Supplementary Information

Molecular docking and dynamic simulation analysis of natural polyphenols for identifying potential PTP1B inhibitors for type 2 diabetes

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Table S1 Binding energy of docked ligands

SR NO	COMPOUND ID	COMPOUND NAME	BINDING ENERGY (Kcal/mol)
1	3	Malvidin 3-O-(6"-p-coumaroyl-glucoside)	-8.2
2	5	Delphinidin 3-O-(6"-acetyl-galactoside)	-7.3
3	6	Cyanidin 3-O-(6"-acetyl-galactoside)	-8
4	8	Cyanidin 3-O-galactoside	-7.6
5	9	Cyanidin 3-O-glucoside	-7.5
6	10	Cyanidin 3-O-rutinoside	-8.5
7	11	Cyanidin 3-O-sophoroside	-7.9
8	12	Pelargonidin 3-O-glucoside	-8
9	13	Cyanidin 3-O-(6"-malonyl-glucoside)	-8.2
10	14	Peonidin	-7.8
11	15	Peonidin 3-O-glucoside	-7.4
12	16	Peonidin 3-O-rutinoside	-8.4
13	17	Pelargonidin 3-O-rutinoside	-8.5
14	18	Pelargonidin	-8
15	19	Cyanidin	-8.3
16	20	Malvidin 3,5-O-diglucoside	-6.6
17	21	Cyanidin 3-O-glucosyl-rutinoside	-7.6
18	22	Pelargonidin 3-O-sophoroside	-7.8
19	23	Pelargonidin 3-O-glucosyl-rutinoside	-8.3
20	24	Cyanidin 3-O-(6"-succinyl-glucoside)	-8.2
21	25	Pelargonidin 3-O-(6"-succinyl-glucoside)	-8.1
22	27	Delphinidin 3-O-galactoside	-7.3
23	28	Delphinidin 3-O-glucoside	-7.4
24	29	Delphinidin 3-O-arabinoside	-7.8
25	31	Petunidin 3-O-galactoside	-7.7
26	32	Cyanidin 3-O-arabinoside	-7.8
27	33	Petunidin 3-O-glucoside	-7.4
28	34	Peonidin 3-O-galactoside	-7.4
29	35	Petunidin 3-O-arabinoside	-7.6
30	36	Malvidin 3-O-glucoside	-7.5
31	37	Malvidin 3-O-arabinoside	-7.6

32	39	Delphinidin 3-O-(6"-acetyl-glucoside)	-8
33	40	Petunidin 3-O-(6"-acetyl-galactoside)	-7.7
34	41	Peonidin 3-O-(6"-acetyl-galactoside)	-7.7
35	42	Cyanidin 3-O-(6"-acetyl-glucoside)	-7.8
36	43	Malvidin 3-O-(6"-acetyl-galactoside)	-7.9
37	44	Petunidin 3-O-(6"-acetyl-glucoside)	-7.7
38	46	Malvidin 3-O-(6"-acetyl-glucoside)	-7.5
39	47	Peonidin 3-O-(6"-acetyl-glucoside)	-7.9
40	48	Pelargonidin 3-O-arabinoside	-8
41	49	Delphinidin 3-O-rutinoside	-8.4
42	50	Cyanidin 3-O-sambubioside	-7.9
43	51	Pelargonidin 3-O-(6"-malonyl-glucoside)	-8.1
44	52	Peonidin 3-O-(6"-p-coumaroyl-glucoside)	-9
45	53	Cyanidin 3-O-xyloside	-7.7
46	54	Malvidin 3-O-galactoside	-7.7
47	55	Peonidin 3-O-arabinoside	-7.6
48	56	Petunidin 3-O-rutinoside	-8.2
49	57	Delphinidin 3-O-xyloside	-7.4
50	58	Petunidin 3-O-(6"-p-coumaroyl-glucoside)	-8.9
51	59	Pelargonidin 3-O-galactoside	-7.9
52	60	Pelargonidin 3-O-sambubioside	-7.8
53	61	Delphinidin 3-O-sambubioside	-7.8
54	62	Cyanidin 3-O-xylosyl-rutinoside	-8.4
55	63	Vitisin A	-7.1
56	64	Delphinidin 3-O-(6"-p-coumaroyl-glucoside)	-8.6
57	65	Pigment A	-7.7
58	68	Cyanidin 3-O-(6"-p-coumaroyl-glucoside)	-9
59	69	Cyanidin 3-O-sambubioside 5-O-glucoside	-7.2
60	70	Cyanidin 3-O-(6"-caffeoyl-glucoside)	-8
61	71	Cyanidin 3,5-O-diglucoside	-7.1
62	72	Pinotin A	-7.9
63	73	Delphinidin 3,5-O-diglucoside	-7.7
64	74	Pelargonidin 3,5-O-diglucoside	-7.7
65	75	Malvidin 3-O-(6"-caffeoyl-glucoside)	-8.7
66	76	Cyanidin 3-O-(6"-dioxalyl-glucoside)	-8.2
67	83	Delphinidin 3-O-glucosyl-glucoside	-8
68	84	Cyanidin 3-O-(6"-malonyl-3"-glucosyl-glucoside)	-8.1
69	95	Delphinidin 3-O-feruloyl-glucoside	-8.5
70	96	Petunidin 3,5-O-diglucoside	-6.5
71	97	Petunidin 3-O-rhamnoside	-7.7
72	104	Butein	-8.3
73	105	Xanthohumol	-7.1
74	108	Phloretin	-7.5

75	109	Phloridzin	-7.5
76	111	Phloretin 2'-O-xylosyl-glucoside	-7.3
77	112	3-Hydroxyphloretin 2'-O-xylosyl-glucoside	-8.7
78	113	3-Hydroxyphloretin 2'-O-glucoside	-7.9
79	116	Dihydroquercetin 3-O-rhamnoside	-7.1
80	117	Dihydroquercetin	-8.1
81	119	Dihydromyricetin 3-O-rhamnoside	-7.1
82	124	(+)-Catechin	-8
83	125	(-)-Epicatechin	-7.9
84	126	(+)-Gallocatechin	-8.1
85	127	(-)-Epigallocatechin	-7.8
86	128	(-)-Epicatechin 3-O-gallate	-7.6
87	129	(-)-Epigallocatechin 3-O-gallate	-7.5
88	133	Theaflavin	-7.7
89	134	Theaflavin 3-O-gallate	-9.1
90	135	Theaflavin 3'-O-gallate	-8.7
91	136	Theaflavin 3,3'-O-digallate	-9.6
92	137	(+)-Gallocatechin 3-O-gallate	-7.7
93	139	(+)-Catechin 3-O-gallate	-8.4
94	150	Procyanidin dimer B1	-8.9
95	151	Procyanidin dimer B2	-8.9
96	152	Procyanidin dimer B3	-7.8
97	153	Procyanidin dimer B4	-6.8
98	154	Procyanidin dimer B5	-8.8
99	155	Procyanidin dimer B7	-8.7
100	156	Prodelphinidin dimer B3	-7.3
101	157	Procyanidin trimer C1	-7.5
102	161	Procyanidin trimer EEC	-7.6
103	168	Procyanidin trimer T2	-7.6
104	169	Procyanidin trimer C2	-7.2
105	195	(-)-Epicatechin-(2a-7)(4a-8)-epicatechin 3-O-galactoside	-7.5
106	196	Cinnamtannin A2	-7.5
107	199	(+)-Catechin 3-O-glucose	-7.1
108	201	Naringenin	-9.1
109	202	Eriodictyol	-7.9
110	203	Hesperetin	-9.2
111	206	Eriocitrin	-9
112	207	Hesperidin	-8.6
113	208	Naringin	-7.4
114	209	Narirutin	-7.5
115	210	Neoeriocitrin	-8.9
116	211	Neohesperidin	-8.3
117	213	Poncirin	-7.3

118	214	Didymin	-8.8
119	215	Narirutin 4'-O-glucoside	-8.9
120	216	Naringin 4'-O-glucoside	-9.4
121	217	Naringin 6'-malonate	-9.4
122	219	Naringenin 7-O-glucoside	-8.6
123	220	Pinocembrin	-9.2
124	221	8-Prenylnaringenin	-7.9
125	222	6-Prenylnaringenin	-7.9
126	223	6-Geranylnaringenin	-7.8
127	224	Isoxanthohumol	-7.8
128	225	Eriodictyol 7-O-glucoside	-9
129	226	Sakuranetin	-7.7
130	228	Apigenin	-9.1
131	229	Luteolin	-9.2
132	232	Diosmin	-8.9
133	233	Isorhoifolin	-9.4
134	234	Neodiosmin	-8.2
135	235	Rhoifolin	-8.8
136	236	Sinensetin	-6.6
137	237	Nobiletin	-6.5
138	238	Tangeretin	-6.5
139	239	Luteolin 7-O-diglucuronide	-9.2
140	240	Chrysin	-9.2
141	243	Luteolin 7-O-rutinoside	-9.2
142	244	Tetramethylscutellarein	-6.8
143	245	Luteolin 7-O-glucoside	-8.8
144	246	Apigenin 7-O-glucoside	-8.6
145	247	Apigenin 6,8-di-C-glucoside	-7.6
146	251	Luteolin 7-O-glucuronide	-9.2
147	252	Apigenin 7-O-glucuronide	-9.1
148	253	Luteolin 7-O-malonyl-glucoside	-8.6
149	254	Luteolin 6-C-glucoside	-7.8
150	257	Luteolin 7-O-(2-apiosyl-glucoside)	-8.8
151	260	Luteolin 7-O-(2-apiosyl-6-malonyl)-glucoside	-8
152	261	Apigenin 7-O-apiosyl-glucoside	-8
153	263	7,3',4'-Trihydroxyflavone	-9
154	264	7,4'-Dihydroxyflavone	-8.8
155	265	Geraldone	-8.7
156	266	Baicalein	-8.7
157	267	Apigenin 6-C-glucoside	-7.6
158	268	Hispidulin	-7.8
159	269	Cirsimaritin	-7.4
160	271	5,6-Dihydroxy-7,8,3',4'-tetramethoxyflavone	-6.7

161	272	Pebrellin	-6.5
162	273	Gardenin B	-6.5
163	274	Nepetin	-7.7
164	275	Jaceosidin	-7.5
165	276	Cirsilineol	-7.3
166	277	Eupatorin	-6.7
167	278	6-Hydroxyluteolin	-8.2
168	279	6-Hydroxyluteolin 7-O-rhamnoside	-8.5
169	280	Scutellarein	-8.2
170	281	Apigenin 7-O-(6"-malonyl-apiosyl-glucoside)	-8.7
171	283	Chrysoeriol 7-O-apiosyl-glucoside	-7.9
172	284	Chrysoeriol 7-O-(6"-malonyl-apiosyl-glucoside)	-8.1
173	285	Chrysoeriol 7-O-glucoside	-8.7
174	286	Chrysoeriol 7-O-(6"-malonyl-glucoside)	-8.7
175	287	Apigenin 7-O-diglucuronide	-9
176	288	Rhoifolin 4'-O-glucoside	-8.9
177	290	Kaempferol	-8.2
178	291	Quercetin	-8.1
179	292	Quercetin 3-O-galactoside	-7.9
180	293	Quercetin 3-O-glucoside	-7.9
181	294	Quercetin 3-O-xyloside	-8.1
182	295	Quercetin 3-O-rhamnoside	-7.4
183	296	Quercetin 3-O-rutinoside	-8.5
184	297	Quercetin 3-O-sophoroside	-7.9
185	298	Quercetin 3-O-arabinoside	-8.1
186	299	Quercetin 3-O-xylosyl-glucuronide	-8.7
187	303	Isorhamnetin 3-O-glucoside 7-O-rhamnoside	-8
188	304	Isorhamnetin 3-O-rutinoside	-7.5
189	305	Kaempferol 3-O-glucuronide	-7.2
190	306	Isorhamnetin 7-O-rhamnoside	-7.8
191	307	Quercetin 3,4'-O-diglucoside	-8.4
192	308	Myricetin 3-O-rutinoside	-7.3
193	309	Myricetin	-7.9
194	310	Morin	-7.9
195	311	Kaempferide	-8.6
196	312	Myricetin 3-O-galactoside	-7.8
197	313	Myricetin 3-O-glucoside	-8.4
198	314	Quercetin 3-O-glucosyl-xyloside	-8.6
199	315	Quercetin 3-O-acetyl-rhamnoside	-7.6
200	316	Kaempferol 3-O-galactoside	-8
201	317	Galangin	-8.3
202	318	Isorhamnetin	-8
203	319	Kaempferol 3-O-glucoside	-8

204	320	Kaempferol 3-O-rutinoside	-8.4
205	321	Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	-8.6
206	322	Kaempferol 3-O-glucosyl-rhamnosyl-glucoside	-8.7
207	323	Quercetin 3-O-glucosyl-rhamnosyl-galactoside	-7.7
208	324	Quercetin 3-O-glucosyl-rhamnosyl-glucoside	-8.6
209	325	Rhamnetin	-7.4
210	326	Isorhamnetin 3-O-glucoside	-7.7
211	327	Myricetin 3-O-rhamnoside	-7.8
212	328	Quercetin 3-O-rhamnosyl-galactoside	-7.9
213	330	Quercetin 3-O-glucuronide	-7.8
214	331	Isorhamnetin 3-O-glucuronide	-7.8
215	332	Myricetin 3-O-arabinoside	-7.5
216	334	Quercetin 7,4'-O-diglucoside	-9
217	335	Quercetin 4'-O-glucoside	-8.5
218	336	Isorhamnetin 4'-O-glucoside	-8.6
219	337	3,7-Dimethylquercetin	-7.8
220	338	Kaempferol 3-O-sophoroside	-7.5
221	339	Kaempferol 3,7-O-diglucoside	-8.2
222	341	Kaempferol 3-O-sophoroside 7-O-glucoside	-7.2
223	349	Quercetin 3-O-(6"-malonyl-glucoside)	-8.6
224	350	Kaempferol 3-O-(6"-malonyl-glucoside)	-7.9
225	351	Kaempferol 3-O-rhamnoside	-8.4
226	352	Quercetin 3-O-(6"-malonyl-glucoside) 7-O-glucoside	-7.4
227	356	Patuletin 3-O-glucosyl-(1->6)-[apiosyl(1->2)]-glucoside	-8.1
228	357	Spinacetin 3-O-glucosyl-(1->6)-[apiosyl(1->2)]-glucoside	-7.4
229	358	Patuletin 3-O-(2"-feruloylglucosyl)(1->6)-[apiosyl(1->2)]-glucoside	-9.2
230	359	Spinacetin 3-O-(2"-p-coumaroylglucosyl)(1->6)-[apiosyl(1->2)]-glucoside	-7.7
231	360	Spinacetin 3-O-(2"-feruloylglucosyl)(1->6)-[apiosyl(1->2)]-glucoside	-8.1
232	361	Spinacetin 3-O-glucosyl-(1->6)-glucoside	-7.2
233	362	Jaceidin 4'-O-glucuronide	-7.5
234	363	5,3',4'-Trihydroxy-3-methoxy-6:7-methylenedioxyflavone 4'-O-glucuronide	-8.3
235	364	5,4'-Dihydroxy-3,3'-dimethoxy-6:7-methylenedioxyflavone 4'-O-glucuronide	-8.1
236	367	Kaempferol 3-O-xylosyl-glucoside	-8.6
237	368	Kaempferol 3-O-acetyl-glucoside	-8.1
238	369	Quercetin 3-O-xylosyl-rutinoside	-7.6
239	370	Kaempferol 3-O-xylosyl-rutinoside	-8.5
240	375	Kaempferol 7-O-glucoside	-8.6
241	376	Kaempferol 3-O-galactoside 7-O-rhamnoside	-7.8
242	377	Kaempferol 3-O-(6"-acetyl-galactoside) 7-O-rhamnoside	-7.4

243	378	Quercetin 3-O-galactoside 7-O-rhamnoside	-7.9
244	379	Quercetin 3-O-(6"-acetyl-galactoside) 7-O-rhamnoside	-7.8
245	380	Kaempferol 3-O-(2"-rhamnosyl-galactoside) 7-O-rhamnoside	-7.6
246	381	Kaempferol 3-O-(2"-rhamnosyl-6"-acetyl-galactoside) 7-O-rhamnoside	-7.7
247	382	6,8-Dihydroxykaempferol	-8.1
248	383	Isorhamnetin 3-O-galactoside	-7.7
249	384	Quercetin 3-O-rhamnosyl-rhamnosyl-glucoside	-8.9
250	385	Kaempferol 3-O-rhamnosyl-rhamnosyl-glucoside	-8.6
251	386	Methylgalangin	-8.5
252	387	Kaempferol 3,7,4'-O-triglucoside	-8.3
253	392	3-Methoxynobiletin	-6.3
254	393	3-Methoxysinensetin	-6.6
255	394	Daidzein	-8.4
256	395	Formononetin	-8.5
257	396	Genistein	-8.6
258	397	Biochanin A	-8.7
259	398	Glycitein	-8.2
260	399	Coumestrol	-8.6
261	400	Glycitin	-7.7
262	401	6"-O-Acetyldaidzin	-8.4
263	402	6"-O-Malonylgenistin	-8.2
264	403	Daidzin	-7.7
265	404	Genistin	-7.7
266	405	6"-O-Acetylgenistin	-8.3
267	406	6"-O-Acetylglycitin	-8
268	407	6"-O-Malonyldaidzin	-8.1
269	408	6"-O-Malonylglycitin	-7.8
270	411	Ellagic acid glucoside	-8
271	412	Protocatechuic acid	-6.3
272	413	Gallic acid	-6.3
273	414	Vanillic acid	-6.2
274	416	Gentisic acid	-6.2
275	417	Ellagic acid	-7.7
276	418	4-Hydroxybenzoic acid	-6
277	420	Syringic acid	-5.9
278	421	5-O-Galloylquinic acid	-7
279	422	Ellagic acid arabinoside	-8.6
280	423	Ellagic acid acetyl-xyloside	-7.9
281	424	Ellagic acid acetyl-arabinoside	-7.9
282	427	Benzoic acid	-6
283	428	2-Hydroxybenzoic acid	-6.2
284	429	3-Hydroxybenzoic acid	-6.2

285	430	2,3-Dihydroxybenzoic acid	-6.4
286	431	2,4-Dihydroxybenzoic acid	-6.2
287	433	4-Hydroxybenzoic acid 4-O-glucoside	-6.4
288	434	Protocatechuic acid 4-O-glucoside	-6
289	435	Gallic acid 4-O-glucoside	-6.8
290	436	3,5-Dihydroxybenzoic acid	-6.2
291	437	2,6-Dihydroxybenzoic acid	-6
292	438	Gallic acid 3-O-gallate	-7.5
293	439	Gallic acid ethyl ester	-6.1
294	440	Valoneic acid dilactone	-8.6
295	444	Galloyl glucose	-7.2
296	454	p-Coumaric acid	-6.8
297	455	5-p-Coumaroylquinic acid	-7
298	456	4-p-Coumaroylquinic acid	-7.2
299	457	Caffeic acid	-6.7
300	458	Feruloyl glucose	-6.8
301	459	Ferulic acid	-6.8
302	460	Caffeoyl tartaric acid	-7.1
303	461	Rosmarinic acid	-7.6
304	462	o-Coumaric acid	-7
305	463	m-Coumaric acid	-6.8
306	464	Sinapic acid	-6.6
307	465	p-Coumaroyl glucose	-6.8
308	466	p-Coumaroylquinic acid	-7.3
309	467	3-Caffeoylquinic acid	-7.2
310	468	Verbascoside	-7.5
311	469	4-Caffeoylquinic acid	-7.1
312	470	p-Coumaroyl tartaric acid	-7.1
313	471	2,5-di-S-Glutathionyl caftaric acid	-6.5
314	472	Feruloyl tartaric acid	-7.2
315	473	Caffeic acid ethyl ester	-6.5
316	474	Cinnamoyl glucose	-6.8
317	475	5-Caffeoylquinic acid	-7.1
318	476	3-p-Coumaroylquinic acid	-7.3
319	477	2-S-Glutathionyl caftaric acid	-7.3
320	478	5-Feruloylquinic acid	-7.5
321	479	4-Feruloylquinic acid	-7.3
322	480	3-Feruloylquinic acid	-7.3
323	481	5-Sinapoylquinic acid	-6.6
324	482	4-Sinapoylquinic acid	-7.6
325	483	3-Sinapoylquinic acid	-7.2
326	484	3,5-Dicaffeoylquinic acid	-8.3
327	485	Isoferulic acid	-6.7

328	486	Caffeoyl glucose	-7.2
329	487	p-Coumaric acid 4-O-glucoside	-7.2
330	488	Caffeic acid 4-O-glucoside	-7.3
331	489	Ferulic acid 4-O-glucoside	-7.2
332	491	p-Coumaric acid ethyl ester	-6.7
333	503	Hydroxycaffeic acid	-6.5
334	506	Chicoric acid	-8.2
335	507	5-5'-Dehydrodiferulic acid	-8.4
336	508	5-8'-Dehydrodiferulic acid	-6.9
337	509	1,2-Disinapoylgentiobiose	-7.8
338	510	1-Sinapoyl-2-feruloylgentiobiose	-7.8
339	511	1,2-Diferuloylgentiobiose	-7.6
340	512	1,2,2'-Trisinapoylgentiobiose	-8.5
341	513	1,2'-Disinapoyl-2-feruloylgentiobiose	-8.5
342	514	1-Sinapoyl-2,2'-diferuloylgentiobiose	-8.1
343	515	1,2,2'-Triferuloylgentiobiose	-7.3
344	516	8-O-4'-Dehydrodiferulic acid	-6.4
345	518	5-8'-Benzofuran dehydrodiferulic acid	-7.2
346	520	3,4-Dicaffeoylquinic acid	-7.7
347	522	3,4-Diferuloylquinic acid	-8.1
348	523	3,5-Diferuloylquinic acid	-8
349	527	4,5-Dicaffeoylquinic acid	-8.3
350	532	Avenanthramide 2p	-8.3
351	533	Avenanthramide 2c	-8.4
352	534	Avenanthramide 2f	-8
353	539	p-Coumaroyl malic acid	-7.8
354	540	p-Coumaroyl glycolic acid	-7.2
355	549	Cinnamic acid	-6.9
356	551	Caffeoyl aspartic acid	-6.7
357	553	p-Coumaroyl tyrosine	-7.2
358	557	Sinapine	-6.7
359	559	Avenanthramide K	-7.6
360	563	24-Methylcholestanol ferulate	-8.7
361	564	24-Methylcholesterol ferulate	-8.8
362	565	24-Methyllathosterol ferulate	-9.3
363	566	Stigmastanol ferulate	-8.6
364	567	Sitosterol ferulate	-8.3
365	568	Schottenol ferulate	-8.7
366	569	24-Methylenecholestanol ferulate	-9.2
367	572	3,4-Dihydroxyphenylacetic acid	-6.4
368	573	4-Hydroxyphenylacetic acid	-6.5
369	574	Homovanillic acid	-6.6
370	575	Homoveratric acid	-6.4

371	576	Methoxyphenylacetic acid	-5.9
372	578	Dihydro-p-coumaric acid	-6.7
373	579	Dihydrocaffeic acid	-6.6
374	582	Piceatannol	-7.8
375	584	e-Viniferin	-8.8
376	585	Pterostilbene	-7.2
377	586	d-Viniferin	-8.7
378	588	Pallidol	-8.3
379	589	Piceatannol 3-O-glucoside	-8.3
380	590	Pinosylvin	-8.2
381	591	Resveratrol 5-O-glucoside	-8.2
382	592	Resveratrol	-8
383	593	Resveratrol 3-O-glucoside	-8.3
384	594	Secoisolariciresinol	-6.7
385	595	Matairesinol	-7.4
386	596	Lariciresinol	-7.1
387	597	Pinoresinol	-7.5
388	598	Syringaresinol	-7.2
389	599	Isolariciresinol	-6.9
390	600	Arctigenin	-6.8
391	601	Trachelogenin	-6.7
392	602	Medioresinol	-7.8
393	603	1-Acetoxypinoresinol	-6.9
394	605	Sesamin	-8.6
395	606	Sesamolin	-9.2
396	607	Sesamolinol	-8.4
397	608	Sesaminol	-8.8
398	612	Sesamol	-6.2
399	614	7-Hydroxymatairesinol	-7
400	615	Isohydroxymatairesinol	-7.4
401	616	Secoisolariciresinol-sesquilignan	-7.8
402	617	Cyclolariciresinol	-6.9
403	618	7-Oxomatairesinol	-7.2
404	619	Todolactol A	-6.9
405	620	Conidendrin	-8.8
406	621	7-Hydroxysecoisolariciresinol	-6.9
407	622	Nortrachelogenin	-7.6
408	623	Lariciresinol-sesquilignan	-8.1
409	624	Anhydro-secoisolariciresinol	-7.9
410	625	Dimethylmatairesinol	-6.6
411	626	Episesamin	-8.6
412	627	Episesaminol	-9.1
413	630	Ferulaldehyde	-6.4

414	631	Sinapaldehyde	-6.6
415	632	4-Vinylguaiacol	-6
416	633	4-Ethylguaiacol	-6.1
417	634	4-Vinylsyringol	-7.7
418	635	Coumarin	-7.1
419	637	Mellein	-7.4
420	638	Scopoletin	-7.2
421	639	Esculetin	-7.1
422	640	Esculin	-6.9
423	641	Umbelliferone	-6.8
424	642	4-Hydroxycoumarin	-7.4
425	644	2-Methoxy-5-prop-1-enylphenol	-6.7
426	645	Anethole	-6.5
427	646	Eugenol	-6.3
428	647	Acetyl eugenol	-6.3
429	648	[6]-Gingerol	-6.4
430	649	Estragole	-6.2
431	650	Guaiacol	-5.4
432	652	Juglone	-7.3
433	653	1,4-Naphtoquinone	-7.3
434	654	Catechol	-5.3
435	655	Pyrogallol	-5.5
436	656	Phlorin	-6.3
437	657	Phenol	-5.1
438	659	Arbutin	-5.6
439	661	3,4-Dihydroxyphenylglycol	-6
440	666	Carnosic acid	-7.2
441	667	Rosmanol	-6.4
442	668	Carnosol	-6.3
443	669	Epirosmanol	-6.3
444	670	Rosmadial	-6.2
445	671	Thymol	-6.3
446	672	Carvacrol	-6.4
447	673	Tyrosol	-5.9
448	674	Hydroxytyrosol	-5.9
449	675	3,4-DHPEA-AC	-6.3
450	676	p-HPEA-AC	-6.3
451	677	Oleuropein	-7.5
452	678	Demethyloleuropein	-7.1
453	679	3,4-DHPEA-EA	-7
454	680	Ligstroside	-7.1
455	681	3,4-DHPEA-EDA	-6.4
456	682	Hydroxytyrosol 4-O-glucoside	-6.2

457	683	Oleoside dimethylester	-5.8
458	684	Oleoside 11-methylester	-6
459	686	p-HPEA-EDA	-6.6
460	688	Oleuropein-aglycone	-6.8
461	689	Ligstroside-aglycone	-6.8
462	691	5-Heneicosylresorcinol	-5.4
463	692	5-Heptadecylresorcinol	-5.6
464	694	5-Nonadecylresorcinol	-5.9
465	695	5-Pentacosenylresorcinol	-5.9
466	696	5-Pentacosylresorcinol	-5.7
467	697	5-Pentadecylresorcinol	-6.2
468	698	5-Tricosenylresorcinol	-6
469	699	5-Tricosylresorcinol	-6
470	703	3-Methylcatechol	-5.7
471	704	4-Methylcatechol	-5.9
472	705	4-Ethylcatechol	-6
473	706	4-Vinylphenol	-5.8
474	707	4-Ethylphenol	-5.9
475	713	Curcumin	-8.1
476	714	Demethoxycurcumin	-8.1
477	715	Bisdemethoxycurcumin	-7.2
478	717	Bergapten	-8.1
479	718	Psoralen	-8
480	719	Xanthotoxin	-7
481	720	Isopimpinellin	-7.1
482	722	Syringaldehyde	-6
483	723	Protocatechuic aldehyde	-6.4
484	724	Vanillin	-6
485	725	4-Hydroxybenzaldehyde	-6
486	726	Gallic aldehyde	-6.3
487	727	p-Anisaldehyde	-5.9
488	729	3-Methoxyacetophenone	-6.2
489	730	2,3-Dihydroxy-1-guaiacylpropanone	-6