,4-dimethoxybenzoic acid
10.09	313.0707	$C_{17}H_{14}O_6$	38.9	-3.50	Koparin 2'-methyl ether
10.09	357.0601	$C_{18}H_{14}O_8$	39.2	-4.11	Psoromic acid
10.09	359.0770	$C_{18}H_{16}O_8$	48.4	-0.79	Rosmarinate
10.09	715.1301	$C_{36}H_{28}O_{16}$	38.2	-0.56	Theaflavin monogallates

RT: retention time (minutes)

Table S2. Compounds identified in the hot water extract of *Melissa officinalis* in MS^E-positive ionization mode.

RT (min)	m/z	Formula	Score	Mass Error (ppm)	Identified Compound
0.84	705.1852	$C_{36}H_{32}O_{15}$	35.9	5.40	Occidentoside
0.91	325.1137	$C_{19}H_{17}ClN_2O$	32.3	10.74	Prazepam
0.91	353.0912	$C_{16}H_{17}ClN_2O_5$	39.9	3.76	N-(Carbethoxyacetyl)-4-chloro-L-tryptophan
0.91	365.1039	$C_{12}H_{22}O_{11}$	40.3	-4.44	D-(+)-Turanose
0.91	434.1189	$C_{21}H_{21}O_{10}$+	34.6	-4.19	Luteolinidin 3-O-glucoside
0.91	443.1227	$C_{17}H_{22}N_4O_8S$	38.3	-0.96	S-(4-Nitrobenzyl)glutathione
0.91	487.1638	$C_{17}H_{30}N_2O_{12}S$	33.5	9.44	Mycothiol
0.91	527.1582	$C_{18}H_{32}O_{16}$	36.6	-0.20	Maltotriose
7.25	285.0767	$C_{16}H_{12}O_5$	49.7	3.22	Thevetiaflavone
7.25	311.0568	$C_{17}H_{10}O_6$	49.8	5.60	Maximaisoflavone A
7.25	369.0303	$C_{10}H_{13}N_2O_{11}P$	37	-7.21	Orotidine, 5'-phosphate (OMP)
7.25	509.1082	$C_{26}H_{20}O_{11}$	45.3	0.66	Fluorescein monoglucuronide
7.25	537.1026	$C_{27}H_{20}O_{12}$	41.7	-0.29	Sagecoumarin
7.29	481.1139	$C_{25}H_{20}O_{10}$	43.7	1.98	2,3-Dehydrosilychristin
8.06	625.1419	$C_{27}H_{28}O_{17}$	44.2	3.13	Kaempferol 3-glucuronide-7-glucoside
10.09	181.0514	$C_9H_8O_4$	53.8	10.10	3-(3,5-Dihydroxyphenyl)-2-propenoic acid
10.09	232.0294	$C_{10}H_{11}Cl_2NO$	31	1.71	2,4-dichloro-N-propylbenzamide
10.09	237.0085	$C_5H_8N_4O_3S_2$	38.1	-10.73	Methazolamide
10.09	278.0351	$C_9H_{11}NO_7S$	37.2	8.00	DOPA sulfate
10.09	343.0827	$C_{18}H_{14}O_7$	41.1	4.36	Phyllocoumarin
10.09	357.0582	$C_{18}H_{12}O_8$	38.4	-6.42	Xerocomic acid
10.09	361.0930	$C_{18}H_{16}O_8$	43.4	3.26	Rosmarinate
10.09	385.0526	$C_{15}H_{16}N_2O_6S_2$	40.4	0.95	Ticarcillin
10.09	455.0300	$C_{20}H_{16}Cl_2O_8$	31	1.02	Gangleoidin acetate
10.09	521.1051	$C_{27}H_{20}O_{11}$	37.8	-5.22	Melitric acid B
10.09	523.1228	$C_{25}H_{24}O_{11}$	38.1	3.49	Epicatechin pentaacetate
10.09	721.1778	$C_{36}H_{32}O_{16}$	37.8	2.01	Sagerinic acid
10.23	463.0877	$C_{21}H_{18}O_{12}$	47.4	1.36	Kaempferol 3-glucuronide
11.19	323.0571	$C_{18}H_{10}O_6$	46.3	6.41	7,7'-Dihydroxy-6,8'-bicoumarin
11.23	341.0664	$C_{18}H_{12}O_7$	53.7	2.42	Salvianolic acid D

RT: retention time (minutes)

Table S3. Compounds identified in the hot water extract of *Melissa officinalis* in survey-negative ionization mode.

RT (min)	m/z	Formula	Score	Mass Error (ppm)	Identified Compound
0.86	701.1906	$C_{24}H_{42}O_{21}$	46.1	-0.27	Stachyose
0.86	195.0512	$C_6H_{12}O_7$	40.5	0.78	Gluconic acid
0.95	179.0554	$C_6H_{12}O_6$	39.9	-3.90	myo-Inositol
0.95	341.1082	$C_{12}H_{22}O_{11}$	41.3	-2.13	D-Lactose
0.95	503.1608	$C_{18}H_{32}O_{16}$	38.2	-1.86	Raffinose
1.29	191.0201	$C_6H_8O_7$	48.1	1.92	Citric acid
3.16	197.0456	$C_9H_{10}O_5$	41.8	-0.45	Vanillylmandelic acid
5.93	305.0695	$C_{15}H_{14}O_7$	37	9.33	Epigallocatechin
5.94	179.0345	$C_9H_8O_4$	41.6	-2.48	Aspirin
8.69	447.0927	$C_{21}H_{20}O_{11}$	35.7	-1.38	Petunidin-3-O-arabinoside
8.80	521.1291	$C_{24}H_{26}O_{13}$	41.2	-1.77	Centaurein
9.90	187.0977	$C_9H_{16}O_4$	39.3	0.63	Nonic acid
10.08	359.0771	$C_{18}H_{16}O_8$	54	-0.44	Rosmarinate
10.19	461.0723	$C_{18}H_{18}N_6O_5S_2$	37.1	3.44	Cefamandole
11.29	343.0821	$C_{18}H_{16}O_7$	37.9	-0.60	Eupatorin
11.54	453.1174	$C_{23}H_{22}N_2O_6S$	35.6	10.65	Nap-Met-OH
12.76	715.1331	$C_{36}H_{28}O_{16}$	38.4	3.74	Theaflavin monogallates

RT: retention time (minutes)

Table S4. Compounds identified in the hot water extract of *Melissa officinalis* in survey-positive ionization mode.

RT (min)	m/z	Formula	Score	Mass Error (ppm)	Identified Compound
0.86	381.0808	$C_{14}H_{20}O_{10}S$	36.4	-11.13	4-Methoxybenzyl O-(2-sulfoglucoside)
0.95	248.1145	$C_{10}H_{17}NO_6$	38.7	6.55	Linamarin
0.95	281.0700	$C_{11}H_{12}N_4O_3S$	38.7	-1.11	Sulfamethopyrazine
1.27	224.1295	$C_{12}H_{17}NO_3$	36	6.19	Cerulenin
1.32	274.0953	$C_{12}H_{19}NO_2S_2$	37.7	8.34	Brugine
1.37	268.1061	$C_{10}H_{13}N_5O_4$	48.4	7.90	Adenosine
3.20	237.0094	$C_5H_8N_4O_3S_2$	35.7	-7.06	Methazolamide
4.35	163.0402	$C_9H_6O_3$	47.6	7.78	Umbelliferone
5.47	195.0784	$C_{14}H_{10}O$	35.7	-10.35	1-Phenanthrol
5.99	163.0400	$C_9H_6O_3$	40.4	6.50	3-Hydroxycoumarin
7.24	311.0567	$C_{17}H_{10}O_6$	50	5.45	Maximaisoflavone A
8.83	163.0401	$C_9H_6O_3$	47.2	6.91	4-Hydroxycoumarin
9.07	197.1190	$C_{11}H_{16}O_3$	48.3	8.84	Benzenemethanol, 2-(2-hydroxypropoxy)-3-methyl-
10.11	181.0510	$C_9H_8O_4$	48.9	8.34	Phenylmalonic acid
10.11	278.0346	$C_9H_{11}NO_7S$	37.1	5.99	DOPA sulfate
10.20	287.0564	$C_{15}H_{10}O_6$	37.6	5.01	Maritimetin
10.20	463.0881	$C_{21}H_{18}O_{12}$	47.1	2.11	Kaempferol 3-glucuronide
11.06	469.3316	$C_{30}H_{44}O_4$	43	0.68	16beta-16-Hydroxy-3-oxo-1, 12-oleanadien-28-oic acid
11.18	323.0551	$C_{15}H_{14}O_6S$	36.7	-10.14	GN25
11.18	341.0668	$C_{18}H_{12}O_7$	52.3	3.68	Salvianolic acid D

RT: retention time (minutes)

Table S5. Classification of MO-extract compounds

Superclass	Identified Compound
Alkaloids	Brugine
Benzenoids	Sulfamethopyrazine
	2,4-dichloro-N-propylbenzamide
	2-Hydroxy-3,4-dimethoxybenzoic acid
	Aspirin
	Phenylmalonic acid
	GN25
	1-Phenanthrol
	Benzenemethanol, 2-(2-hydroxypropoxy)-3-methyl-
	Xerocomic acid
	Vanillylmandelic acid
Lipids and lipid-like molecules (Lipids)	Nonic acid
	16beta-16-Hydroxy-3-oxo-1,12-oleanadien-28-oic acid
Nucleotides	Adenosine
	Orotidine, 5'-phosphate (OMP)
Organic acids and derivatives	DOPA sulfate
	N-(Carbethoxyacetyl)-4-chloro-L-tryptophan
	Nap-Met-OH
	S-(4-Nitrobenzyl)glutathione
	Ticarcillin
	Citric acid
	Gluconic acid
Organic oxygen compounds (Sugars)	myo-Inositol
	4-Methoxybenzyl O-(2-sulfoglucoside)
	D-(+)-Turanose
	D-Lactose
	Fluorescein monoglucuronide
	Linamarin
	Maltopentaose
	Maltotetraose
	Maltotriose
	Mycothiol
	Raffinose
	Stachyose
Organoheterocyclic compounds	Methazolamide

	Prazepam
	Salvianolic acid D
	Cerulenin
	Cefamandole
Phenylpropanoids and polyketides	2,3-Dehydrosilychristin
	Maritimetin
	3-(3,5-Dihydroxyphenyl)-2-propenoic acid
	Melitric acid B
	Rosmarinate (Rosmarinic Acid)
	3-Hydroxycoumarin
	4-Hydroxycoumarin
	7,7'-Dihydroxy-6,8'-bicoumarin
	Sagecoumarin
	Umbelliferone
	Gangleoidin acetate
	Psoromic acid
	Epicatechin pentaacetate
	Epigallocatechin
	Phyllocoumarin
	Theaflavin monogallates
	Centaurein
	Chrysanthemin
	Kaempferol 3-glucuronide
	Kaempferol 3-glucuronide-7-glucoside
	Luteolinidin 3-O-glucoside
	Petunidin-3-O-arabinoside
	Eupatorin
	Thevetiaflavone
	Maximaisoflavone A
	Koparin 2'-methyl ether
Lignans, neolignans and related compounds (Lignans)	Sagerinic acid
	Occidentoside