Supplementary Information

Table S1. The constituents of *Folium Eriobotryae.*

MolID	Compound Name	CAS	OB	Caco-2	DL
001	(−)-epicatechin	490-46-0	21.97	−0.65	0.77
002	(+)-carvone	2244-16-8	22.23	1.35	0.03
003	(1-methylethyl)-benzene	98-82-8	28.73	1.81	0.02
004	(1-methylpropyl)-benzene	68411-44-9	31.13	1.87	0.02
005	(2*R*)-naringenin 8-C-α-L-rhamnopyranosyl-(1→2) -β-D-glucopyranoside	278614-44-1	45.22	−1.80	0.81
006 *	(2*R*)-naringenin 8-C-α-L-rhamnopyranosyl-(1→2) -β-D-glucopyranoside_qt	—	49.13	−1.23	0.71
007	(2*S*)-naringenin 8-C-α-L-rhamnopyranosyl-(1→2) -β-D-glucopyranoside	278614-43-0	45.48	−1.59	0.78
008 *	(2*S*)-naringenin 8-C-α-L-rhamnopyranosyl-(1→2) -β-D-glucopyranoside_qt	—	18.02	−1.24	0.71
009	(6*R*,7*E*,9*R*)-9-hydroxy-4,7-megastigmadien-3-one 9-*O*-β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside	—	30.35	−1.65	0.72
010	(6*R*,7*E*,9*R*)-9-hydroxy-4,7-megastigmadien-3-one 9-*O*-β-D-glucopyranoside	—	51.53	−0.76	0.34
011	(6*R*,7*E*,9*R*)-9-hydroxy-4,7-megastigmadien-3-one 9-*O*-β-D-xylopyranosyl-(1→6)-β-D-glucopyranoside	—	34.51	−1.70	0.72
012	(6*R*,7*E*,9*R*)-9-hydroxy-4,7-megastigmadien-3-one 9-*O*-β-L-arabinopyranosy-(1→6)-β-D-glucopyranoside	—	45.80	−1.80	0.72
013	(6*R*,7*E*,9*R*)-9-hydroxy-4,7-megastigmadien-3-one	52210-15-8	19.80	0.49	0.07
014	(6*R*,7*E*,9*S*)-9-hydroxy-4,7-megastigmadien-3-one 9-*O*-β-D-glucopyranoside	—	32.01	−1.09	0.34
015 *	(6*r*,9*r*)-3-oxo-r-ionyl-9-o-glc_qt	—	18.63	0.52	0.07
016	(6*S*,7*E*,9*R*)-6,9-dihydroxy-4,7-megastigmadien-3-one	—	48.96	−0.11	0.08
017	(6*s*,9*r*)-roseoside	—	9.73	−1.19	0.36
018	(6*S*,9*R*)-vomifoliol-9-*O*-β-apiofuranosyl-(1"→6')*O*-β-gluopyranoside	—	43.92	−2.29	0.71
019	(6*S*,9*R*)-vomifoliol-9-*O*-β-xylopyranosyl-(1"→6')*O*-β-gluopyranoside	—	41.86	−2.19	0.72
020 *	(6*S*,9*R*)-vomifoliol-9-*O*-β-xylopyranosyl-(1"→6')*O*-β-gluopyranoside_qt	—	28.19	−0.16	0.08
021	(*cis*-trans) farnesol	3790-71-4	5.25	1.26	0.06
022	(*E*)-2-hexenyl-gamma-L-arabinopyranosyl-(1-2)-beta-D-glucopyranoside	—	45.37	−1.51	0.38
023 *	(*E*)-2-hexenyl-gamma-L-arabinopyranosyl-(1-2)-beta-D-glucopyranoside_qt	—	50.63	1.08	0.01
024	(*E*)-3-penten-2-one	3102-33-8	48.40	1.26	0.00
025	(*E*)-6,10-dimethyl-5,9-undecadien-2-one	3796-70-1	5.65	1.45	0.04

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
026	(*trans-trans*)farnesol	106-28-5	27.72	1.26	0.06
027	1-(ethenyloxy)-butane	111-34-2	30.68	1.45	0.01
028	1,1,2-trichloro-ethane	79-00-5	13.05	1.82	0.00
029	1,1'-bicyclohexyl	92-51-3	24.33	1.77	0.04
030	1,2,3,4-tetramethyl-benzene	25619-60-7	34.70	1.88	0.03
031	1,2,3,5-tetramethyl-benzene	527-53-7	54.69	1.88	0.03
032	1,2,4,5-tetramethyl-benzene	—	37.65	1.86	0.03
033	1,2,4-trimethyl-benzene	95-63-6	32.41	1.84	0.02
034	1,2-benzenedicarboxylic,bis(2-methylpropyl)ester	—	20.96	0.74	0.13
035	1,2-diethyl-benzene	—	7.79	1.88	0.02
036	1,2-dimethyl-naphthalene	573-98-8	76.49	1.89	0.05
037	1,3,3-trimethyl-bicyclo[2.2.1]heptan-2-ol	1632-73-1	32.19	1.30	0.05
038	1,3,5-trimethyl-benzene	108-67-8	14.21	1.85	0.02
039	1,3-bis(1-methylethyl)-benzene	99-62-7	21.00	1.85	0.03
040	1,3-diethyl-benzene	25340-17-4	11.13	1.86	0.02
041	1,3-dimethyl-naphthalene	575-41-7	12.13	1.87	0.05
042	1,4-bis(1-methylethyl)-benzene	100-18-5	11.28	1.87	0.03
043	1,4-dichloro-benzene	106-46-7	1.85	1.84	0.01
044	1,4-dimethoxy-2,3-dimethylbenzene	39021-83-5	10.83	1.39	0.04
045	1,4-methanoazulene,decahydro-4,8,8-trimethyl-9-methylene	475-20-7	23.49	1.79	0.11
046	1,6,7-trimethyl-naphthalene	2245-38-7	77.35	1.90	0.06
047	1,8-dimethyl-naphthalene	569-41-5	38.72	1.87	0.05
048	10,10-dimethyl-2,6-bis(methylene)-dicyclo[7.2.0] undecane	—	54.71	1.82	0.09
049	11H-benzo[b]fluorene	243-17-4	17.84	1.94	0.21
050	1-dodecanol	112-53-8	10.62	1.24	0.03
051	1-ethyl-2-methyl-benzene	611-14-3	29.21	1.83	0.02
052	1-ethyl-3,5-dimethyl-benzene	934-74-7	26.59	1.87	0.02
053	1-ethyl-3-methyl-benzene	620-14-4	20.10	1.86	0.02
054	1-hexadecanol	36653-82-4	48.54	1.31	0.08
055	1-hexadecene	629-73-2	60.36	1.86	0.06
056	1-hexyl-cyclohexen	—	65.55	1.86	0.03
057	1-methyl-2(1-methylethyl)-benzene	527-84-4	50.74	1.84	0.02
058	1-methyl-2-propyl-benzene	1074-17-5	18.36	1.85	0.02

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
059	1-methyl-3-(1-methylethyl)-benzene	535-77-3	17.91	1.83	0.02
060	1-methyl-4-(1-methylethyl)-benzene	99-87-6	9.64	1.88	0.02
061	1-methyl-naphthalene	90-12-0	40.40	1.86	0.04
062	1-methyl-phenanthrene	832-69-9	12.29	1.92	0.11
063	1-nonanal	124-19-6	46.74	1.32	0.02
064	1-*O*-feruloyl-β-D-glucopyranoside	—	47.54	−0.97	0.32
065 *	1-*O*-feruloyl-β-D-glucopyranoside_qt	—	17.95	0.41	0.06
066	1-penten-3-ol	616-25-1	3.54	1.04	0.00
067	1-tetradecanol	112-72-1	28.24	1.27	0.05
068	1-tridecene	2437-56-1	72.77	1.83	0.03
069	1-undecanol	112-42-5	65.96	1.24	0.03
070	1-verbenone	1196-01-6	5.06	1.27	0.06
071	1β-hydroxyeuscaphic acid	—	24.03	−0.38	0.69
072	2,2,3,3-tetramethylhexane	13475-81-5	31.28	1.80	0.02
073	2,2,4,4-tetramethyl-3-pentanone	815-24-7	32.64	1.40	0.02
074	2,2-dimethylbutane	75-83-2	1.79	1.77	0.01
075	2,3,5,8-tetramethyldecane	192823-15-7	62.96	1.82	0.04
076	2,3,5-trimethyl-phenol	697-82-5	35.09	1.60	0.03
077	2,3-dihydro-4,6-dimethyl-1H-indene	1685-82-1	31.35	1.89	0.04
078	2,3-dihydro-5-methyl-1H-indene	874-35-1	30.80	1.89	0.03
079	2,3-dimethyl-naphthalene	581-40-8	33.81	1.90	0.05
080	2,3-diphenyl-2-cyclopropen-1-one	886-38-4	47.63	1.42	0.11
081	2,4,6-trimethyl-pyridine	108-75-8	31.25	1.61	0.02
082	2,4-bis(1,1-dimethylethyl)-phenol	—	30.38	1.67	0.06
083	2,4-heptadienal	96-76-4	32.01	1.33	0.01
084	2,6,10-trimethyl-14-pentadecanone	502-69-2	41.74	1.44	0.10
085	2,6,10-trimethyltetradecane	31295-56-4	33.27	1.82	0.06
086	2,6,11-trimethyldodecane	—	27.04	1.83	0.04
087	2,6-dimethoxy-4-(2-propenyl)phenol 1-*O*-β-D-glucopyranoside	—	17.14	−0.47	0.28
088	2,6-dimethoxy-4-(2-propenyl)phenol	6627-88-9	17.74	1.26	0.05
089	2,6-dimethyloctane	2051-30-1	34.59	1.80	0.01
090	2,6-dimethylpyridine	108-48-5	30.37	1.58	0.01
091	23-*cis*-*p*-coumaroyltormentic acid	—	43.93	−0.65	0.32
092	23-*trans*-*p*-coumaroyltormentic acid	—	20.45	−0.64	0.32

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
093	2-butanone,4-(2,6,6-trimethyl-2-cyclohexen-1-ylidene)	56052-61-0	37.64	1.43	0.05
094	2-butenal	4170-30-3	55.96	1.14	0.00
095	2-ethyl-1-hexanol	104-76-7	11.53	1.17	0.01
096	2-ethyl-naphthalene	91-57-6	54.27	1.88	0.05
097	2-hexadecen-1-ol, 3,7,11,15-tetramethyl-	7541-49-3	47.57	1.26	0.13
098	2-hexadecenoic acid	629-56-1	44.46	1.10	0.10
099	2-hexanoylfuran	14360-50-0	62.88	1.22	0.03
100	2-hexenoic acid	1191-04-4	13.25	0.81	0.01
101	2-methoxy-4-vinylphenol	7786-61-0	22.15	1.38	0.03
102	2-methyl butyric acid	116-53-0	17.70	0.74	0.01
103	2-methyl-5-(1-methylethyl)-phenol	499-75-2	25.09	1.60	0.03
104	2-methyl-aziridine	75-55-8	1.85	1.23	0.00
105	2-methyl-decane	90622-57-4	62.50	1.81	0.02
106	2-methyl-naphthalene	—	26.85	1.85	0.04
107	2-naphthalenamine	91-59-8	47.38	1.13	0.04
108	2-propenal	25314-61-8	19.89	1.07	0.00
109	2-propenamide	107-13-1	11.33	0.70	0.00
110	2-propyn-ol	—	2.44	0.78	0.00
111	2α,19α-dihydroxy-3-oxo-urs-12-en-28-oic acid	—	46.95	−0.30	0.71
112	2α,3α,19α,23-tetrahydroxy-olean-12-en-28-oic acid	—	16.65	−0.59	0.69
113	2α,3α,19α-trihydroxy-12-oleanen-28-oic acid	—	30.03	−0.18	0.72
114	2α,3α,23-trihydroxyolean-12-en-28-oic acid	102519-34-6	41.34	−0.27	0.72
115	2α,3α,24-trihydroxyolean-12-en-28-oic acid	150821-16-2	13.24	−0.20	0.72
116	2α,3α-dihydroxyurs-12-en-28-oic acid	—	45.16	0.21	0.74
117	2α,3α-dihydroxyursolic acid	—	37.73	0.25	0.74
118	2α,3β,13β-trihydroxyurs-11-en-28-oic acid	—	17.85	−0.44	0.68
119	2α,3β,19α,23-tetrahydroxyurs-12-en-28-oic acid	—	22.73	−0.70	0.69
120	3,4-dimethoxy-phenol	95-65-8	16.66	1.09	0.03
121	3,6-dimethyldecane	17312-53-7	42.83	1.80	0.02
122	3,6-dimethyl-phenanthrene	1576-67-6	20.84	1.95	0.13
123	3,7,11-trimethyl-[*S*-(*Z*)]-1,6,10-dodecatrien-3-ol	—	6.21	1.45	0.06
124	3,7-dimethylnonane	17302-32-8	70.51	1.81	0.02
125	3,8-dimethyl-decane	17312-55-9	33.07	1.81	0.02
126	3,8-dimethylundecane	17301-30-3	27.11	1.81	0.03
127	3-carene	13466-78-9	27.36	1.87	0.04

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
128	3-epicorosolic acid methyl ester	—	14.35	0.30	0.72
129	3-epicorosolic acid	52213-27-1	17.74	0.55	0.76
130	3-epiursolic acid	989-30-0	39.92	0.51	0.75
131	3-ethyl-3-methylheptane	17302-01-1	23.90	1.82	0.02
132	3-ethyloctane	5881-17-4	24.77	1.78	0.01
133	3-methyl-1-butanol	123-51-3	50.77	1.01	0.00
134	3-methyl-2-cyclopenten-1-one	2758-18-1	32.04	1.22	0.01
135	3-*O*-*cis*-*p*-coumaroyltormentic acid	121072-40-0	33.35	−0.19	0.34
136	3-*O*-*trans*-caffeoyltormentic acid	—	36.33	−0.07	0.32
137	3-*O*-*trans*-*p*-coumaroylrotundic acid	—	10.02	−0.10	0.34
138	3-*O*-*trans*-*p*-coumaroyltormentic acid	121064-78-6	46.94	−0.17	0.34
139	3-oxo-α-ionyl-9-*O*-β-D-apiofuranosyl(1→6)-β-D-glucopyranside	—	7.82	−1.39	0.72
140	3-oxo-α-ionyl-9-*O*-β-D-glucopyranside	—	43.92	−0.85	0.34
141 *	3-oxo-α-ionyl-9-*O*-β-D-glucopyranside_qt	—	72.83	0.54	0.07
142	3α-*trans*-feruloyloxy-2α-hydroxyurs-12-en-28-oic acid	—	22.12	0.01	0.31
143	3β,6α,19α-trihydroxyurs-12-en-28-oic acid	—	17.69	−0.06	0.71
144	3β,6β,19α-trihydroxyurs-12-en-28-oic acid	—	15.31	−0.37	0.71
145	4-(1-methylethyl)-phenol	99-89-8	63.08	1.56	0.02
146	4,6-dimethylundecane	17312-82-2	6.15	1.82	0.03
147	4,8,12-tetradecatrienal,5,9,13-trimethyl	66408-55-7	42.84	1.55	0.09
148	4-allylanisole	140-67-0	44.01	1.74	0.03
149	4-ethyl-decane	1636-44-8	12.88	1.80	0.02
150	4-hexenylacetic acid	—	73.88	0.92	0.02
151	4-methoxy-1,3-benzenediamine	615-05-4	31.77	0.03	0.03
152	4-methyl-1,3-benzenediamine	95-80-7	34.04	0.20	0.02
153	4-methyl-cyclohexene	591-47-9	15.09	1.78	0.01
154	4-*O*-caffeoylquinic acid	905-99-7	28.59	−0.95	0.33
155	5-(2-propenyl)-1,3-benzodioxole	94-59-7	32.67	1.45	0.05
156	5,6-dimethylundecane	17615-91-7	50.24	1.81	0.03
157	5,9-undecadion-2-one,6,10-dimethyl	689-67-8	34.67	0.26	0.06
158	5-ethenyl-2-methyl-pyridine	20260-76-8	49.16	1.58	0.02
159	6-methyl-5-hepten-2-one	110-93-0	31.12	1.31	0.01
160	6α,19α-dihydroxyursolic acid	—	23.23	−0.43	0.71

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
161	9,12-octadecadienoic acid (*Z*,*Z*)-,methyl ester	112-63-0	28.07	1.43	0.17
162	9-ethyl-9H-carbazol-3-amine	132-32-1	14.68	1.24	0.13
163	9-octadecenoic acid,(*Z*)-,methyl ester	112-62-9	43.98	1.43	0.17
164	acetamide	60-35-5	2.81	0.56	0.00
165	alpha,4-dimethyl-benzenmethanol	536-50-5	37.51	1.21	0.02
166	alpha-bisabobol	502-61-4	23.78	1.38	0.07
167	alpha-farnesene	—	11.55	1.92	0.05
168	amygdalin	29883-15-6	7.77	−1.96	0.61
169 *	amygdalin_qt	—	32.59	0.68	0.02
170	anisic aldehyde	123-11-5	38.50	1.05	0.02
171	arjunic acid	31298-06-3	21.80	−0.22	0.72
172	arjunolic acid	465-00-9	43.27	−0.27	0.72
173	benzaldehyde	100-52-7	12.65	1.31	0.01
174	benzene	71-43-2	2.87	1.78	0.01
175	benzenemethanol	100-51-6	54.08	1.08	0.01
176	benzyl benzoate	120-51-4	42.89	1.33	0.09
177	benzyl salicylate	118-58-1	16.13	1.09	0.10
178	beta-cadinene	523-47-7	19.09	1.87	0.08
179	beta-damascone	23726-91-2	30.85	1.36	0.05
180	biphenyl	92-52-4	17.74	1.90	0.04
181	borneol	507-70-0	46.99	1.21	0.05
182	butyl benzoate	136-60-7	37.92	1.28	0.04
183	butylated hydroxyanisole	25013-16-5	56.06	1.40	0.05
184	butylated hydroxytoluene	128-37-0	30.93	1.75	0.07
185	butyl-benzene	104-51-8	15.55	1.88	0.02
186	cadindiene	29350-73-0	17.05	1.87	0.08
187	camphene	79-92-5	12.50	1.80	0.04
188	camphor	76-22-2	24.25	1.27	0.05
189	caryophyllene	87-44-5	29.67	1.83	0.09
190	chlorogenic acid	327-97-9	63.12	−1.07	0.33
191	cinchonain IIb	—	24.81	−1.51	0.18
192	cinchonain Ia	85081-24-9	13.92	−0.55	0.93
193	cinchonain Ib	85022-69-1	30.62	−0.74	0.93
194	cinchonain Ic	85081-22-7	22.82	−0.55	0.93
195	cinchonain Id 7-*O*-β-glucopyranoside	—	39.36	−2.10	0.61

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
196	cinchonain Id	85022-67-9	15.22	−0.52	0.93
197	*cis*-3-hexen-1-ol	928-96-1	35.69	1.06	0.01
198	*cis*-linalooloxide	5989-33-3	25.90	0.99	0.04
199	*cis*-verbenol	1845-30-3	32.58	1.25	0.06
200	colosolic acid	4547-24-4	39.30	0.03	0.74
201	corchoionoside C	185414-25-9	15.22	−1.30	0.36
202 *	corchoionoside C_qt	—	24.51	−0.14	0.08
203	corosolic acid methyl ester	—	15.48	0.26	0.72
204	coumaran	496-16-2	25.01	1.67	0.03
205	cyclohexane	110-82-7	10.45	1.77	0.01
206	cyclohexanone	108-94-1	53.50	1.19	0.01
207	cyclohexene,1-methyl-4-(5-methy-1-menthylene-4-hexenyl)-(s)-	—	21.65	1.89	0.22
208	cyclopentane	287-92-3	1.84	1.78	0.00
209	daucosterol	474-58-8	23.47	−0.15	0.63
210	decane	124-18-5	52.49	1.78	0.01
211	delta 7-stigmastenol	6869-99-4	40.40	1.30	0.75
212	delta-cadinol	36564-42-8	14.84	1.44	0.09
213	dibenz[a,h]anthracene	53-70-3	9.38	2.02	0.62
214	dibenzofuran	132-64-9	9.90	1.75	0.08
215	dibutyl phthalate	84-74-2	78.06	0.79	0.13
216	dihydroactinidiolide	17092-92-1	38.23	1.18	0.07
217	diisobutyl phthalate	84-69-5	41.87	0.85	0.13
218	dimethyl phthalate	131-11-3	66.69	0.44	0.06
219	diphenyl ether	101-84-8	8.62	1.75	0.05
220	docosane	629-97-0	12.59	1.84	0.18
221	eicosane	112-95-8	46.94	1.82	0.13
222	elemicin	487-11-6	45.85	1.34	0.06
223	ellagic acid	476-66-4	7.04	−0.49	0.43
224	epicatechin-(4β→2)-phloroglucinol	—	43.82	−0.59	0.64
225	eriobofuran	97218-06-9	36.60	1.19	0.17
226	eriobotrin	—	43.20	−0.87	0.62
227	eriojaposide A	—	29.74	−1.57	0.71
228	eriojaposide B	—	47.09	−1.45	0.73
229 *	eriojaposide B_qt	—	18.20	0.51	0.07

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
230	ethyl cyclohexane	—	9.75	1.77	0.01
231	ethylbenzene	100-41-4	9.05	1.81	0.01
232	eugenyl β-rutinoside	—	17.84	−1.31	0.68
233 *	eugenyl β-rutinoside_qt	—	7.87	1.45	0.04
234	euscaphic acid	53155-25-2	17.69	−0.22	0.71
235	farnesane	3891-98-3	43.13	1.91	0.05
236	farnesiferol A	511-33-1	8.30	0.72	0.64
237	farnesyl acetate	29548-30-9	37.26	1.40	0.11
238	farnesylacetone	762-29-8	16.60	1.46	0.10
239	ferulic acid	1135-24-6	67.39	0.61	0.06
240	furfural	98-01-1	5.36	1.09	0.01
241	geranic acid	459-80-3	21.86	1.04	0.03
242	hex-2-enal	505-57-7	31.30	1.26	0.01
243	hexachloro-ethane	67-72-1	24.89	1.80	0.02
244	hexadecane	544-76-3	21.36	1.82	0.06
245	hexadecanoic acid, methyl ester	112-39-0	11.62	1.38	0.12
246	hexanoic acid	142-62-1	31.23	0.83	0.01
247	hexanol	111-27-3	67.53	1.06	0.01
248	hydrocinnamic acid	65-85-0	42.40	0.90	0.03
249	hydrocoumarin	119-84-6	52.62	1.19	0.04
250	hyperoside	482-36-0	34.90	−1.34	0.77
251	hyptadienic acid	128397-09-1	32.62	0.90	0.01
252	indane	496-11-7	19.36	1.87	0.02
253	indene	95-13-6	50.05	1.82	0.03
254	indole	120-72-9	33.82	1.78	0.03
255	isobutylamine	78-81-9	32.73	1.03	0.00
256	isocyanato-methane	624-83-9	51.66	1.06	0.00
257	isoeriobotrin	—	15.31	−0.60	0.62
258	isohumbertiol-3-*O*-{α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)-[α-L-(4-*trans*-feruloyl) rhamnopyranosyl(1→6)]}-β-D-glucopyranoside	—	7.02	−2.83	0.17
259 *	isohumbertiol-3-*O*-{α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)-[α-L-(4-*trans*-feruloyl) rhamnopyranosyl(1→6)]}-β-D-glucopyranoside_qt	—	7.02	−1.29	0.47

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
260	isohumbertiol-3-*O*-{α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)-[α-L-rhamnopyranosyl(1→6)]}-β-D-glucopyranoside	—	11.36	−2.70	0.38
261	isoquercitrin	482-35-9	17.72	−1.44	0.77
262	isorhamnetin-3-*O*-galactoside	6743-92-6	63.56	−1.24	0.80
263	isorhamnetin-3-*O*-glucoside	5041-82-7	90.59	−1.45	0.80
264 *	isorhamnetin-3-*O*-glucoside_qt	—	17.25	0.33	0.31
265	kaempferol 3-*O*-α-L-(2",4"-di-*Z*-*p*-coumaroyl)-rhamnoside	—	17.63	−0.98	0.40
266	kaempferol	520-18-3	65.70	0.27	0.24
267	kaempferol-3-*O*-galactoside	23627-87-4	28.23	−1.14	0.74
268	kaempferol-3-*O*-glucoside	480-10-4	66.61	−1.11	0.74
269	kaempferol-3-*O*-neohesperidoside	32602-81-6	41.08	−2.22	0.75
270	kaempferol-3-*O*-rhamnoside	482-39-3	59.10	−0.77	0.70
271	kaempferol-3-*O*-sophoroside	19895-95-5	18.50	−2.57	0.71
272	kaempferol-3-*O*-α-L-(2",4"-di-E-feruloyl)-rhamnoside	—	6.17	−0.66	0.31
273	kaempferol-3-*O*-α-L-(2",4"-di-E-*p*-coumaroyl)-rhamnoside	—	7.67	−0.70	0.40
274	kaempferol-3-*O*-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside	—	42.64	−2.15	0.75
275	kaempferol-3-rutinoside	17650-84-9	22.50	−2.26	0.74
276	limonene	138-86-3	19.72	1.86	0.02
277	linalool	78-70-6	25.24	1.22	0.02
278	linamarin	554-35-8	34.59	−0.90	0.09
279	linguersinol 9'-*O*-β-D-xylopyranoside	—	37.15	−0.91	0.83
280	linguersinol	—	48.60	−0.17	0.54
281	linolenyl alcohol	506-44-5	48.38	1.39	0.12
282	loquatifolin A	116174-69-7	42.19	−1.71	0.59
283 *	loquatifolin A_qt	—	47.60	1.38	0.06
284	malic acid	6915-15-7	34.60	−1.06	0.02
285	maslinic acid	4373-41-5	55.84	0.04	0.74
286	menthol	89-78-1	36.33	1.24	0.03
287	methyl arjunolate	22452-82-0	56.25	−0.05	0.70
288	methyl betulinate	25493-95-2	43.41	0.85	0.76
289	methyl chlorogenate	—	11.49	−0.94	0.36
290	methyl corosolate	4518-70-1	29.88	0.30	0.72
291	methyl maslinate	22425-82-7	42.79	0.32	0.72

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
292	methyl mercaptan	74-93-1	30.64	1.40	0.00
293	methyl salicylate	119-36-8	47.71	0.83	0.03
294	methyl ursolate	32208-45-0	47.63	0.92	0.74
295	methyl vinyl ketone	78-94-4	49.96	1.16	0.00
296	methylbenzene	108-88-3	44.09	1.80	0.01
297	methyl-cyclohexyl-dimethyl oxygensilane	—	44.03	1.48	0.03
298	m-tert-butyl-phenol	585-34-2	50.18	1.56	0.03
299	m-xylene	108-38-3	10.49	1.85	0.01
300	myrcene	123-35-3	22.06	1.87	0.02
301	myristicin	607-91-0	47.76	1.34	0.07
302	myrtanol	53369-17-8	28.48	1.17	0.06
303	nerol	106-25-2	21.95	1.17	0.02
304	nerolidol	7212-44-4	6.43	1.45	0.06
305	nerolidol-3-*O*-[α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)]-β-D-glucopyranoside	—	34.22	−1.86	0.55
306	nerolidol-3-*O*-{[α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)]-α-L-(4-*trans*-feruloyl)-rhamnopyranosyl(1→6)}-β-D-glucopyranoside	—	29.11	−2.75	0.17
307	nerolidol-3-*O*-{[α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)]-α-L-rhamnopyranosyl(1→6)}-β-D-glucopyranoside	—	29.62	−2.63	0.36
308	nerolidol-3-*O*-α-L-rhamnopyranosyl(1→2)-[α-L-rhamnopyranosyl(1→6)]-β-D-glucopyranoside	—	17.83	−1.84	0.59
309	nerolidol-3-*O*-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside	—	44.57	−1.06	0.68
310	nerolidol-3-*O*-α-L-rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside	—	38.33	−2.01	0.55
311	nerolidol-3-*O*-α-L-rhamnopyranosyl(1→6)-α-L-rhamnopyranosyl(1→2)-β-D-glucopyranoside	—	8.84	−1.88	0.59
312	*n*-heptadecane	629-78-7	37.15	1.84	0.07
313	nitro-cyclohexane	—	9.81	1.35	0.02
314	*N*-methyl-*N*-nitroso-benzenamine	614-00-6	27.05	0.95	0.02
304	nerolidol	7212-44-4	6.43	1.45	0.06
305	nerolidol-3-*O*-[α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)]-β-D-glucopyranoside	—	34.22	−1.86	0.55
306	nerolidol-3-*O*-{[α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)]-α-L-(4-*trans*-feruloyl)-rhamnopyranosyl(1→6)}-β-D-glucopyranoside	—	29.11	−2.75	0.17

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
307	nerolidol-3-*O*-{[α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)]-α-L-rhamnopyranosyl(1→6)}-β-D-glucopyranoside	—	29.62	−2.63	0.36
308	nerolidol-3-*O*-α-L-rhamnopyranosyl(1→2)-[α-L-rhamnopyranosyl(1→6)]-β-D-glucopyranoside	—	17.83	−1.84	0.59
309	nerolidol-3-*O*-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside	—	44.57	−1.06	0.68
310	nerolidol-3-*O*-α-L-rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside	—	38.33	−2.01	0.55
311	nerolidol-3-*O*-α-L-rhamnopyranosyl(1→6)-α-L-rhamnopyranosyl(1→2)-β-D-glucopyranoside	—	8.84	−1.88	0.59
312	*n*-heptadecane	629-78-7	37.15	1.84	0.07
313	nitro-cyclohexane	—	9.81	1.35	0.02
314	*N*-methyl-*N*-nitroso-benzenamine	614-00-6	27.05	0.95	0.02
315	N-nitrosodimethylamine	62-75-9	32.76	1.20	0.00
316	nonanoic acid	112-05-0	16.49	0.94	0.02
317	octanoic acid	124-07-2	9.93	0.90	0.02
318	oleanolic acid	508-02-1	66.91	0.61	0.76
319	*O*-xylene	95-47-6	47.04	1.82	0.01
320	palmitic acid ethyl ester	628-97-7	43.92	1.38	0.14
321	palmitic acid	57-10-3	39.33	1.09	0.10
322	*p*-aminotoluene	106-49-0	13.70	1.08	0.01
323	*p*-cymene	—	40.91	1.84	0.02
324	pentadecane	629-62-9	6.56	1.81	0.05
325	phenanthrene	85-01-8	55.31	1.89	0.10
326	phenethyl alcohol	60-12-8	54.12	1.12	0.02
327	phenylacetaldehyde	122-78-1	22.17	1.31	0.02
328	pinocarvone	16812-40-1	55.27	1.32	0.06
329	piperidine	110-89-4	51.47	1.46	0.01
330	pomolic acid	13849-91-7	75.44	0.26	0.73
331	procyanidin B	—	16.08	1.02	0.74
332	procyanidin B1	20315-25-7	32.34	−1.06	0.66
333	procyanidin B2	29106-49-8	15.72	−1.05	0.66
334	procyanidin B4	29106-51-2	11.72	−0.85	0.66
335	procyanidin C1	37064-30-5	35.78	−2.02	0.10
336	procyanidin C2	—	25.35	−2.05	0.10

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
337	propanoic acid, anhydride	123-62-6	17.20	0.78	0.01
336	procyanidin c2	—	25.35	−2.05	0.10
337	propanoic acid,anhydride	123-62-6	17.20	0.78	0.01
338	*p*-xylene	106-42-3	42.90	1.84	0.01
339	pyrene	129-00-0	29.04	1.93	0.19
340	quercetin	117-39-5	31.36	0.04	0.28
341	quercetin-3-*O*-sophoroside	18609-17-1	48.08	−2.67	0.67
342	quercetin-3-rhamnoside	522-12-3	11.61	−0.85	0.74
343	quercetin-3-sambubioside	83048-35-5	40.37	−2.46	0.74
344	quercetin-4'-*O*-β-D-galactoside	—	7.22	−1.26	0.81
345	quercetin-7-α-L-rhamnoside	—	17.74	−1.14	0.76
346	quinoline	91-22-5	39.70	1.56	0.03
347	rhamnocitrin	569-92-6	17.41	0.39	0.27
348	roseoside	54835-70-0	9.71	−1.23	0.36
349	roxburic acid	108657-25-6	19.59	−0.57	0.69
350	rutin	153-18-4	62.82	−2.50	0.68
351	safranal	116-26-7	14.61	1.42	0.04
352	sanguisorba,officinalis-7	—	35.32	−0.25	0.71
353	sanguisorba,officinalis-8	—	17.76	−0.52	0.69
354	tartaric acid	526-83-0	57.03	−1.85	0.02
355	terpineol	8000-41-7	15.69	1.33	0.03
356	tert-butyl-benzene	98-06-6	45.26	1.85	0.02
357	tetradecanoic acid	544-63-8	59.01	1.06	0.07
358	thymol	89-83-8	27.15	1.65	0.03
359	tormentic acid methyl ester	13850-15-2	17.82	0.10	0.69
360	tormentic acid	13850-16-3	33.73	−0.20	0.71
361	*trans*-2-hexenol	928-95-0	27.85	1.10	0.01
362	*trans*-cinnamaldehyde	14371-10-9	29.96	1.37	0.02
363	*trans*-farnesol	—	44.45	1.26	0.06
364	*trans*-linalool oxide	34995-77-2	17.60	0.99	0.07
365	tricosane	638-67-5	5.02	1.88	0.21
366	tricosanoic acid	2433-96-7	23.50	1.21	0.30
367	tridecane	629-50-5	18.23	1.84	0.03
368	trimethylamine	75-50-3	4.57	1.87	0.00
369	undecane	1120-21-4	17.71	1.83	0.02

Table S1. *Cont.*

MolID	Compound Name	CAS	OB	Caco-2	DL
370	ursolic acid	77-52-1	9.95	0.79	0.65
371	ursolic acid lactone	—	15.61	0.54	0.76
372	uvaol	545-46-0	17.56	0.87	0.76
373	valeric acid	109-52-4	29.97	0.75	0.01
374	vomifoliol	23526-45-6	22.38	−0.05	0.08
375	vomifoliol-9-o-β-D-apiofuranosyl(1→6)-β-D-glucopyranside	—	39.33	−1.65	0.71
376	α-cadinol	481-34-5	36.26	1.32	0.09
377	α-ionone	127-41-3	20.14	1.38	0.05
378	α-pinene	80-56-8	25.08	1.82	0.05
379	α-ylangene	14912-44-8	18.56	1.83	0.12
380	β-farnesene	18794-84-8	17.73	1.90	0.05
381	β-ionone	79-77-6	36.33	1.41	0.05
382	β-pinene	127-91-3	37.62	1.82	0.05
383	β-sesquiphellandrene	20307-83-9	22.33	1.89	0.06
384	β-sitosterol	83-46-5	45.04	1.33	0.75
385	γ-hexanolide	695-06-7	52.44	1.11	0.01
386	quercetin-3-*O*-galactosyl-(1→6)-glucoside	—	3.45	−3.03	0.64
387	betulinic acid	472-15-1	17.10	0.55	0.78
388	δ-oleanolic acid	6713-26-4	12.51	0.58	0.76
389 *	caffeic acid	331-39-5	51.08	0.24	0.05

* deglycosylated molecule.