NETWORK ANALYSIS OF NEUROPROTECTIVE RECEPTORS AND MOLECULAR DOCKING INSIGHTS INTO AMARANTHUS-DERIVED COMPOUNDS

Table S1

Tested ligands from *Amaranthus*-derived compounds.

Number	Compounds	CID	Class
1	Quercetin	5280343	flavonoid
2	Isoquercetin	5280804	flavonoid
3	Hyperoside	5281643	flavonoid
4	Rutin	5280805	flavonoid
5	Kaempferol	5280863	flavonoid
6	Myricetin	5281672	flavonoid
7	Apigenin	5280443	flavonoid
8	Catechin	9064	flavonoid
9	Naringenin	439246	flavonoid
10	Kaempferol-3-O-glucoside	5282102	flavonoid
11	Myricetin-3-O-rutinoside	21577860	flavonoid
12	kaempferol-3-O-rutinoside	5318767	flavonoid
13	Luteolin-7-O-glucoside	5280637	flavonoid
14	Rhamnetin	5281691	flavonoid
15	Dihydrokaempferol	122850	flavonoid
16	Dihydroquercetin	439533	flavonoid
17	Gallocatechin	65084	flavonoid
18	Isorhamnetin	5281654	flavonoid
19	Apigenin glucoside	5280704	flavonoid
20	Isorhamnetin 3-vicianoside	44258010	flavonoid
21	Quercetin 3-arabinoside	10252339	flavonoid
22	Naringin	442428	flavonoid
23	6-hydroxykaempferol	5281638	flavonoid
24	Quercetin-3-O-neohesperidoside	5491657	flavonoid
25	Kaempferol-3-O-neohesperidoside	5318761	flavonoid
26	Isorhamnetin-3-O-glucoside	5318645	flavonoid
27	Isorhamnetin-3-O- eohesperidoside	11664505	flavonoid
28	Quercetol A	44257151	flavonoid
29	Hydrangenol	119199	flavonoid
30	Quercitrin	5280459	flavonoid
31	Hesperidin	10621	flavonoid
32	Dihydromyricetin	161557	flavonoid
33	Epicatechin	72276	flavonoid
34	Luteolin	5280445	flavonoid
35	Caffeic acid	689043	phenolic acid
36	2-O-caffeoylglucaric acid	5459979	phenolic acid
37	Ferulic acid	445858	phenolic acid
38	4-hydroxycinnamic acid	637542	phenolic acid
39	Caffeoylquinic acid	1794427	phenolic acid
40	Isoferulic acid	736186	phenolic acid
41	3,4,5-trihydroxybenzoic acid	370	phenolic acid
42	4-hydroxy-3-methoxybenzoic acid	8468	phenolic acid
43	3,5-dimethoxy-4-hydroxybenzoic acid	10742	phenolic acid
44	4-hydroxybenzoic acid	135	phenolic acid
45	2-hydroxybenzoic acid	338	phenolic acid
46	2,3,7,8-tetrahydroxy-chromeno [5,4,3-cde] chromene-5,10-dione	5281855	phenolic acid
47	3,4-dihydroxybenzoic acid	72	phenolic acid
48	2,4-dihydroxybenzoic acid	1491	phenolic acid
49	2,5-dihydroxybenzoic acid	3469	phenolic acid
50	3-methoxy-4-hydroxy cinnamic acid	709	phenolic acid
51	3-hydroxy cinnamic acid	637541	phenolic acid
52	4-hydroxy-3,5-dimethoxy cinnamic acid	637775	phenolic acid
53	O-coumaric acid	637540	phenolic acid
54	4-O-caffeoylquinic acid	9798666	phenolic acid
55	4-O-feruloylquinic acid	10177048	phenolic acid
56	Ferulic acid 4-glucoside	13916049	phenolic acid
57	Caffeoylglucaricacid	129660947	phenolic acid
58	Bourgeanic acid	10905154	phenolic acid
59	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	62603	phenolic acid
60	p-hydroxyl benzoic acid	21426294	phenolic acid
61	Butanoic acid	264	carboxylic acid
62	Dodecanedioic acid	12736	carboxylic acid
63	Glutaric acid	743	carboxylic acid
64	2-hydroxyoctanoic acid	94180	carboxylic acid
65	Malic acid	525	carboxylic acid
66	Malonic acid	867	carboxylic acid
67	Lactic acid	612	carboxylic acid
68	Pentonic acid	10264	carboxylic acid
69	10-undecynoic acid	31039	carboxylic acid
70	Erythronic acid	2781043	carboxylic acid
71	Erythro-pentonic acid	21636776	carboxylic acid
72	Succinic acid	1110	carboxylic acid
73	2-Isopropylmalic acid	77	carboxylic acid
74	Pantothenic acid	6613	carboxylic acid
75	Benzoic acid	243	carboxylic acid
76	Phenylacetic acid	999	carboxylic acid
77	Phthalic acid	1017	carboxylic acid
78	Dodecanoic acid	3893	carboxylic acid
79	Myristic acid	11005	carboxylic acid
80	Hexadecanoic acid	985	carboxylic acid
81	Linoleic acid (essential)	5280450	carboxylic acid
82	2-pyrrolidone-5-carboxylic acid	499	carboxylic acid
83	Citric acid	311	carboxylic acid
84	Mannonic acid	3246006	carboxylic acid
85	Maleic acid	444266	carboxylic acid

(*continues*)

Table S1
Continued.

Number	Compounds	CID	Class
86	Glyceric acid	752	carboxylic acid
87	2-oxopentanoic acid	74563	carboxylic acid
88	Fumaric acid	444972	carboxylic acid
89	Propenoic acid, acrylic acid	6581	carboxylic acid
90	Pentanoic acid	7991	carboxylic acid
91	Margaric acid, heptadecanoic acid	10465	carboxylic acid
92	Oxalic acid	971	carboxylic acid
93	Shikimic acid	8742	carboxylic acid
94	Glyoxylic acid	760	carboxylic acid
95	3-Hydroxy-3-methylglutaric acid	1662	carboxylic acid
96	Octanoic acid	379	carboxylic acid
97	Oleic acid	445639	carboxylic acid
98	Pyroglutamic acid (5-oxoproline)	7405	carboxylic acid
99	Citramalic acid	1081	carboxylic acid
100	Adipic acid	196	carboxylic acid
101	Threonic acid	151152	carboxylic acid
102	α-hydroxyglutaric acid	43	carboxylic acid
103	2-hydroxysebacic acid	128458	carboxylic acid
104	Methylmaleic acid	643798	carboxylic acid
105	Itaconic acid	811	carboxylic acid
106	Aconitic acid	643757	carboxylic acid
107	Chloroacetic acid	300	carboxylic acid
108	Acetic acid	176	carboxylic acid
109	n-decanoic acid	2969	carboxylic acid
110	2-thiophenecarboxylic acid, 5-nonyl-	587962	carboxylic acid
111	Ascorbic acid	54670067	carboxylic acid
112	Neopentyl trifluoroacetate	522588	carboxylic acid
113	3,4,5-trihydroxystilbene	9964599	stilbene
114	Phlorizin	6072	stilbene
115	Betanin (betanidin 5-*O*-β-glucoside)	6540685	betalain
116	Betalamic acid	5281176	betalain
117	Phenol,2-methyl-5-[1-methylethyl]-	10364	phenolic
118	2-Methoxy-4-vinylphenol	332	phenolic
119	Phenol, 2,6-bis(1,1-dimethylethyl)-	31405	phenolic
120	2-Tert-Butyl-4-(1,1,3,3-Tetramethylbutyl) phenol	605573	phenolic
121	2-methylphenol	335	phenolic
122	Syringaldehyde	8655	phenolic aldehyde
123	Sinapoyltyramine	25245053	phenolic amide
124	Squalene	638072	terpene
125	Borneol	64685	terpene
126	Izoborneol	6321405	terpene
127	(+)-α-tocopherol	2116	terpene
128	Phytol	5280435	terpene
129	Hydroxytremetone	186059	terpene
130	Lapachenole	174859	terpene
131	α-vetivone	442405	terpene
132	Valerenic acid	6440940	terpene
133	1,7-octadien-3-ol	545738	terpene
134	α-pinène	6654	terpene
135	Camphene	6616	terpene
136	β-Pinène	10290825	terpene
137	α-phellandrene	7460	terpene
138	Eucalyptol	2758	terpene
139	α-thujone	261491	terpene
140	Camphor	2537	terpene
141	α-Terpineol	17100	terpene
142	Bornyl acetate	93009	terpene
143	Spathulenol	92231	terpene
144	β-elemene	6918391	terpene
145	β-eudesmol	91457	terpene
146	Dehydroabietic acid	94391	terpene acid
147	Trigonelline	5570	alkaloid
148	Caffeine	2519	alkaloid
149	D-arabinonic acid	122045	aldonic acid
150	Azelainic acid	2266	aldonic acid
151	β-DL-arabinopyranose	439764	sugar
152	β-L-galactopyranose	6971007	sugar
153	D-galactose	6036	sugar
154	β-D-xylopyranose	125409	sugar
155	β-D-glucopyranose	64689	sugar
156	β-DL-lyxopyranose	642638	sugar
157	Levoglucosan	2724705	sugar
158	3-α-mannobiose	11013287	sugar
159	D-(-)-tagatofuranos	12306016	sugar
160	L-(-)-sorbose	6904	sugar
161	α-l-(-)sorbofuranose	12306007	sugar
162	D-(-)-ribofuranose	5779	sugar
163	D-(-)-fructofuranose	439163	sugar
164	D-(-)-fructopyranose	2723872	sugar
165	D-(+)-turanose	54301978	sugar
166	D-(+)-talofuranose	53664879	sugar
167	Gluconic acid, gamma-lacton	439994	sugar
168	Glucofuranose	11105941	sugar
169	Mannose, D-mannopyranose	18950	sugar
170	Glucose	5793	sugar
171	Sucrose	5988	sugar
172	Trehalose	7427	sugar
173	Arabinose	439195	sugar
174	n-acetyl-d-galactosamine	35717	sugar
175	L-(-)-arabitol	439255	sugar alcohol
176	D-mannitol	6251	sugar alcohol
177	Ribitol	6912	sugar alcohol
178	β-erythrotetrofuranose	21581150	sugar alcohol

(*continues*)

Table S1
Continued.

Number	Compounds	CID	Class
179	Inositol	892	sugar alcohol
180	Sorbitol, D-sorbitol	5780	sugar alcohol
181	Glycerol	753	sugar alcohol
182	D-(+)-ribono-1,4-lactone	111064	sugar lactone
183	2(3H)-furanone	140765	sugar lactone
184	Lyxonic acid-1,4-lactone	11829598	sugar lactone
185	Oleic acid amide	5283387	amide
186	Allantoic acid	203	amide
187	Butanamide, 3,3-dimethyl-	219625	amide
188	N-allyloxymethylacrylamide	n/a	amide
189	Dodecanamide	14256	amide
190	Ergost-7-en-3beta-ol	12308940	sterol
191	Chondrillasterol	5283663	sterol
192	Stigmasterol	5280794	sterol
193	Trihydroxyoctadecadienoic acid	129730334	fatty acid
194	Hydroperoxyoctadecadienoic acid	85768813	fatty acid
195	Hydroxyoctadecatrienoic acid	86007827	fatty acid
196	Hydroxyoctadecadienoic acid	21159005	fatty acid
197	9,12-octadecadienoic acid	3931	fatty acid
198	cis,cis,cis-9,12,15-octadecatrienoic acid	5280934	fatty acid
199	Lauryl acetate	8205	fatty acid ester
200	Tetradecyl acetate	12531	fatty acid ester
201	Niacinamide	936	vitamin B3
202	2-Acetyl-1-hydroxyanthraquinone	12033048	anthraquinone
203	Scopoletin	5280460	coumarin
204	Dopaxanthin	135438589	carotenoid
205	Uracil	1174	pyramidine
206	2,4(1H,3H)-pyromidinedione	6451479	pyramidine
207	Adenosine	60961	nucleoside
208	Uridine	6029	nucleoside
209	5-methylcytosine	65040	nucleic acid base
210	2-nonen-1-ol, (E)	5364941	alcohol
211	3-buten-2-ol	11716	alcohol
212	3-methyl-3-oxetanemethanol	137837	alcohol
213	Ethanolamine	700	amino alcohol
214	Xylonic acid-1,4-lactone	439799	lactone
215	2-pentadecanone, 6,10,14-trimethyl-	10408	ketone
216	Ethanone, 1-cyclobutyl-	76398	ketone
217	5-hepten-3-one, 5-ethyl-4-methyl	5365028	ketone
218	Tridecanoic acid, 3-hydroxy-, ethyl ester	575914	ester
219	Nonanoic acid, methyl ester	15606	ester
220	Ethyl 4-bromohexanoate	20288702	ester
221	Decane, 1,1-diethoxy-	101363	ether
222	Ethanol, 2-butoxy-	8133	ether
223	Indole-3-acetonitrile	351795	indole
224	2,2-dimethyl-propyl 2,2-dimethyl-propanesulfinyl sulfone	551399	sulfony
225	Furan, 3-(chloromethyl)-	11126228	furan
226	Benzofuran, 2,3-dihydro-	10329	benzofuran
227	Carbamothioic acid	167559	thiol
228	Adenine	190	purine
229	Diphenylamine	11487	aromatic amine
230	Naphthalene	931	aromatic hydrocarbone
231	4-(2-aminoethyl)phenol	5610	Phenethylamines
232	Pentachlorobutene	181316	chlorinated alkene
233	Arabino-hexos-2-ulose (2-ketoglucose)	159630	ketose
234	Glycerophosphoglycerol	439964	phospholipid
235	Dopa	6047	amino acid
236	4-Aminobenzoic acid	978	aromatic acid
237	Bicyclo[3.2.2]nonane-1,5-dicarboxylic acid, 5-ethyl ester	578603	norbornane
238	1*H*-Cyclopenta(*b*)quinoline, 2,3,5,6,7,8-hexahydro-9-amino-	604519	cyclopentaquinoline
239	Butane, 2,2-Dimethyl-	6403	alkene
240	Epibromohydrine	18430	bromohydrins

(*continues*)

Table S2

ID mapping result for 32 selected proteins.

Number	Protein (PDF Table)	PDB ID (PDF Table)	Entry	Reviewed	Entry	Protein	Gene	Organism	Length
1	Nrf2-Keap1	8XGV	Q14145	reviewed	KEAP1_HUMAN	Kelch-like ECH-associated protein 1 (Cytosolic inhibitor of Nrf2) (INrf2) (Kelch-like protein 19)	KEAP1 INRF2 KIAA0132 KLHL19	Homo sapiens (Human)	624
2	P2X7R	5XW6	Q99572	reviewed	P2RX7_HUMAN	P2X purinoceptor 7 (P2X7) (ATP receptor) (P2Z receptor) (Purinergic receptor)	P2RX7	Homo sapiens (Human)	595
3	5-HT1A	7E2Y/ 8PKM	P63096	reviewed	GNAI1_HUMAN	Guanine nucleotide-binding protein G(i) subunit alpha-1 (Adenylate cyclase-inhibiting G alpha protein)	GNAI1	Homo sapiens (Human)	354
4	D3	3PBL	P35462	reviewed	DRD3_HUMAN	D(3) dopamine receptor (Dopamine D3 receptor)	DRD3	Homo sapiens (Human)	400
5	D2	6CM4	P14416	reviewed	DRD2_HUMAN	D(2) dopamine receptor (Dopamine D2 receptor)	DRD2	Homo sapiens (Human)	443
6	MORs	7UL4/ 4DKL/5C1M	P35372	reviewed	OPRM_HUMAN	Mu-type opioid receptor	OPRM1 MOR1	Homo sapiens (Human)	400
7	KORs	–	–	–	–	–	–	–	–
8	DORs	–	–	–	–	–	–	–	–
9	NOP	–	–	–	–	–	–	–	–
10	mGlu2	5CNI	Q14416	reviewed	GRM2_HUMAN	Metabotropic glutamate receptor 2 (mGluR2)	GRM2 GPRC1B MGLUR2	Homo sapiens (Human)	872
11	mGlu3	5CNK	Q14832	reviewed	GRM3_HUMAN	Metabotropic glutamate receptor 3 (mGluR3)	GRM3 GPRC1C MGLUR3	Homo sapiens (Human)	879
12	GPR26		Q8NDV2	reviewed	GPR26_HUMAN	G-protein coupled receptor 26	GPR26	Homo sapiens (Human)	337
13	GPR56	7SF8	Q9Y653	reviewed	AGRG1_HUMAN	Adhesion G-protein coupled receptor G1 (G-protein coupled receptor 56) (Protein TM7XN1) [Cleaved into: ADGRG1 N-terminal fragment (ADGRG1 NT) (GPR56 N-terminal fragment) (GPR56 NT) (GPR56(N)) (GPR56 extracellular subunit) (GPR56 subunit alpha); ADGRG1 C-terminal fragment (ADGRG1 CT) (GPR56 C-terminal fragment) (GPR56 CT) (GPR56(C)) (GPR56 seven-transmembrane subunit) (GPR56 7TM) (GPR56 subunit beta)]	ADGRG1 GPR56 TM7LN4 TM7XN1 UNQ540/ PRO1083	Homo sapiens (Human)	693
14	GPR52	6LI2	Q9Y2T5	reviewed	GPR52_HUMAN	G-protein coupled receptor 52	GPR52	Homo sapiens (Human)	361
15	GPR158	7SHE	Q5T848	reviewed	MGLYR_HUMAN	Metabotropic glycine receptor (mGlyR) (G-protein coupled receptor 158)	GPR158 KIAA1136	Homo sapiens (Human)	1215
16	TAAR1	8W8A	Q96RJ0	reviewed	TAAR1_HUMAN	Trace amine-associated receptor 1 (TaR-1) (Trace amine receptor 1)	TAAR1 TA1 TAR1 TRAR1	Homo sapiens (Human)	339

(*continues*)

Table S2
Continued.

Number	Protein (PDF Table)	PDB ID (PDF Table)	Entry	Reviewed	Entry	Protein	Gene	Organism	Length
17	TAAR5		O14804	reviewed	TAAR5_ HUMAN	Trace amine-associated receptor 5	TAAR5 PNR	Homo sapiens (Human)	337 AA
18	CB1	5TGZ/5XRA	P21554	reviewed	CNR1_ HUMAN	Cannabinoid receptor 1 (CB-R) (CB1) (CANN6)	CNR1 CNR	Homo sapiens (Human)	472
19	CB2	2HFF	P34972	reviewed	CNR2_ HUMAN	Cannabinoid receptor 2 (CB-2) (CB2) (hCB2) (CX5)	CNR2 CB2A CB2B	Homo sapiens (Human)	360
20	M1	6ZFZ	P11229	reviewed	ACM1_ HUMAN	Muscarinic acetylcholine receptor M1	CHRM1	Homo sapiens (Human)	460
21	M2	5ZKC	P08172	reviewed	ACM2_ HUMAN	Muscarinic acetylcholine receptor M2	CHRM2	Homo sapiens (Human)	466
22	GABAb	4MR7	O75899	reviewed	GABR2_ HUMAN	Gamma-aminobutyric acid type B receptor subunit 2 (GABA-B receptor 2) (GABA-B-R2) (GABA-BR2) (GABABR2) (Gb2) (G-protein coupled receptor 51) (HG20)	GABBR2 GPR51 GPRC3B	Homo sapiens (Human)	941
23	GABAb	4MR7	Q9UBS5	reviewed	GABR1_ HUMAN	Gamma-aminobutyric acid type B receptor subunit 1 (GABA-B receptor 1) (GABA-B-R1) (GABA-BR1) (GABABR1) (Gb1)	GABBR1 GPRC3A	Homo sapiens (Human)	961
24	NK1	6HLP	P25103	reviewed	NK1R_ HUMAN	Substance-P receptor (SPR) (NK-1 receptor) (NK-1R) (Tachykinin receptor 1)	TACR1 NK1R TAC1R	Homo sapiens (Human)	407
25	CCK2	7F8W	P32239	reviewed	GASR_ HUMAN	Gastrin/cholecystokinin type B receptor (CCK-B receptor) (CCK-BR) (Cholecystokinin-2 receptor) (CCK2-R)	CCKBR CCKRB	Homo sapiens (Human)	447
26	Leucine transporter	2A65	–	–	–	–	–	–	–
27	NET	8TGL	P54219	reviewed	VMAT1_ HUMAN	Chromaffin granule amine transporter (Solute carrier family 18 member 1) (Vesicular amine transporter 1) (VAT1)	SLC18A1 VAT1 VMAT1	Homo sapiens (Human)	525
28	SERT	5I6X	P31645	reviewed	SC6A4_ HUMAN	Sodium-dependent serotonin transporter (SERT) (5HT transporter) (5HTT) (Solute carrier family 6 member 4)	SLC6A4 HTT SERT	Homo sapiens (Human)	630
29	DAT	–	–	–	–	–	–	–	–
30	Mineralocorticoid receptor	2AA2	P08235	reviewed	MCR_ HUMAN	Mineralocorticoid receptor (MR) (Nuclear receptor subfamily 3 group C member 2)	NR3C2 MCR MLR	Homo sapiens (Human)	984
31	MAO	2XCG	P27338	reviewed	AOFB_ HUMAN	Amine oxidase [flavin-containing] B (EC 1.4.3.21) (EC 1.4.3.4) (Monoamine oxidase type B) (MAO-B)	MAOB	Homo sapiens (Human)	520
32	Glycogen synthase kinase 3s	4PTE	P49841	reviewed	GSK3B_ HUMAN	Glycogen synthase kinase-3 beta (GSK-3 beta) (EC 2.7.11.26) (Serine/threonine-protein kinase GSK3B) (EC 2.7.11.1)	GSK3B	Homo sapiens (Human)	420

Note: the yellow lines are the unavailable data in ID Uniprot.

Table S3
Binding affinity and %BSS of top ten selected ligands.

Ligand Number	ΔG (kcal/mol); % BSS (%) of PDB Codes Receptor								
	2XCG	4MR7	5C1M	5CNI	5CNK	5I6X	5TGZ	6CM4	8PKM
2	–	–10.4; 67	–11.0; 92	–	–11.6; 58	–	–	–	–
3	–	–11.0; 50	–10.2; 83	–	–12.8; 50	–	–	–10.8; 56	–
5	–	–	–	–7.8; 75	–	–	–	–	–
6	–	–	–9.7; 67	–	–10.6; 75	–	–	–	–
7	–9.2; 90	–	–	–	–	–	–	–	–
10	–	–	–11.7; 83	–	–11.2; 58	–	–	–	–
11	–	–	–	–	–	–	–9.1; 64	–	–
13	–	–11.5; 67	–10.7; 50	–	–	–11.1; 64	–9.3; 64	–10.4; 56	–10.0; 53
15	–	–	–	–7.8; 88	–	–	–	–	–
16	–	–	–	–	–10.5; 67	–	–	–	–9.7; 47
19	–	–10.9; 50	–11.0; 83	–	–	–	–9.7; 64	–	–
20	–	–10.4; 67	–	–	–	–	–9.0; 55	–11.5; 56	–
21	–	–11.3; 100	–9.9; 67	–	–11.5; 58	–	–	–10.4; 67	–
22	–	–11.2; 50	–	–	–	–	–9.5; 64	–	–
23	–	–	–	–	–	–10.7; 79	–	–	–9.5; 40
24	–	–	–	–	–	–	–9.2; 73	–10.1; 67	–
25	–	–10.4; 83	–	–	–	–	–9.2; 73	–10.1; 67	–
26	–	–10.4; 50	–	–	–	–	–	–10.1; 67	–
27	–	–10.4; 33	–	–	–	–	–9.2; 73	–	–
28	–	–	–9.9; 67	–	–	–11.3; 36	–	–	–
29	–	–	–	–7.8; 88	–	–	–	–	–
30	–	–	–	–	–11.8; 67	–11.6; 36	–	–	–
31	–	–10.6; 50	–	–	–	–	–9.3; 55	–10.8; 67	–
32	–	–	–9.6; 50	–	–10.9; 75	–	–	–	–9.6; 53
33	–	–	–	–	–	–11.1; 71	–	–	–
34	–9.3; 90	–	–	–	–10.5; 67	–	–	–	–
35	–8.6; 80	–	–	–	–	–	–	–	–
36	–	–	–	–8.2; 50	–	–11.5; 64	–	–	–
37	–8.5; 80	–	–	–	–	–	–	–	–
38	–8.2; 70	–	–	–	–	–	–	–	–
39	–	–	–	–9.3; 63	–	–10.7; 43	–	–	–10.4; 47
46	–	–	–	–8.0; 100	–10.7; 83	–	–	–	–
51	–8.1; 80	–	–	–	–	–	–	–	–
53	–8.0; 80	–	–	–	–	–	–	–	–
54	–	–	–	–9.0; 75	–10.5; 75	–10.7; 59	–	–	–9.7; 40
55	–	–	–	–	–	–11.2; 57	–	–	–9.9; 33
56	–	–	–9.6; 67	–	–	–	–	–	–
57	–	–10.6; 100	–	–	–11.2; 58	–	–	–	–9.6; 33
74	–	–	–	–7.8; 100	–	–	–	–	–
113	–7.6; 90	–	–	–	–	–	–	–	–9.6; 47
115	–	–12.0; 67	–	–	–	–	–9.0; 55	–10.2; 56	–
116	–7.5; 30	–	–	–7.9; 75	–	–	–	–	–
165	–	–	–	–9.3; 100	–	–	–	–	–
190	–	–	–	–	–	–10.7; 71	–	–	–
192	–	–	–	–	–	–	–	–10.5; 67	–
203	–7.6; 0	–	–	–	–	–	–	–	–
204	–	–	–11.8; 75	–	–	–11.5; 64	–	–	–10.1; 47
218	–8.4; 70	–	–	–	–	–	–	–	–
234	–	–	–	–8.3; 75	–	–	–	–	–

(–) means the ligands exclude the top ten ligand of respective receptor.

Table S4
Druglikeness and medicinal chemistry of selected ligand.

Ligand Number	Parameters									
	LRF	G	V	E	M	BS	P	B	LS	SA
2	no	no	no	no	no	0.17	1	1	no	5.32
3	no	no	no	no	no	0.17	1	1	no	5.32
5	yes	yes	yes	yes	yes	0.55	0	0	yes	3.14
6	yes	yes	no	no	no	0.55	1	1	yes	3.27
7	yes	yes	yes	yes	yes	0.55	0	0	yes	2.96
10	no	yes	no	no	no	0.17	0	0	no	5.29
11	no	no	no	no	no	0.17	1	1	no	6.56
13	no	yes	no	no	no	0.17	1	1	no	5.17
15	yes	yes	yes	yes	yes	0.55	0	0	yes	3.42
16	yes	yes	yes	yes	yes	0.55	1	1	yes	3.51
19	yes	yes	no	no	no	0.55	0	0	no	5.12
20	no	no	no	no	no	0.17	0	0	no	6.46
21	no	yes	no	no	no	0.17	1	1	no	5.04
22	no	no	no	no	no	0.17	0	0	no	6.16
23	yes	yes	yes	yes	yes	0.55	1	1	yes	3.18
24	no	no	no	no	no	0.17	1	1	no	6.53
25	no	no	no	no	no	0.17	0	0	no	6.49
26	no	yes	no	no	no	0.17	0	0	no	5.44
27	no	no	no	no	no	0.17	0	0	no	6.65
28	yes	yes	yes	yes	yes	0.55	0	0	no	4.65
29	yes	yes	yes	yes	yes	0.55	0	0	yes	2.98
30	no	yes	no	no	no	0.17	1	1	no	5.28
31	no	no	no	no	no	0.17	0	0	no	6.34
32	yes	yes	no	no	no	0.55	1	1	yes	3.55
33	yes	yes	yes	yes	yes	0.55	1	1	yes	3.5
34	yes	yes	yes	yes	yes	0.55	1	1	yes	3.02
35	yes	yes	yes	yes	no	0.56	1	2	no	1.81
36	no	no	no	no	no	0.11	1	2	no	4.12
37	yes	yes	yes	yes	no	0.85	0	1	no	1.93
38	yes	yes	yes	yes	no	0.85	0	1	no	1.61
39	yes	no	no	no	no	0.11	1	2	no	4.16
46	yes	yes	no	no	yes	0.55	1	3	yes	3.17
51	yes	yes	yes	yes	no	0.85	0	1	no	1.74
53	yes	yes	yes	yes	no	0.85	0	1	no	1.85
54	yes	no	no	no	no	0.11	1	2	no	4.13
55	yes	no	no	no	no	0.11	0	1	no	4.22
56	yes	no	no	no	yes	0.56	0	1	no	4.5
57	no	no	no	no	no	0.11	1	3	no	4.16
74	yes	no	yes	yes	yes	0.56	0	0	no	2.44
113	yes	yes	yes	yes	yes	0.55	1	2	no	2.06
115	no	no	no	no	no	0.11	0	0	no	6.03
116	yes	no	yes	yes	yes	0.55	0	2	no	3.58
165	no	no	no	no	no	0.17	0	0	yes	5.35
190	yes	no	yes	no	no	0.55	0	1	no	6.05
192	yes	no	yes	no	no	0.55	0	1	no	6.21
203	yes	yes	yes	yes	no	0.55	0	1	no	2.62
204	yes	yes	no	no	no	0.11	1	2	no	4.48
218	yes	yes	no	yes	yes	0.55	0	0	no	3.23
234	yes	no	no	no	no	0.56	0	1	no	4.81

L: Lipinski's Rule of Five; G: Ghose; V: Veber; E: Egan; M: Muegge; BS: Bioavailabilty Score; P: PAINS; B: BRENK; LS: Leadlikeness; SA: Syntethic Accessibility; P and B indicating number of alerts.