cosmetics

MDPI

Supplementary Material

Table S1. Compounds in ginger rhizome extracts based on the results of liquid chromatography-mass spectrometry/ mass spectrometry analysis

No.	Retention Time [min]	Name	Molecular Weight (g/mol)	Formula	Error [ppm]	Abundance (%)		
						Gajah	Red	Emprit
1	1.040	L-Histidine	155.069	$C_6H_9N_3O_2$	-0.93	0.28±0.14a	0.37±0.15a	0.2685±0.1222a
2	1.040	L-(+)-Arginine	174.112	$C_6H_{14}N_4O_2$	-0.80	0.40±0.25a	1.75±0.74b	-
3	1.056	L-(-)-Serine	105.043	$C_3H_7NO_3$	1.49	0.17±0.07a	-	-
4	1.069	Choline	103.100	$C_5H_{13}NO$	1.74	4.04±2.00a	3.50±1.33a	4.2852±2.0211a
5	1.069	D-Asparagine	132.053	$C_4H_8N_2O_3$	-0.87	-	-	0.6726±0.0000a
6	1.075	D-Xylonic acid	166.047	$C_5H_{10}O_6$	-4,29	0.16±0.07a	-	-
7	1.083	D-β-homoserine	119.058	$C_4H_9NO_3$	0.25	0.29±0.16a	0.37±0.00a	0.3236±0.1890a
8	1.084	D-Glutamine	146.069	$C_5H_{10}N_2O_3$	-1.12	0.54±0.27b	0.14±0.05a	-
9	1.087	γ-Aminobutyric acid	103.064	$C_4H_9NO_2$	1.83	0.25±0.12b	0.136±0.05a	-
10	1.095	L-Glutamic acid	147.053	$C_5H_9NO_4$	-1.31	0.69±0.24b	0.09±0.03a	0.33±0.19ab
11	1.104	L-(+)-Valine	117.079	$C_5H_{11}NO_2$	0.81	-	-	0.32±0.16a
12	1.105	L-Pyroglutamic acid	129.043	$C_5H_7NO_3$	0.09	-	0.10±0.04a	-
13	1.107	β-D-ructofuranosyl	324.105	$C_{12}H_{20}O_{10}$	-1.34	0.32±0.19a	-	-
14	1.112	D-(+)-Proline	115.063	$C_5H_9NO_2$	0.33	0.55±0.29a	0.98±0.41a	0.63±0.31a
15	1.121	L-Theanine	174.100	$C_7H_{14}N_2O_3$	-0.48	0.10±0.03a	-	-
16	1.136	Mannoheptulose	210.074	$C_7H_{14}O_7$	-1.94	0.18±0.10a	-	-
17	1.143	α,α-Trehalose	342.116	$C_{12}H_{22}O_{11}$	0.13	0.44±0.21a	-	0.34±0.12a
18	1.158	D-(+)-Galactose	180.063	$C_6H_{12}O_6$	-3.33	1.17±0.84a	-	-
19	1.205	D-(+)-Pipecolinic acid	129.079	$C_6H_{11}NO_2$	-1.04	1.37±0.66a	7.62±3.16b	7.94±0.00b
20	1.205	Adenosine	267.096	$C_{10}H_{13}N_5O_4$	-1.24	-	-	0.87±0.00a
21	1.208	5'-O-β-D-Glucosylpyridoxine	331.126	C14 H21 N O8	-1.20	0.19±0.09a	0.12±0.04a	0.18±0.09a
22	1.209	Malic acid	134.021	$C_4H_6O_5$	-6.56	1.28±0.60a	1.31±0.00a	0.94±0.66a
23	1.211	L-Valine	117.079	$C_5H_{11}NO_2$	0.29	1.56±0.00a	1.53±0.68a	-

Numbers followed by the same letter consecutively indicate values that are not significantly different ($p>0.05$).

Table S1 ***(continuation).*** Compounds in ginger rhizome extracts based on the results of liquid chromatography-mass spectrometry/ mass spectrometry analysis

No.	Retention Time [min]	Name	Molecular Weight (g/mol)	Formula	Error [ppm]	Abundance (%)		
						Gajah	Red	Emprit
24	1.212	2-Methylamino-isobutyric acid	117.079	$C_5H_{11}NO_2$	0.81	-	-	1.47±1.14a
25	1.217	Citric acid	192.026	$C_6H_8O_7$	-2.65	0.09±0.05a	0.14±0.06a	0.28±0.21a
26	1.237	L-(-)-Methionine	149.051	$C_5H_{11}NO_2S$	-1.68	-	0.63±0.31a	-
27	1.246	L-Tyrosine	181.074	$C_9H_{11}NO_3$	-1.90	-	0.95±0.51a	-
28	1.248	N-Benzylformamide	135.068	C_8H_9NO	-1.29	-	0.24±0.00a	-
29	1.249	4-Hydroxycinnamic acid	164.047	$C_9H_8O_3$	-0.62	-	0.19±0.08a	-
30	1.688	L-Isoleucine	131.094	$C_6H_{13}NO_2$	-2.11	1.04±0.61a	2.19±1.55a	1.52±1.13a
31	2.588	L-Phenylalanine	165.079	$C_9H_{11}NO_2$	-1.28	0.64±0.35a	0.95±0.38a	0.53±0.28a
32	4.923	D-Tryptophan	204.090	$C_{11}H_{12}N_2O_2$	-1.47	0.60±0.00a	1.73±0.00b	-
33	5.119	trans-3-Indoleacrylic acid	187.063	$C_{11}H_9NO_2$	-1.48	0.26±0.13a	0.69±0.35a	0.39±0.26a
34	5.516	D-(+)-Tryptophan	204.090	$C_{11}H_{12}N_2O_2$	-1.20	-	-	1.20±0.00a
35	7.130	Catechin	290.079	$C_{15}H_{14}O_6$	1.32	-	0.14±0.05a	-
36	8.731	2-(acetylamino)-3-(1H-indol-3-yl)-propanoic acid	246.100	$C_{13}H_{14}N_2O_3$	0.14	-	0.11±0.04a	-
37	9.987	N-Desmethyltramadol	249.172	$C_{15}H_{23}NO_2$	-2.00	-	0.18±0.09a	-
38	10.398	Trp-Trp	390.168	$C_{22}H_{22}N_4O_3$	-2.39	0.24±0.09a	-	-
39	10.917	Dibenzo-18-crown-6	360.158	$C_{20}H_{24}O_6$	1.05	-	-	0.66±0.17a
40	12.187	Myricanone	356.161	$C_{21}H_{24}O_5$	-2.50	0.75±0.37b	0.11±0.04a	-
41	12.313	Isoamyl-4-methoxycinnamate	248.141	$C_{15}H_{20}O_3$	-2.52	-	0.10±0.03a	0.28±0.12b
42	12.978	Pulegone	152.120	$C_{10}H_{16}O$	-1.33	0.66±0.30a	0.62±0.50a	-
43	13.178	12-epi-Salvinorin A	432.179	$C_{23}H_{28}O_8$	0.29	0.76±0.39a	-	-
44	14.735	Mycophenolate mofetil	433.209	$C_{23}H_{31}NO_7$	-2.85	0.23±0.11a	-	-
45	14.736	Falcarindiol	260.177	$C_{17}H_{24}O_2$	-2.27	1.15±1.11a	0.59±0.45a	0.70±0.26a
46	14.889	Methyl cinnamate	162.068	$C_{10}H_{10}O_2$	-1.93	0.42±0.21a	0.18±0.08a	0.20±0.07a

Numbers followed by the same letter consecutively indicate values that are not significantly different ($p>0.05$).

Table S1 ***(continuation).*** Compounds in ginger rhizome extracts based on the results of liquid chromatography-mass spectrometry/ mass spectrometry analysis

No.	Retention Time [min]	Name	Molecular Weight (g/mol)	Formula	Error [ppm]	Abundance (%)		
						Gajah	Red	Emprit
47	14.899	6-Paradol	278.187	$C_{17}H_{26}O_3$	-2.44	0.61±0.00a	0.27±0.00a	-
48	15.280	Embelin	294.182	$C_{17}H_{26}O_4$	-2.65	-	0.17±0.06a	-
49	15.471	6-Gingerol	294.183	$C_{17}H_{26}O_4$	-1.72	-	-	1.51±2.16a
50	15.481	Ethyl cinnamate	176.083	$C_{11}H_{12}O_2$	-1.60	1.01±0.91a	1.08±0.86a	1.90±1.15a
51	15.481	1-Naphthol	144.057	$C_{10}H_8O$	-1.04	0.18±0.09a	0.19±0.08a	0.29±0.11a
52	15.482	4-Methoxybenzaldehyde	136.052	$C_8H_8O_2$	-1.07	1.13±1.16a	1.08±1.11a	2.16±1.62a
53	16.141	d-Corlin	400.188	$C_{23}H_{28}O_6$	-2.68	0.26±0.10a	-	-
54	16.426	Crocetin	328.167	$C_{20}H_{24}O_4$	-2.58	0.31±0.08a	-	-
55	16.542	β,β-Dimethylacrylshikonin	370.141	$C_{21}H_{22}O_6$	-1.87	0.22±0.11a	-	0.19±0.11a
56	16.706	p-Cymene	134.109	$C_{10}H_{14}$	-1.33	3.15±2.05a	2.69±2.61a	1.41±0.59a
57	16.707	p-Xylene	106.078	C_8H_{10}	1.61	0.34±0.16a	0.38±0.17a	-
58	16.864	Curcumin	368.125	$C_{21}H_{20}O_6$	-1.81	-	-	0.18±0.07a
59	16.988	4'-Methoxyacetophenone	150.068	$C_9H_{10}O_2$	-1.89	-	-	0.29±0.1a
60	16.995	Octinoxate	290.187	$C_{18}H_{26}O_3$	-2.72	0.57±0.28a	0.66±0.25b	1.73±0.64a
61	16.999	Bisoprolol	325.225	$C_{18}H_{31}NO_4$	-2.33	-	0.13±0.05a	0.47±0.23b
62	17.100	Citral	152.120	$C_{10}H_{16}O$	-1.58	0.85±0.57a	1.10±0.56a	0.45±0.22a
63	17.804	Testosterone	288.208	$C_{19}H_{28}O_2$	-2.08	-	0.14±0.06a	-
64	18.359	11-nor-9-carboxy-δ-9-tetrahydrocannabiol	344.196	$C_{21}H_{28}O_4$	-8.99	-	-	0.19±0.08a
65	18.380	6-β-hydroxy testosterone	304.203	$C_{19}H_{28}O_3$	-2.16	2.24±1.05a	2.54±2.29a	-
66	18.410	8-Shogaol	276.172	$C_{17}H_{24}O_3$	-2.09	1.28±0.00b	0.71±0.00a	-
67	18.568	6-Gingerdione	292.167	$C_{17}H_{24}O_4$	-2.52	0.94±0.00a	1.44±0.00a	1.4896±0.00a

Numbers followed by the same letter consecutively indicate values that are not significantly different ($p>0.05$).

Table S1 ***(continuation).*** Compounds in ginger rhizome extracts based on the results of liquid chromatography-mass spectrometry/ mass spectrometry analysis

No.	Retention Time [min]	Name	Molecular Weight (g/mol)	Formula	Error [ppm]	Abundance (%)		
						Gajah	Red	Emprit
68	18.591	Nandrolone	274.193	$C_{18}H_{26}O_2$	-1.99	0.28±0.14a	0.14±0.06a	-
69	18.849	Dehydrocostus Lactone	230.130	$C_{15}H_{18}O_2$	-2.26	0.71±0.38a	-	-
70	18.999	4-Shogaol	276.172	$C_{17}H_{24}O_3$	-2.69	-	-	1.26±0.00a
71	19.118	Methenolone	302.224	$C_{20}H_{30}O_2$	-3.08	-	-	0.94±0.00a
72	19.344	4-Methylumbelliferone	176.047	$C_{10}H_8O_3$	-127	-	0.18±0.07a	0.23±0.09a
73	19.858	Steviol	318.219	$C_{20}H_{30}O_3$	-2.57	-	0.13±0.05a	0.23±0.10a
74	19.998	Pregnane-3,20-dione	316.239	$C_{21}H_{32}O_2$	-2.44	-	-	0.31±0.11a
75	20.028	Ubiquinol 10	320.198	$C_{19}H_{28}O_4$	-2.33	1.20±1.15a	1.06±0.91a	-
76	20.325	10-Hydroxy-3-methoxy-1,3,5,7-cadinatetraen-9-one	260.141	$C_{16}H_{20}O_3$	-1.73	-	0.14±0.05a	-
77	20.334	Zerumbone	218.167	$C_{15}H_{22}O$	-2.06	0.30±0.14a	0.15±0.06a	0.27±0.12a
78	20.597	5a-Pregnane-3,20-dione	316.240	$C_{21}H_{32}O_2$	-1.86	-	0.33±0.00a	-
79	21.089	10-Shogaol	350.245	$C_{21}H_{34}O_4$	-2.16	-	-	0.36±0.18a
80	21.095	20-α-Dhydrodydrogesterone	332.234	$C_{21}H_{32}O_3$	-2.70	3.38±2.99a	3.34±3.25a	7.06±4.52a
81	21.106	(E)-4-Methoxycinnamic acid	178.063	$C_{10}H_{10}O_3$	-1.74	-	0.27±0.09a	-
82	21.205	α-Curcumene	202.172	$C_{15}H_{22}$	-1.35	-	-	0.15±0.06a
83	21.213	Curcumene	202.172	$C_{15}H_{22}$	-1.43	0.61±0.38a	0.75±0.26a	-
84	21.225	4-Vinylcyclohexene	108.094	C_8H_{12}	1.17	-	0.19±0.08a	-
85	22.021	Pentylbenzene	148.125	$C_{11}H_{16}$	-0.88	-	0.29±0.11a	0.40±0.15a
86	22.023	(E,E)-α-Farnesene	204.188	$C_{15}H_{24}$	-1.73	-	3.11±2.98a	6.04±4.74a
87	22.136	Ferulic acid	194.058	$C_{10}H_{10}O_4$	-1.03	0.25±0.13a	0.28±0.10a	-
88	22.504	R-(+)-Tolterodine	325.240	$C_{22}H_{31}NO$	-2.65	-	-	0.30±0.13a
89	23.235	Ubiquinone-2	318.182	$C_{19}H_{26}O_4$	-2.16	0.80±0.39a	1.05±0.44b	-
90	23.702	Drostanolone propionate	360.265	$C_{23}H_{36}O_3$	-3.08	-	-	0.55±0.23a

Numbers followed by the same letter consecutively indicate values that are not significantly different ($p>0.05$).

Table S1 ***(continuation).*** Compounds in ginger rhizome extracts based on the results of liquid chromatography-mass spectrometry/ mass spectrometry analysis

No.	Retention Time [min]	Name	Molecular Weight (g/mol)	Formula	Error [ppm]	Abundance (%)		
						Gajah	Red	Emprit
91	25.164	Epristeride	399.276	$C_{25}H_{37}NO_3$	-2.18	-	-	0.77±0.32a
92	25.220	17-α-21-dihydroxypregnenolone	348.229	$C_{21}H_{32}O_4$	-2.42	1.30±0.66a	0.74±0.52b	-
93	25.221	Hydroxyprogesterone	330.218	$C_{21}H_{30}O_3$	-3.59	-	-	0.69±0.26a
94	25.614	Corticosterone	346.213	$C_{21}H_{30}O_4$	-2.84	1.54±1.34a	1.13±0.81a	-
95	26.264	1-Heptadecanoyl-glycero-3-phospate	424.260	$C_{20}H_{41}O_7P$	2.66	-	0.14±0.05a	-
96	26.613	ent-cassa-12,15-diene	272.250	$C_{20}H_{32}$	-2.19	-	-	0.28±0.16a
97	27.156	Hecogenin	430.308	$C_{27}H_{42}O_4$	-1.14	-	0.77±0.30a	-
98	27.653	Calcitroic acid	374.245	$C_{23}H_{34}O_4$	-2.68	0.23±0.00a	-	0.28±0.13a

Table S2. Examples of test and control ligand structures

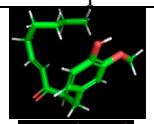
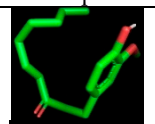
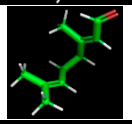
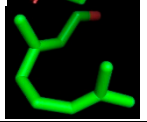
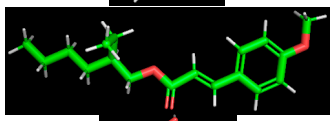
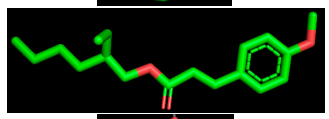
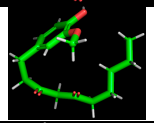
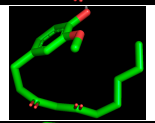
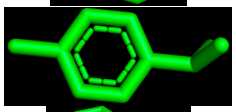
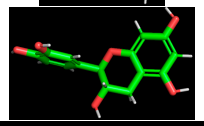
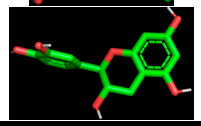
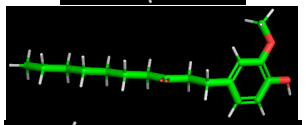
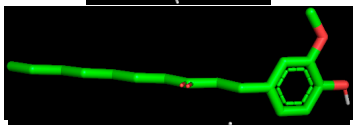
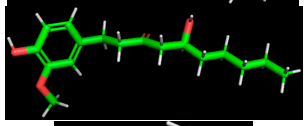
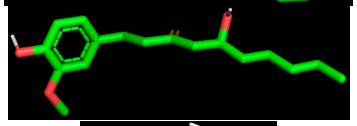
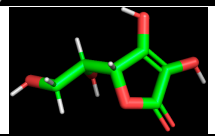
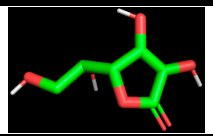
No.	Ligand	Chemical Formula	Before Preparation	After Preparation
1	10-Shogaol	$C_{21}H_{32}O_3$		
2	Citral	$C_{10}H_{16}O$		
3	Octinoxate	$C_{18}H_{26}O_3$		
4	6-Gingerdione	$C_{17}H_{24}O_4$		
5	p-Cymene	$C_{10}H_{14}$		
6	4-Shogaol	$C_{15}H_{20}O_3$		
7	Catechin	$C_{15}H_{14}O_6$		
8	6-Paradol	$C_{17}H_{26}O_3$		
9	6-Gingerol	$C_{17}H_{26}O_4$		
10	Ascorbic acid	$C_6H_8O_6$		

Table S3. The affinity energy of the ligand-receptor complex

Ligand	Affinity Energy (kcal/mol)				Ligand	Affinity Energi (kcal/mol)			
	2TCL	2PE4	3F19	5M8R		2TCL	2PE4	3F19	5M8R
L-Histidine	-6.1	-5.0	-6.0	-5.3	α,α-Trehalose	-6.2	-6.2	-6.7	-5.9
L-(+)-Arginine	-6.1	-4.8	-6.0	-5.0	D-(+)-Galactose	-6.3	-5.3	-5.9	-5.3
L-(-)-Serine	-4.2	-4.0	-4.2	-4.2	D-(+)-Pipecolinic Acid	-5.8	-5.3	-6.1	-5.5
Choline	-4.5	-3.5	-3.8	-4.0	Adenosine	-7.0	-6.9	-7.8	-6.2
D-Asparagine	-5.4	-4.9	-5.4	-4.8	5'-O-β-D-Glucosylpyridoxine	-7.1	-6.9	-8.1	-6.9
D-Xylonic acid	-5.9	-5.0	-5.3	-5.2	Malic Acid	-5.4	-4.8	-5.0	-5.1
D-(+)-Proline	-5.2	-5.0	-5.2	-4.9	L-Isoleucine	-5.6	-5.1	-5.3	-5.0
L-Theanine	-6.1	-5.5	-5.9	-5.1	L-Phenylalanine	-6.6	-6.4	-6.8	-6.1
Mannoheptulose	-6.3	-5.6	-6.4	-5.3	D-Tryptophan	-7.2	-6.7	-7.8	-6.8
trans-3-Indoleacrylic Acid	-6.7	-6.4	-7.6	-7.0	Falcarindiol	-5.6	-6.2	-7.1	-5.8
Catechin	-8.8	-7.9	-9.7	-8.4	Methyl Cinnamate	-6.0	-6.1	-6.7	-5.6
2-(Acetylamino)-3-(1H-Indol-3-yl)-Propanoic Acid	-7.1	-6.7	-8.0	-7.4	6-Paradol	-5.7	-6.8	-7.9	-5.5
N-Desmethyltramadol	-6.5	-6.0	-8.9	-6.4	Embelin	-6.2	-7.0	-7.3	-6.1
Trp-Trp	-8.6	-9.0	-10.2	-8.4	6-Gingerol	-6.1	-6.7	-8.0	-6.8
Dibenzo-18-crown-6	-7.3	-7.3	-7.1	-7.4	Ethyl Cinnamate	-6.1	-6.1	-7.0	-5.5
Myricanone	-6.0	-7.1	-6.4	-6.6	1-Naphthol	-6.9	-6.7	-7.3	-6.3
Isoamyl-4-methoxycinnamate	-6.0	-6.5	-7.8	-6.9	4-Methoxybenzaldehyde	-5.7	-5.3	-5.8	-5.8
Pulegone	-5.6	-6.6	-6.9	-5.8	d-Corlin	-14.6	-13.9	-16.0	-13.4
12-epi-Salvinorin A	-6.9	-7.6	-8.9	-8.0	Crocetin	-6.2	-6.9	-8.0	-6.7
Mycophenolate Mofetil	-7.3	-7.0	-9.1	-7.0	p-Cymene	-5.9	-6.6	-6.5	-5.8
6-β-Hydroxytestosterone	-5.8	-7.2	-7.4	-7.6	p-Xylene	-5.3	-5.5	-5.5	-4.9
8-Shogaol	-6.0	-6.9	-8.0	-6.4	Curcumin	-6.4	-7.7	-8.8	-7.7

Note: 2TCL: collagenase, 2PE4: hyaluronidase, 3F19: elastase, 5M8R: tyrosinase

Table S3 ***(continuation)*****.** The affinity energy of the ligand-receptor complex

Ligand	Affinity Energy (kcal/mol)				Ligand	Affinity Energy (kcal/mol)			
	2TCL	2PE4	3F19	5M8R		2TCL	2PE4	3F19	5M8R
6-Gingerdione	-5.9	-6.4	-7.9	-6.6	4'-Methoxyacetophenone	-6.1	-5.7	-6.3	-5.5
Nandrolone	-6.3	-8.1	-7.2	-7.4	Octinoxate	-6.1	-7.2	-7.8	-6.3
Dehydrocostus Lactone	-6.7	-7.2	-7.7	-7.5	Bisoprolol	-6.3	-5.9	-7.5	-6.1
4-Shogaol	-6.1	-6.8	-7.6	-6.3	Citral	-5.3	-5.3	-6.3	-5.8
Methenolone	-6.3	-7.2	-7.5	-7.5	Testosterone	-5.9	-7.3	-7.3	-7.6
4-Methylumbelliferone	-6.7	-6.4	-7.2	-6.6	10-Hydroxy-3-methoxy-1,3,5,7-cadinatetraen-9-one	-6.8	-7.1	-7.1	-6.4
Steviol	-5.7	-7.0	-7.2	-8.4	Zerumbone	-5.2	-5.9	-6.8	-8.0
Pregnane-3,20-dione	-6.1	-8.0	-7.6	-8.3	5a-Pregnane-3,20-dione	-6.0	-8.1	-7.6	-8.3
D-β-Homoserine	-4.8	-4.3	-4.3	-4.5	L-Valine	-5.4	-4.7	-5.1	-4.9
D-Glutamine	-6.0	-5.1	-5.5	-5.1	2-(Methylamino)-isobutyric Acid	-4.8	-4.7	-4.6	-4.6
γ-Aminobutyric acid	-4.7	-4.5	-4.2	-4.3	Citric Acid	-6.2	-5.6	-6.0	-5.5
L-Glutamic Acid	-5.8	-5.0	-5.3	-5.0	L-(-)-Methionine	-4.6	-4.5	-4.8	-4.3
L-(+)-Valine	-5.1	-4.8	-5.1	-4.9	L-Tyrosine	-6.8	-6.0	-6.8	-5.9
Ubiquinol 10	-8.4	-11.3	-11.9	-11.5	10-Shogaol	-5.5	-7.0	-7.7	-6.6
Drostanolone Propionate	7.2	-7.9	-8.2	-8.8	20-α-Dhydrodydrogesterone	-10.6	-11.4	-13.0	-10.6
Epristeride	-6.6	-8.5	-8.1	-8.2	(E)-4-Methoxycinnamic Acid	-6.1	-6.1	-7.2	-6.9
Hydroxyprogesterone	-6.5	-7.1	-7.6	-8.8	α-Curcumene	-6.6	-7.0	-8.2	-6.7
Corticosterone	-6.1	-7.4	-7.8	-8.5	4-Vinylcyclohexene	-5.6	-6.0	-5.4	-4.7
Ascorbic Acid	-6.4	-5.6	-6.1	-6.0	Pentylbenzene	-5.7	-6.5	-5.4	-5.1
L-Pyroglutamic Acid	-5.7	-5.0	-5.9	-5.1	N-Benzylformamide	-5.8	-5.7	-5.9	-5.8
β-D-Fructofuranose	-5.9	-5.1	-6.2	-5.0	R-(+)-Tolterodine	-7.1	-7.3	-7.1	-6.4
ent-Cassa-12,15-diene	-5.6	-7.9	-8.0	-8.2	(E,E)-α-Farnesene	-6.1	-6.6	-7.3	-5.6
Hecogenin	-7.8	-8.9	-9.7	-8.5	Ferulic Acid	-6.8	-5.9	-7.2	-6.4
Calcitroic Acid	-6.6	-7.6	-7.8	-7.5					

Note: 2TCL: collagenase, 2PE4: hyaluronidase, 3F19: elastase, 5M8R: tyrosinase