

Exploring flavonoids as multi-target therapeutic agents in Alzheimer’s disease: Insights from Network Pharmacology, Molecular Docking, and Dynamics

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SUPPLEMENTARY MATERIAL

Tables:

Table 1. Physicochemical and drug-likeness properties of all the selected flavonoids

S.No.	Selected flavonoids	MW	logp	Alogp	HBA	HBD	TPSA	AMR	nRB	nAtom	nAcidic Group	RC	nRigid B	nArom Ring	nHB	SAlerts	Rule of Five
1	Apiforol	274.273	0.77	-0.724	5	4	90.15	77.51	1	34	0	3	21	2	9	0	0
2	Arbutin	272.254	-0.652	-1.814	7	5	119.61	66.87	3	35	0	2	17	1	12	0	0
3	Aromadendrin	288.256	0.455	-0.806	6	4	107.22	79.87	1	33	0	3	22	2	10	0	0
4	Astragalin	448.382	-0.249	-2.771	11	7	186.37	114.53	4	52	0	4	31	2	18	1	2
5	Baicalein	270.241	2.629	-0.224	5	3	86.99	80.15	1	30	0	3	21	2	8	2	0
6	Butein	272.257	1.806	0.261	5	4	97.99	81.48	3	32	0	2	18	2	9	3	0

7	Calophyllolide	416.473	4.723	2.704	5	0	61.83	129.03	4	55	0	4	30	2	5	4	0
8	Cianidanol	290.272	0.852	-0.936	6	5	110.38	81.07	1	35	0	3	22	2	11	1	0
9	Coutareagenin	300.267	1.807	-0.145	6	3	96.22	85.57	2	34	0	3	22	2	9	3	0
10	Cyanidin	287.061	0	0	6	5	101.15	0	1	32	0	3	22	2	11	2	0
11	Dalbergichromene	254.285	3.259	1.037	3	1	38.69	82.48	2	33	0	3	19	2	4	0	0
12	Dalbergin	268.268	2.806	0.981	4	1	55.76	82.36	2	32	0	3	20	2	5	2	0
13	Delphinidin	303.052	0	0	7	6	121.38	0	1	33	0	3	23	2	13	2	1
14	Didymin	594.568	-1.029	-3.427	14	7	214.06	147.3	7	76	0	5	39	2	21	0	3
15	Diosmin	608.552	-0.762	-4.06	15	8	234.29	150.53	7	75	0	5	40	2	23	1	3
16	Equol	242.274	1.182	0.715	3	2	49.69	75.9	1	32	0	3	19	2	5	0	0
17	Eriocitrin	596.541	-1.002	-4.055	15	9	245.29	143.87	6	74	0	5	40	2	24	1	3
18	Eriodicytol	288.256	1.138	-0.717	6	4	107.22	80.13	1	33	0	3	22	2	10	1	0
19	Fisetin	286.240	1.915	-0.681	6	4	107.22	81.83	1	31	0	3	22	2	10	2	0
20	Galangin	270.241	2.2	-0.117	5	3	86.99	80.23	1	30	0	3	21	2	8	1	0
21	Gallocatechin	306.271	1.2	-1.499	7	6	130.61	82.67	1	36	0	3	23	2	13	1	1
22	Genistein	270.241	1.043	-0.387	5	3	86.99	78.92	1	30	0	3	21	2	8	1	0
23	Genistin	432.383	-0.263	-2.478	10	6	166.14	111.62	4	51	0	4	30	2	16	1	1
24	Glabridin	324.376	2.266	0.981	4	2	58.92	99.71	1	44	0	4	26	2	6	0	0
25	Glycitein	284.268	1.364	-0.323	5	2	75.99	83.96	2	33	0	3	21	2	7	1	0
26	Hesperetin	302.283	1.03	-0.653	6	3	96.22	85.17	2	36	0	3	22	2	9	0	0
27	Hesperidin	610.568	-1.11	-3.99	15	8	234.29	148.91	7	77	0	5	40	2	23	0	3
28	Homoeriodicytol	302.283	1.03	-0.653	6	3	96.22	85.17	2	36	0	3	22	2	9	0	0
29	Isorhamnetin	316.267	1.726	-1.179	7	4	116.45	88.48	2	35	0	3	23	2	11	1	0
30	Kaempferitrin	578.526	-0.149	-3.862	14	8	225.06	144.48	5	71	0	5	40	2	22	1	3
31	Kaempferol	286.240	1.486	-0.681	6	4	107.22	81.83	1	31	0	3	22	2	10	1	0
32	Malvidin	331.083	0	0	7	4	99.38	0	3	39	0	3	23	2	11	1	0
33	Morin	302.240	1.405	-1.244	7	5	127.45	83.44	1	32	0	3	23	2	12	1	0
34	Myricetin	318.239	2.182	-1.807	8	6	147.68	85.04	1	33	0	3	24	2	14	2	1
35	Naringenin Chalcone	272.257	0.79	-0.154	5	3	86.99	78.53	1	32	0	3	21	2	8	0	0
36	Naringenin	272.257	2.017	0.261	5	4	97.99	81.48	3	32	0	2	18	2	9	2	0
37	Naringin	580.541	-1.35	-3.492	14	8	225.06	142.26	6	73	0	5	39	2	22	0	3
38	Narirutin	580.541	-1.35	-3.492	14	8	225.06	142.26	6	73	0	5	39	2	22	0	3

39	Nobiletin	402.400	2.821	-1.526	8	0	81.68	115.2	7	51	0	3	24	2	8	1	0
40	Pachypodol	344.320	1.939	-1.05	7	2	94.45	98.55	4	41	0	3	23	2	9	1	0
41	Pelargonidin	271.064	0	0	5	4	80.92	0	1	31	0	3	21	2	9	1	0
42	Peonidin	301.075	0	0	6	4	90.15	0	2	35	0	3	22	2	10	1	0
43	Petunidin	317.078	0	0	7	5	110.38	0	2	36	0	3	23	2	12	2	0
44	Phloretin	274.273	1.803	-0.003	5	4	97.99	80.65	4	34	0	2	17	2	9	1	0
45	Phlorizin	436.415	0.068	-2.094	10	7	177.14	113.35	7	55	0	3	26	2	17	1	1
46	Poncirin	594.568	-1.029	-3.427	14	7	214.06	147.3	7	76	0	5	39	2	21	0	3
47	Procyanidin	594.528	1.502	-2.069	13	10	229.99	161.19	4	69	0	6	44	4	23	1	3
48	Rhamnazin	330.293	2.047	-1.115	7	3	105.45	93.51	3	38	0	3	23	2	10	1	0
49	Rhoifolin	578.526	-1.002	-3.562	14	8	225.06	143.89	6	71	0	5	39	2	22	1	3
50	Rutin	610.524	-0.735	-4.581	16	10	265.52	147.17	6	73	0	5	41	2	26	2	3
51	Scutellarein	286.240	1.915	-0.787	6	4	107.22	81.76	1	31	0	3	22	2	10	2	0
52	Sinensetin	372.374	2.581	-1.028	7	0	72.45	108.55	6	47	0	3	23	2	7	1	0
53	Sophoraflavonolosside	610.524	-1.786	-4.518	16	10	265.52	146.95	7	73	0	5	40	2	26	1	3
54	Tangeretin	372.374	2.581	-1.028	7	0	72.45	108.55	6	47	0	3	23	2	7	1	0
55	Wogonin	284.268	2.092	-0.16	5	2	75.99	85.19	2	33	0	3	21	2	7	1	0

*Note: Molecular weight (Mw), Partition coefficient (logP), Octanol-water partition coefficient (AlogP), H-bond acceptor (HBA), H-bond donor (HBD), Total polar surface area (TPSA), Atom molar refractivity (AMR), Number of rotatable bonds (nRB), Rotatable bond count (RC), Number of rigid bonds (nRigidB), and Number of hydrogen bonds (nHB).

Table 2. ADMET profile of the selected flavonoids

S.no	Selected Flavonoids	Water solubility	Caco2 permeability	Intestinal absorption (human)	Skin Permeability	P-glycoprotein substrate	P-glycoprotein I inhibitor	P-glycoprotein II inhibitor	VDss (human)	Fraction unbound (human)	BBB permeability	CNS permeability
1	Apiforol	-3.296	1.03	88.861	-2.735	Yes	No	No	0.958	0.257	-8.06	-2.269
2	Arbutin	-1.607	0.009	38.027	-2.801	No	No	No	0.026	0.784	-0.962	-3.557
3	Aromadendrin	-2.967	0.996	59.072	-2.735	Yes	No	No	1.16	0.278	-0.588	-3.014
4	Astragalin	-2.863	0.306	48.052	-2.735	Yes	No	No	1.444	0.218	-1.514	-3.908

5	Baicalein	-3.302	1.117	94.268	-2.735	Yes	No	No	-0.004	0.156	-1.061	-2.21
6	Butein	-3.177	-0.021	72.567	-2.736	Yes	No	No	0.741	0.232	-0.895	-2.395
7	Calophyllolide	-5.699	1.121	98.504	-2.702	No	Yes	Yes	0.47	0.147	-0.823	-1.678
8	Cianidanol	-3.117	-0.283	68.829	-2.735	Yes	No	No	1.027	0.235	-1.054	-3.298
9	Coutareagenin	-3.406	-0.339	84.993	-2.735	Yes	No	No	-0.231	0	-1.25	-2.395
10	Cyanidin	-2.935	-0.35	87.303	-2.735	Yes	No	No	0.952	0.243	-1.234	-2.218
11	Dalbergichromene	-3.596	1.534	94.254	-2.783	No	No	No	0.146	0.006	-0.02	-1.748
12	Dalbergin	-3.599	1.233	94.665	-2.741	No	No	No	-0.312	0.054	-0.094	-2.048
13	Delphinidin	-2.918	-0.833	77.385	-2.735	Yes	No	No	0.863	0.312	-1.62	-3.523
14	Didymin	-3.155	0.547	41.134	-2.735	Yes	No	No	0.501	0.096	-1.578	-4.655
15	Diosmin	-2.929	0.305	29.319	-2.735	Yes	No	No	1.428	0.105	-1.795	-4.836
16	Equol	-3.24	1.218	94.189	-2.858	Yes	No	No	0.42	0.085	0.324	-1.99
17	Eriocitrin	-2.941	-1.101	26.972	-2.735	Yes	No	No	1.529	0.148	-1.831	-4.859
18	Eriodicytol	-3.253	-0.094	74.687	-2.735	Yes	No	No	0.377	0.106	-0.827	-3.142
19	Fisetin	-3.181	0.058	83.752	-2.735	Yes	No	No	0.718	0.166	-1.039	-2.282
20	Galangin	-3.335	0.999	93.985	-2.735	Yes	No	No	0.816	0.142	-0.748	-2.068
21	Gallocatechin	-2.969	-0.375	54.128	-2.735	Yes	No	No	1.301	0.274	-2.969	-0.375
22	Genistein	-3.595	0.9	93.387	-2.735	Yes	No	No	0.094	0.087	-0.71	-2.048
23	Genistin	-2.759	0.066	37.511	-2.735	Yes	No	No	0.274	0.211	-1.417	-3.687
24	Glabridin	-3.646	1.284	94.164	-2.886	Yes	Yes	No	0.613	0.046	0.087	-1.8
25	Glycitein	-3.289	1.175	94.681	-2.742	Yes	No	No	-0.046	0.036	-0.322	-2.216
26	Hesperetin	-3.047	0.294	70.277	-2.737	Yes	No	No	0.746	0.118	-0.719	-2.976
27	Hesperidin	-3.014	0.505	31.481	-2.735	Yes	No	No	0.996	0.101	-1.715	-4.807
28	Homoeriodicytol	-3.042	0.342	73.251	-2.736	Yes	No	No	0.789	0.119	-0.708	-2.987
29	Isorhamnetin	-3	-0.003	76.014	-2.735	Yes	No	No	1.123	0.091	-1.135	-3.188
30	Kaempferitrin	-3.646	1.284	94.164	-2.886	Yes	Yes	No	1.487	0.129	-1.823	-4.673
31	Kaempferol	-3.04	0.032	74.29	-2.735	Yes	No	No	1.274	0.178	-0.939	-2.228
32	Malvidin	-3.07	-0.381	88.785	-2.735	Yes	No	No	0.762	0.137	-1.355	-3.374
33	Morin	-2.978	-0.294	75.408	-2.735	Yes	No	No	1.229	0.214	-1.18	-3.389
34	Myricetin	-2.915	0.095	65.93	-2.735	Yes	No	No	1.317	0.238	-1.493	-3.709
35	Naringenin	-3.224	1.029	91.31	-2.742	Yes	No	No	-0.015	0.064	-0.578	-2.215
36	Naringenin Chalcone	-3.079	-0.267	61.079	-2.735	Yes	No	No	0.724	0.243	-0.908	-2.419
37	Naringin	-2.919	-0.658	25.796	-2.735	Yes	No	No	0.619	0.159	-1.6	-4.773
38	Narirutin	-3.038	0.521	36.625	-2.735	Yes	No	No	1.295	0.121	-1.594	-4.708
39	Nobiletin	-4.949	1.306	98.921	-2.715	No	Yes	Yes	-0.281	0.179	-1.254	-3.142

40	Pachypodol	-3.362	0.008	91.094	-2.741	Yes	No	No	-0.226	0.071	-0.076	-3.147
41	Pelargonidin	-3.083	-0.089	87.294	-2.735	Yes	No	No	0.649	0.2	-1.061	-2.029
42	Peonidin	-3.058	-0.133	89.163	-2.735	Yes	No	No	0.563	0.109	-1.256	-2.297
43	Petunidin	-2.943	-0.47	84.429	-2.735	Yes	No	No	0.837	0.182	-1.415	-3.48
44	Phloretin	-3.077	-0.325	60.5	-2.735	Yes	No	No	0.765	0.253	-0.927	-2.535
45	Phlorizin	-2.493	0.189	37.825	-2.735	Yes	Yes	No	0.667	0.27	-1.133	-3.983
46	Poncirin	-2.97	0.612	30.305	-2.735	Yes	Yes	No	-0.058	0.146	-1.584	-4.721
47	Procyanidin	-2.892	0.131	55.527	-2.735	Yes	Yes	Yes	0.193	0.284	-1.783	-4.106
48	Rhamnazin	-3.399	-0.002	-86.863	-2.735	Yes	No	No	-0.067	0.043	-1.186	-3.193
49	Rhoifolin	-2.862	-0.942	24.308	-2.735	Yes	No	No	1.14	0.152	-1.702	-4.798
50	Rutin	-2.892	-0.949	23.446	-2.735	Yes	No	No	1.663	0.187	-1.899	-5.178
51	Scutellarein	-3.156	-0.357	66.687	-2.735	Yes	No	No	0.587	0.192	-1.398	-2.363
52	Sinensetin	-4.682	1.233	98.578	-2.678	No	Yes	Yes	-0.188	0.155	-1.008	-3.016
53	Sophoraflavonolloside	-2.8	-1.097	4.738	-2.735	Yes	No	No	1.083	0.265	-2.104	-4.903
54	Tangeretin	-4.792	1.245	98.478	-2.678	No	Yes	Yes	-0.226	0.188	-1.026	-3.011
55	Wogonin	-3.469	0.969	92.682	-2.737	Yes	No	No	0.034	0.102	-0.232	-2.18

Table 3: *In silico* predicted Toxicity properties of the selected flavonoids

S.No	Selected flavonoids	LD50 in Rat	AMES toxicity	Max. tolerated dose (human)	hERG I inhibitor	hERG II inhibitor	Oral Rat Acute Toxicity (LD50)	Oral Rat Chronic Toxicity (LOAEL)	Hepato-toxicity	Skin Sensitisation	T.Pyriformis toxicity	Minnow toxicity	Carcinogenicity
1	Apiforol	2500 mg/kg	No	0.205	No	No	2.478	2.045	No	No	0.471	2.946	Noncarcinogenic
2	Arbutin	2500 mg/kg	No	0.485	No	No	1.641	3.497	No	No	0.285	4.286	Noncarcinogenic
3	Aromadendrin	2000 mg/kg	No	0.353	No	No	2.169	2.958	No	No	0.297	3.754	Noncarcinogenic
4	Astragalin	5000 mg/kg	No	0.582	No	No	2.546	4.53	No	No	0.285	6.735	Noncarcinogenic
5	Baicalein	3919 mg/kg	No	0.498	No	No	2.325	2.645	No	No	0.42	1.25	Noncarcinogenic

6	Butein	1000 mg/kg	No	0.117	No	No	2.456	2.578	No	No	0.592	2.818	Noncarcinogenic
7	Calophyllolide	2500 mg/kg	No	0.255	No	Yes	3.074	1.249	No	No	0.34	-0.414	Noncarcinogenic
8	Cianidanol	10000 mg/kg	No	0.438	No	No	2.428	2.5	No	No	0.347	3.585	Noncarcinogenic
9	Coutareagenin	2850 mg/kg	Yes	0.519	No	Yes	2.291	2.393	No	No	0.317	1.957	Noncarcinogenic
10	Cyanidin	5000 mg/kg	No	0.497	No	No	2.464	2.542	No	No	0.29	2.548	Noncarcinogenic
11	Dalbergichromene	500 mg/kg	No	0.026	No	No	2.188	1.517	No	No	1.082	1.043	Noncarcinogenic
12	Dalbergin	2850 mg/kg	No	0.097	No	Yes	2.012	0.889	No	No	0.467	0.581	Noncarcinogenic
13	Delphinidin	5000 mg/kg	No	0.506	No	No	2.553	2.929	No	No	0.286	3.311	Noncarcinogenic
14	Didymin	2300 mg/kg	No	0.462	No	Yes	2.538	3.143	No	No	0.285	6.002	Noncarcinogenic
15	Diosmin	5000 mg/kg	No	0.565	No	Yes	2.512	3.343	No	No	0.285	5.348	Noncarcinogenic
16	Equol	500 mg/kg	No	-0.497	No	No	2.384	1.924	No	No	0.849	1.76	Noncarcinogenic
17	Eriocitrin	12000 mg/kg	No	0.474	No	Yes	2.514	3.357	No	No	0.285	7.621	Noncarcinogenic
18	Eriodicytol	2000 mg/kg	No	0.014	No	No	2.03	2.475	No	No	0.332	2.972	Noncarcinogenic
19	Fisetin	159 mg/kg	No	0.579	No	No	2.465	1.921	No	No	0.376	2.273	Noncarcinogenic
20	Galangin	3919 mg/kg	No	0.333	No	No	2.45	2.323	No	No	0.382	2.385	Noncarcinogenic
21	Gallocatechin	10000 mg/kg	No	0.506	No	No	2.492	2.927	No	No	0.286	4.235	Noncarcinogenic
22	Genistein	2500 mg/kg	No	0.478	No	No	2.268	2.189	No	No	0.377	1.941	Noncarcinogenic
23	Genistin	2500 mg/kg	No	0.412	No	No	2.643	4.406	No	No	0.285	5.016	Noncarcinogenic
24	Glabridin	500 mg/kg	No	-0.395	No	Yes	2.523	1.148	No	No	0.737	0.126	Noncarcinogenic
25	Glycitein	2500 mg/kg	No	0.208	No	Yes	2.17	1.709	No	No	0.417	0.944	Noncarcinogenic
26	Hesperetin	2000 mg/kg	No	0.25	No	No	2.042	2.605	No	No	0.39	2.305	Noncarcinogenic
27	Hesperidin	12000 mg/kg	No	0.525	No	Yes	2.506	3.167	No	No	0.285	7.131	Noncarcinogenic
28	Homoeriodicytol	2000 mg/kg	No	0.271	No	No	2.021	2.635	No	No	0.37	2.062	Noncarcinogenic
29	Isorhamnetin	5000 mg/kg	No	0.576	No	No	2.407	2.499	No	No	0.296	2.206	Noncarcinogenic
30	Kaempferitrin	5000 mg/kg	No	0.519	No	Yes	2.587	3.228	No	No	0.285	7.155	Noncarcinogenic
31	Kaempferol	3919 mg/kg	No	0.531	No	No	2.449	2.505	No	No	0.312	2.885	Noncarcinogenic
32	Malvidin	5000 mg/kg	No	0.554	No	No	2.346	2.412	No	No	0.327	1.224	Noncarcinogenic
33	Morin	3919 mg/kg	No	0.537	No	No	2.413	2.448	No	No	0.308	4.684	Noncarcinogenic
34	Myricetin	159 mg/kg	No	0.51	No	No	2.497	2.718	No	No	0.286	5.023	Noncarcinogenic
35	Naringenin	3600 mg/kg	No	-0.176	No	No	1.791	1.944	No	No	0.369	2.136	Noncarcinogenic
36	Naringenin Chalcone	2000 mg/kg	No	0.298	No	No	2.381	3.32	No	No	0.341	2.535	Noncarcinogenic
37	Naringin	2300 mg/kg	No	0.43	No	Yes	2.495	4.202	No	No	0.285	6.042	Noncarcinogenic
38	Narirutin	2300 mg/kg	No	0.467	No	Yes	2.519	3.203	No	No	0.285	6.491	Noncarcinogenic
39	Nobiletin	5000 mg/kg	No	0.443	No	No	2.459	0.82	No	No	0.315	0.686	Noncarcinogenic
40	Pachypodol	5000 mg/kg	No	0	No	No	2.212	2.115	No	No	0.374	1.32	Noncarcinogenic

41	Pelargonidin	3919 mg/kg	No	0.501	No	No	2.432	2.46	No	No	0.311	1.811	Noncarcinogenic
42	Peonidin	5000 mg/kg	No	0.568	No	No	2.408	2.434	No	No	0.319	1.409	Noncarcinogenic
43	Petunidin	5000 mg/kg	No	0.534	No	No	2.459	2.45	No	No	0.294	2.463	Noncarcinogenic
44	Phloretin	500 mg/kg	No	0.307	No	No	2.381	3.318	No	No	0.34	2.484	Noncarcinogenic
45	Phlorizin	3000 mg/kg	No	0.555	No	No	2.494	4.667	No	No	0.285	6.334	Noncarcinogenic
46	Poncirin	2300 mg/kg	No	0.259	No	Yes	2.545	4.096	No	No	0.285	5.65	Noncarcinogenic
47	Procyanidin	5000 mg/kg	No	0.438	No	Yes	2.482	3.857	No	No	0.285	10.607	Noncarcinogenic
48	Rhamnazin	5000 mg/kg	No	2.286	No	No	2.241	2.04	No	No	0.363	1.493	Noncarcinogenic
49	Rhoifolin	5000 mg/kg	No	0.492	No	Yes	2.498	4.443	No	No	0.285	3.865	Noncarcinogenic
50	Rutin	5000 mg/kg	No	0.452	No	Yes	2.491	3.673	No	No	0.285	7.677	Noncarcinogenic
51	Scutellarein	3919 mg/kg	No	0.626	No	No	2.452	3.135	No	No	0.301	1.99	Noncarcinogenic
52	Sinensetin	5000 mg/kg	No	0.208	No	No	2.503	1.131	No	No	0.384	0.908	Noncarcinogenic
53	Sophoraflavonolloside	5000 mg/kg	No	0.442	No	Yes	2.484	5.146	No	No	0.285	11.883	Noncarcinogenic
54	Tangeretin	5000 mg/kg	No	0.385	No	No	2.368	0.944	No	No	0.355	0.144	Noncarcinogenic
55	Wogonin	3919 mg/kg	No	0.151	No	No	2.265	1.674	No	No	0.423	0.865	Noncarcinogenic

Table 4: Docking XP scores (Kcal/mol) of the selected flavonoids in the compound–target network against the most enriched Alzheimer’s associated target proteins

S.No	Selected flavonoids	4EY7	4AZE	6EQM	1Q4L	1AAP
1	Apiforol	-8.183	-8.326	-6.412	-7.454	-4.91
2	Arbutin	-5.92	-6.168	-5.359	-6.694	-4.447
3	Baicalein	-8.341	-7.767	-4.295	-8.074	-4.681
4	Calophyllolide	-8.2	-8.893	-3.518	-4.138	-2.388
5	Coutareagenin	-7.261	-8.959	-4.943	-7.091	-4.502
6	Dalbergin	-8.129	-8.588	-4.037	-7.243	-4.037
7	Equol	-8.129	-7.878	-6.484	-7.664	-3.749
8	Galangin	-7.597	-8.477	-5.151	-7.431	-4.347
9	Genistein	-7.387	-9.133	-5.683	-8.369	-5.493

10	Glycetin	-7.861	-8.829	-6.171	-7.569	-4.024
11	Hesperetin	-8.661	-7.855	-5.156	-7.848	-5.075
12	Homoeriodictol	-8.538	-7.9	-5.158	-7.408	-4.726
13	Isorhamnetin	-8.296	-8.497	-5.258	-7.786	-5.267
14	Kaempferol	-8.165	-8.662	-5.762	-7.6	-5.176
15	Morin	-7.819	-9.277	-5.221	-7.639	-5.384
16	Naringenin	-8.473	-8.797	-6.573	-7.227	-4.86
17	Naringenin Chalcone	-7.201	-7.942	-5.003	-7.123	-3.574
18	Nobiletin	-8.885	-8.653	-3.539	-5.838	-3.937
19	Pachypodol	-7.447	-7.632	-3.946	-6.916	-4.312
20	Phloretin	-7.493	-8.598	-4.874	-8.465	-3.654
21	Rhamnazin	-8.111	-9.088	-4.822	-8.51	-4.129
22	Scutellarein	-8.322	-9.002	-5.334	-8.394	-4.075
23	Sinensetin	-8.762	-7.769	-3.847	-6.416	-4.247
24	Tangeretin	-8.302	-7.008	-3.682	-6.931	-4.451
25	Wogonin	-8.234	-7.354	-4.273	-7.472	-4.601
26	Donepizil	-12.17	-6.719	-5.434	-6.461	-4.994

*Note: Amyloid precursor protein (APP) with PDB ID: 1AAP, β -site APP cleaving enzyme 1 (BACE1) with PDB ID: 6EQM, Glycogen synthase kinase-3 beta (GSK-3 β) with PDB ID: 1Q4L, Acetylcholinesterase (AChE) with PDB ID: 4EY7 and Dual specificity tyrosine-phosphorylation-regulated kinase 1A (DYRK1A) with PDB ID: 4AZE.

Figures

The top five docked complex:

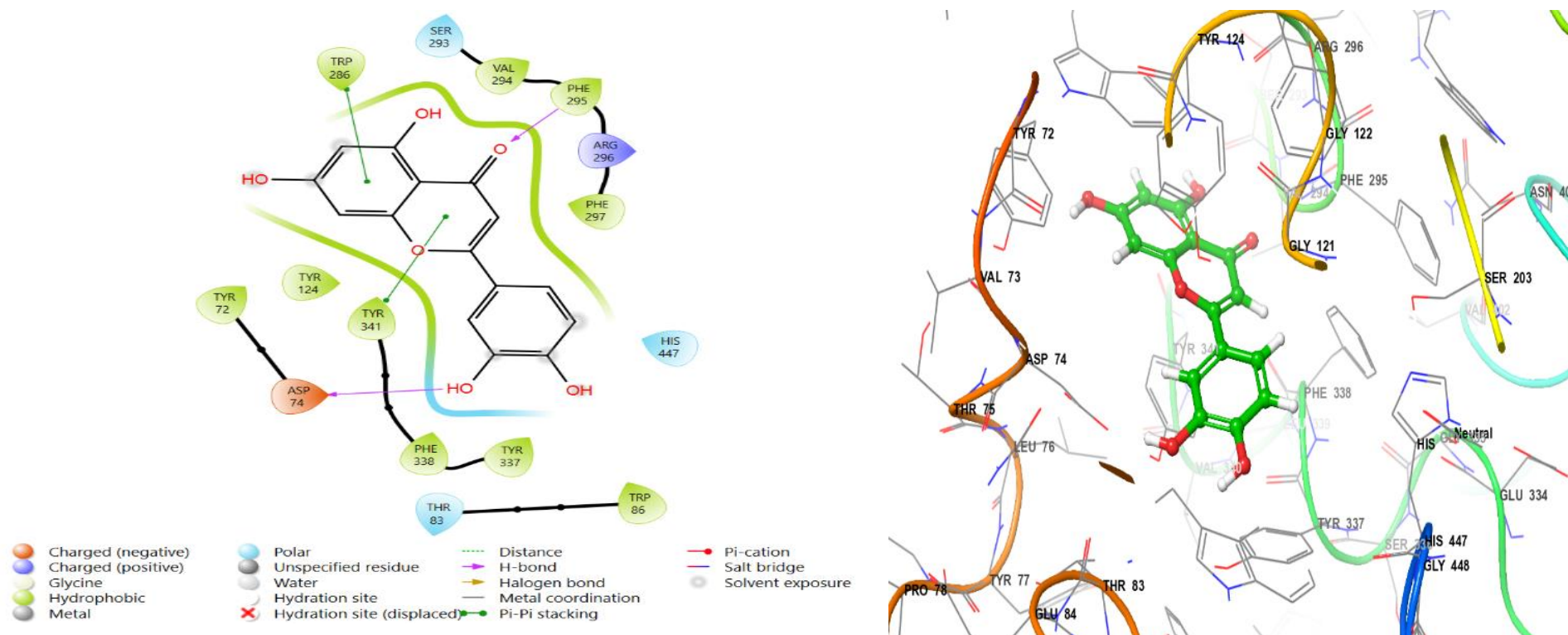


Figure 1. 2D and 3D interactions of Luteolin with Acetylcholinesterase (AChE).

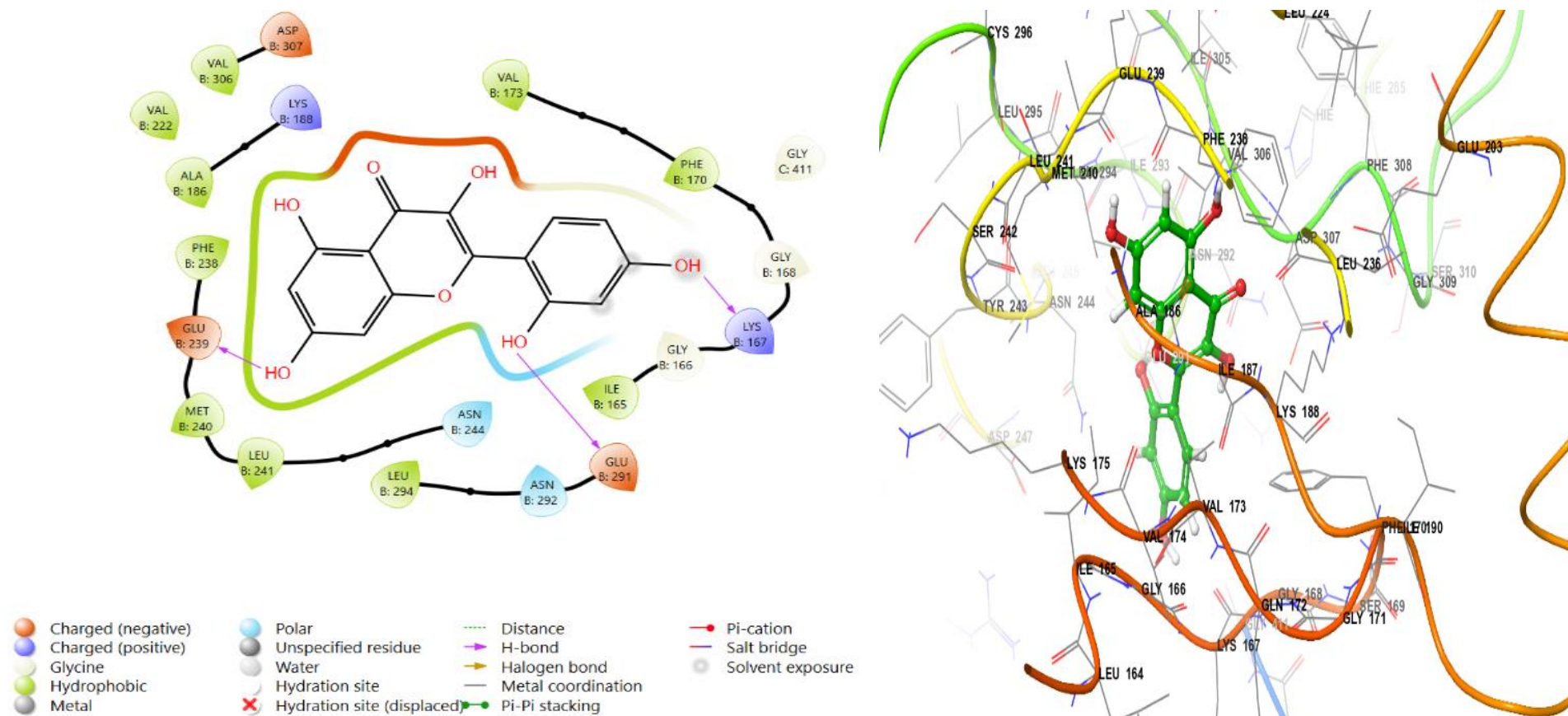


Figure 2. 2D and 3D interactions of Morin with Dual specificity tyrosine-phosphorylation-regulated kinase 1A (DYRK1A).

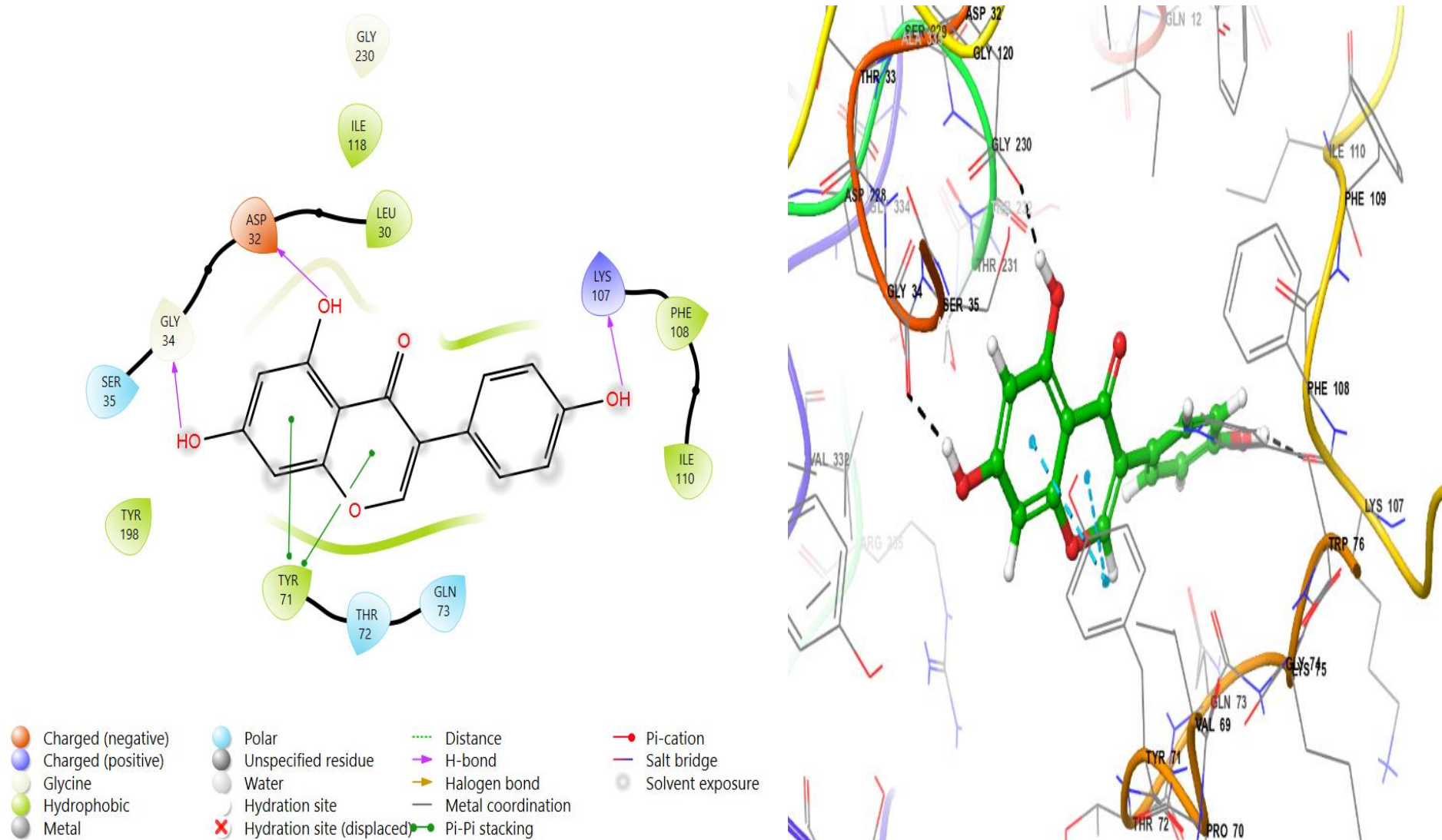


Figure 3. 2D and 3D interactions of Genistein with β -site APP cleaving enzyme 1 (BACE1)

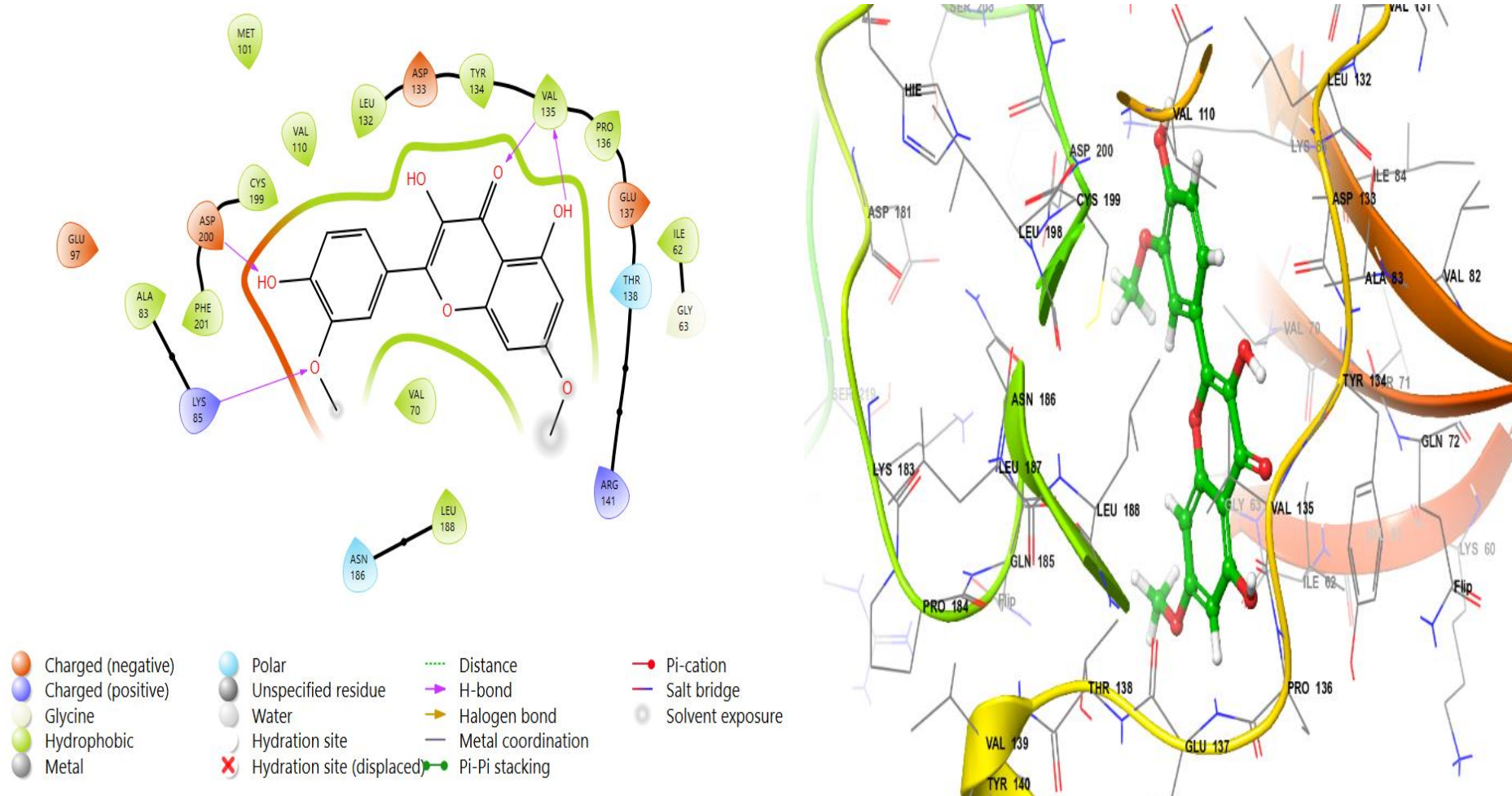


Figure 4. 2D and 3D interactions of Rhamnazin with Glycogen synthase kinase-3 beta (GSK-3 β).

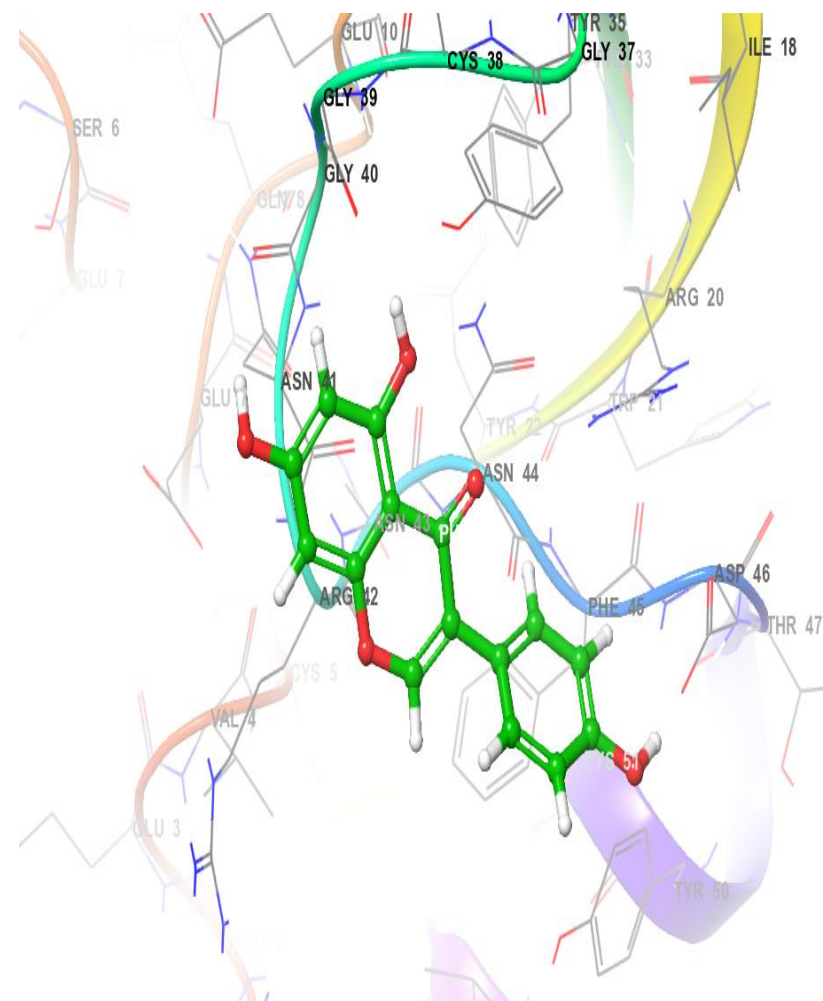
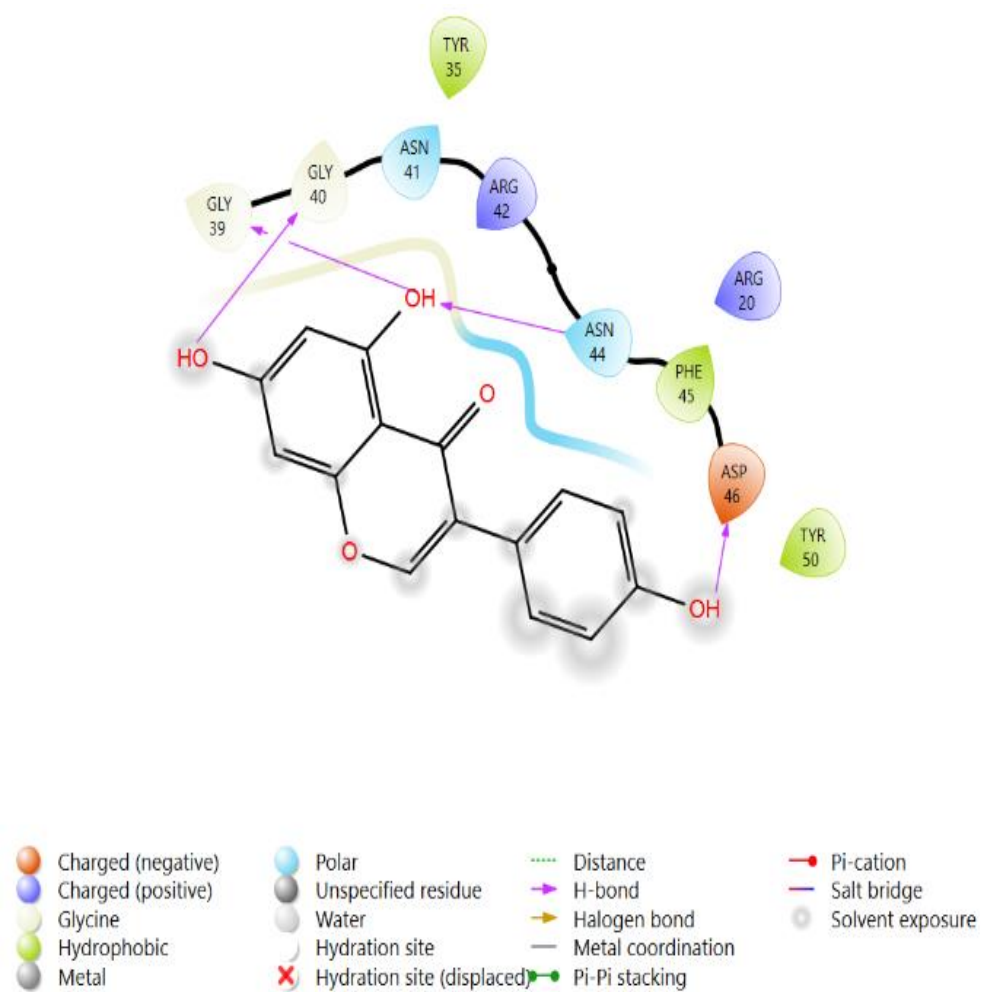


Figure 5. 2D and 3D interactions of Genistein with Amyloid precursor protein (APP).

Other related supplementary material in Excel file:

1. Molecular Function
2. Gene Ontology
3. KEGG Analysis
4. SR Plot KEGG Pathway

Downloaded from the following link: [<http://japsonline.com/19-1737966407-Supplementary-1.xlsx>]