Supplementary material

Monte Carlo optimization based QSAR modeling of angiotensin II receptor antagonists

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Table S1. The SMILES notation of the studied molecules, calculated values for the DCW, experimental data (Ac) – Expr, the values of Ac calculated with the application of CORAL software – Calc, the difference between Expr and Calc – Diff for the built QSPR model.

	SMILES notation	Expr	Split 1				Split 2				Split 3			
			DCW	Calc	Diff	Set	DCW	Calc	Diff	Set	DCW	Calc	Diff	Set
1	O=C(O)c1ccccc1c1ccc(cc1)n1c(cnc1CCC)C(=O)O	7.222	79.32224	6.5632	0.6588	Tr	43.95984	7.0134	0.2086	Tr	71.0841	6.8091	0.4129	Ts
2	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(C)nc1CCC)C(=O)O	6.959	86.81707	6.9975	-0.0385	Tr	46.17449	7.2645	-0.3055	Ts	64.94211	6.4046	0.5544	Tr
3	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)CC)C(=O)O	7	84.76801	6.8788	0.1212	Ts	44.13763	7.0336	-0.0336	Tr	73.92323	6.9961	0.0039	Tr
4	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)C(C)C)C(=O)O	6.444	85.26174	6.9074	-0.4634	Tr	41.30586	6.7125	-0.2685	Tr	69.51122	6.7056	-0.2616	Ts
5	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)C(=C)C)C(=O)O	6.569	80.63282	6.6392	-0.0702	Ts	39.26623	6.4812	0.0878	Tr	68.87184	6.6634	-0.0944	Tr
6	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)CO)C(=O)O	7.237	85.89491	6.9441	0.2929	Tr	46.35552	7.2851	-0.0481	Tr	74.61119	7.0414	0.1956	Tr
7	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)C(C)O)C(=O)O	7.553	87.26991	7.0238	0.5292	Ts	45.22276	7.1566	0.3964	Tr	74.36749	7.0254	0.5276	Tr
8	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)C(C)(C)O)C(=O)O	7.553	91.3052	7.2576	0.2954	Tr	43.45991	6.9567	0.5963	Ts	75.30684	7.0873	0.4657	Ts
9	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)C(C)(O)CC)C(=O)O	7.292	88.91051	7.1188	0.1732	Tr	45.65962	7.2061	0.0859	Tr	76.65003	7.1757	0.1163	Ts
10	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)C(O)(CC)CC)C(=O)O	6.959	90.8365	7.2304	-0.2714	Ts	45.7814	7.22	-0.261	Tr	79.00975	7.3311	-0.3721	Tr
11	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)CO)C(=O)OCC	6.076	69.46414	5.992	0.084	Ts	34.16925	5.9033	0.1727	Ts	62.95394	6.2737	-0.1977	Ts
12	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)C(C)(C)O)C(=O)OCC	6.222	73.6058	6.232	-0.01	Tr	35.16542	6.0163	0.2057	Tr	68.00953	6.6066	-0.3846	Ts
13	O=C(O)c1ccccc1c1ccc(cc1)n1cc(nc1CCC)C(=O)O	4.347	39.26036	4.2418	0.1052	Tr	23.62161	4.7074	-0.3604	Ts	36.12188	4.5064	-0.1594	Tr
14	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCC)C(=O)O)C(=O)O	6.495	82.48114	6.7463	-0.2513	Tr	39.61716	6.521	-0.026	Ts	73.7982	6.9879	-0.4929	Ts
15	O=C(O)c1ccccc1c1ccc(cc1)n1c(CO)c(nc1CCC)C(=O)O	4.699	60.81018	5.4905	-0.7915	Ts	30.06906	5.4384	-0.7394	Tr	50.14812	5.4303	-0.7313	Tr
16	O=C(O)c1ccccc1c1ccc(cc1)n1c(CO)c(nc1CCC)CO	5.569	63.10893	5.6237	-0.0547	Tr	29.01674	5.3191	0.2499	Tr	54.04001	5.6866	-0.1176	Ts
17	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CC)C(C)(C)O)C(=O)O	7.432	101.1405	7.8275	-0.3955	Tr	47.51316	7.4163	0.0157	Tr	81.54817	7.4983	-0.0663	Tr
18	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(nc1CCCC)C(C)(C)O)C(=O)O	7.523	93.47258	7.3832	0.1398	Tr	46.91238	7.3482	0.1748	Ts	77.36705	7.223	0.3	Tr
19	O=C(O)c1cnc(CCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1	8.041	95.56673	7.5045	0.5365	Tr	50.8569	7.7954	0.2456	Ts	87.24201	7.8733	0.1677	Tr
20	O=C(O)c1c(C)nc(CCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1	7.959	101.88	7.8704	0.0886	Tr	52.6822	8.0024	-0.0434	Tr	80.64776	7.439	0.52	Tr
21	O=C(O)c1c(CC)nc(CCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1	7.921	107.5459	8.1987	-0.2777	Tr	51.03318	7.8154	0.1056	Tr	86.62936	7.833	0.088	Tr
22	O=C(O)c1c(nc(CCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1)C(C)C	7.337	94.79179	7.4596	-0.1226	Tr	49.14807	7.6017	-0.2647	Tr	79.25583	7.3474	-0.0104	Tr
23	O=C(O)c1c(nc(CCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1)C(=C)C	7.301	90.16287	7.1914	0.1096	Tr	47.10845	7.3704	-0.0694	Tr	78.61645	7.3052	-0.0042	Ts
24	O=C(O)c1c(CO)nc(CCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1	8.161	105.7651	8.0955	0.0655	Tr	51.77218	7.8992	0.2618	Tr	89.44471	8.0184	0.1426	Ts
25	O=C(O)c1c(nc(CCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1)C(C)O	8.31	95.78719	7.5173	0.7927	Tr	51.71058	7.8922	0.4178	Tr	86.64287	7.8339	0.4761	Tr
26	O=C(O)c1c(nc(CCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1)C(C)(C)O	8.091	99.82248	7.7512	0.3398	Tr	49.94772	7.6924	0.3986	Ts	87.58221	7.8958	0.1952	Tr
27	O=C(OCC)c1c(nc(CCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1)C(C)(C)O	6.699	84.27005	6.8499	-0.1509	Tr	42.25781	6.8204	-0.1214	Tr	76.57539	7.1708	-0.4718	Ts

28	O=C(O)c1cn(c(CCC)n1)c1ccc(cc1)c1ccccc1c1nnn[NH]1	4.854	54.87	5.1463	-0.2923	Tr	22.52675	4.5832	0.2708	Tr	43.60806	4.9995	-0.1455	Tr
29	O=C(O)c1c(nc(CCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1)C(=O)O	7	92.86773	7.3481	-0.3481	Tr	47.05107	7.3639	-0.3639	Tr	83.46154	7.6244	-0.6244	Tr
30	O=C(O)c1nc(CCC)n(c1CO)c1ccc(cc1)c1ccccc1c1nnn[NH]1	5.337	69.91533	6.0181	-0.6811	Tr	32.81745	5.75	-0.413	Ts	59.27702	6.0315	-0.6945	Tr
31	O=C(O)c1c(nc(CC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1)C(C)(C)O	8.276	109.6578	8.3211	-0.0451	Tr	54.00097	8.1519	0.1241	Tr	93.82355	8.3068	-0.0308	Tr
32	O=C(O)c1c(nc(CCCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1)C(C)(C)O	8.022	101.9899	7.8767	0.1453	Ts	53.40019	8.0838	-0.0618	Tr	89.64243	8.0314	-0.0094	Tr
33	OCc1c(Cl)nc(CCCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1	6.921	81.34306	6.6803	0.2407	Tr	43.9963	7.0175	-0.0965	Tr	70.83937	6.793	0.128	Tr
34	O=C(O)c1c(Cl)nc(CCCC)n1c1ccc(cc1)c1ccccc1c1nnn[NH]1	7.657	104.475	8.0207	-0.3637	Tr	51.97948	7.9227	-0.2657	Ts	92.14046	8.196	-0.539	Tr
35	O=C(O)c1ccccc1c1ccc(cc1)n1c(CO)c(Cl)nc1CCCC	6.31	66.05975	5.7947	0.5153	Tr	33.8603	5.8683	0.4417	Ts	55.92727	5.8109	0.4991	Tr
36	O=C(O)c1ccccc1c1ccc(cc1)n1c(c(Cl)nc1CCCC)C(=O)O	6.886	91.27686	7.256	-0.37	Ts	45.80086	7.2222	-0.3362	Tr	76.54587	7.1689	-0.2829	Tr
37	CCCCC1=NNC(=O)N1c1ccc(cc1)c1ccccc1C(=O)O	5.824	79.43141	6.5696	-0.7456	Tr	36.90097	6.213	-0.389	Tr	65.12276	6.4165	-0.5925	Ts
38	CCCCN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1C(=O)O	6.996	82.46716	6.7455	0.2505	Ts	39.51527	6.5095	0.4865	Tr	66.74785	6.5236	0.4724	Tr
39	CCCCC1=NNC(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.377	91.51025	7.2695	0.1075	Tr	44.78026	7.1064	0.2706	Ts	78.75777	7.3146	0.0624	Tr
40	CCCCC1=NN(CC)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.658	97.48826	7.6159	0.0421	Ts	48.0212	7.4739	0.1841	Ts	86.15312	7.8016	-0.1436	Tr
41	CCCCC1=NN(CCC)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.824	98.46942	7.6727	0.1513	Ts	52.25514	7.954	-0.13	Tr	88.44691	7.9527	-0.1287	Tr
42	CCCCC1=NN(CCCC)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	8.292	100.2162	7.774	0.518	Ts	54.36595	8.1933	0.0987	Tr	87.76596	7.9079	0.3841	Ts
43	CCCCC1=NN(CCCCC)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	8.252	102.9572	7.9328	0.3192	Tr	54.57517	8.217	0.035	Tr	88.63473	7.9651	0.2869	Tr
44	CCCCC1=NN(CCCCCC)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	8.06	101.4448	7.8452	0.2148	Tr	52.52567	7.9847	0.0753	Tr	85.80807	7.7789	0.2811	Tr
45	CCCCC1=NN(CCCCCCCC)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	6.77	100.0712	7.7656	-0.9956	Tr	49.69885	7.6641	-0.8941	Ts	81.40452	7.4889	-0.7189	Tr
46	CC(C)N1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.699	98.10604	7.6517	0.0473	Ts	53.29601	8.072	-0.373	Ts	82.06925	7.5327	0.1663	Tr
47	CC(CC)N1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	8	94.24698	7.4281	0.5719	Tr	48.21442	7.4958	0.5042	Tr	81.85072	7.5183	0.4817	Tr
48	CC(C)(C)CC(C)CN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.456	102.1836	7.888	-0.432	Ts	50.91824	7.8024	-0.3464	Tr	80.12654	7.4047	0.0513	Tr
49	O=C(O)CN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.041	94.69608	7.4541	-0.4131	Tr	46.92971	7.3502	-0.3092	Tr	80.0944	7.4026	-0.3616	Tr
50	O=C(OCC)CN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	8.046	98.15735	7.6547	0.3913	Tr	53.38657	8.0823	-0.0363	Tr	86.22467	7.8063	0.2397	Tr
51	CC(C)(C)OC(=O)CN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.796	103.5049	7.9645	-0.1685	Tr	52.16008	7.9432	-0.1472	Tr	84.61495	7.7003	0.0957	Tr
52	O=C(O)CCCCN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.921	106.4583	8.1357	-0.2147	Tr	51.75308	7.8971	0.0239	Tr	95.55463	8.4208	-0.4998	Tr
53	O=C(OC)CCCCN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	8.357	108.0926	8.2304	0.1266	Tr	55.80246	8.3562	0.0008	Tr	92.13096	8.1953	0.1617	Ts
54	O=C(O)CCCCCN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.77	104.4146	8.0172	-0.2472	Tr	51.14865	7.8285	-0.0585	Tr	91.04601	8.1239	-0.3539	Tr
55	O=C(OCC)CCCCCN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	8.009	102.2051	7.8892	0.1198	Tr	51.37034	7.8537	0.1553	Tr	84.35529	7.6832	0.3258	Ts
56	CCCCC1=NN(c2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.229	91.12778	7.2473	-0.0183	Tr	45.5251	7.1909	0.0381	Tr	80.10336	7.4032	-0.1742	Tr
57	CCCCC1=NN(Cc2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.796	100.3242	7.7802	0.0158	Tr	50.38637	7.7421	0.0539	Tr	92.94508	8.249	-0.453	Tr
58	CCCCC1=NN(CCc2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	8.509	107.1048	8.1731	0.3359	Ts	55.13762	8.2808	0.2282	Tr	88.7897	7.9753	0.5337	Tr
59	CCCCC1=NN(CCCc2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.745	96.62508	7.5659	0.1791	Tr	50.70961	7.7787	-0.0337	Tr	83.25974	7.6111	0.1339	Ts
60	CCCCC1=NN(C\C=C\c2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	6.538	92.36784	7.3192	-0.7812	Tr	44.6452	7.0911	-0.5531	Tr	72.85523	6.9258	-0.3878	Tr
61	CCCCC1=NN(CC(=O)c2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	8.102	97.72404	7.6296	0.4724	Tr	46.88834	7.3455	0.7565	Tr	87.75989	7.9075	0.1945	Tr
62	CCCCC1=NN(CC(O)c2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	8.444	99.39157	7.7262	0.7178	Ts	49.7979	7.6754	0.7686	Ts	91.87077	8.1782	0.2658	Tr

63	CCCCC1=NN(c2cccc3ccccc32)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.301	85.48282	6.9202	0.3808	Tr	42.35603	6.8316	0.4694	Tr	71.97633	6.8679	0.4331	Tr
64	CCCCC1=NN(c2cc3ccccc3cc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	6.553	86.36262	6.9712	-0.4182	Tr	42.01938	6.7934	-0.2404	Tr	75.77921	7.1184	-0.5654	Tr
65	COc1cc(c(OC)cc1)C(=O)CN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.678	101.1354	7.8272	-0.1492	Tr	48.46001	7.5237	0.1543	Tr	81.64648	7.5048	0.1732	Tr
66	COc1cc(c(OC)cc1)C(O)CN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.658	102.8029	7.9239	-0.2659	Tr	51.36956	7.8536	-0.1956	Tr	85.75736	7.7756	-0.1176	Ts
67	CCCCC1=NN(CC(OC)c2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.921	99.01791	7.7045	0.2165	Tr	49.48227	7.6396	0.2814	Tr	81.78601	7.514	0.407	Ts
68	CCCCC1=NN(CC(OCC)c2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.824	100.3256	7.7803	0.0437	Tr	52.72558	8.0073	-0.1833	Tr	82.84826	7.584	0.24	Tr
69	CCCCC1=NN(CC(OCCC)c2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.347	95.35676	7.4924	-0.1454	Ts	48.73353	7.5547	-0.2077	Ts	84.6089	7.6999	-0.3529	Tr
70	CCCCC1=NN(CC(OCc2ccccc2)c2ccccc2)C(=O)N1c1ccc(cc1)c1ccccc1c1n[NH]nn1	6.553	77.2816	6.445	0.108	Tr	44.10273	7.0296	-0.4766	Tr	71.44523	6.8329	-0.2799	Tr
71	O=C(O)COC(CN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1)c1ccccc1	7.523	88.39447	7.0889	0.4341	Tr	45.45643	7.1831	0.3399	Ts	77.22898	7.2139	0.3091	Tr
72	O=C(OCC)COC(CN1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1)c1ccccc1	6.745	83.34941	6.7966	-0.0516	Tr	41.65108	6.7516	-0.0066	Tr	70.31978	6.7588	-0.0138	Tr
73	O=C(c1ccccc1)C(C)(C)N1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1	7.367	93.49388	7.3844	-0.0174	Ts	50.50151	7.7551	-0.3881	Ts	81.3723	7.4868	-0.1198	Tr
74	O=C(c1ccccc1)C(Cc1ccccc1)N1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1~	5.237	57.16173	5.2791	-0.0421	Ts	26.12532	4.9912	0.2458	Tr	41.58195	4.8661	0.3709	Tr
75	O=C(OCC)CC(C(=O)c1ccccc1)N1N=C(CCCC)N(C1=O)c1ccc(cc1)c1ccccc1c1n[NH]nn1~	7.444	96.09329	7.5351	-0.0911	Tr	49.72887	7.6675	-0.2235	Tr	83.67609	7.6385	-0.1945	Ts

Table S2. The list of SAks together with their correlation weights for the three runs of the Monte Carlo optimization obtained from QSAR model for angiotensin II receptor antagonism.

SAk(CW)	CW			SAk(CW)	CW			SAk(CW)	CW			SAk(CW)	CW		
	Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3
10001000000	0.16077	-0.42439	0.20815	N...=.....	0.45311	0.28247	-0.66068	P4E0N...8-..	-0.47292	0.65646	1.60204	S3E0N...14-.	-0.28891	0.19965	-0.59669
10011000000	-0.75207	1.87686	2.07301	N...=...1...	0.18221	0.82741	-1.26475	P4E0N...9-..	2.46321	2.29562	0.89768	S3E0N...15-.	2.15066	2.6637	0.56285
(...(.....	0.89648	0.86506	0.38045	N...=...C...	0.45578	0.37066	-0.44456	P4E0O...0-..	0.11336	-0.43227	-0.65839	S3E0N...4-..	-0.2188	2.19907	0.25671
(.....	0.07094	1.38324	-0.99142	N...C...(...	0.17312	0.59148	0.04931	P4E0O...1-..	0.43466	0.33239	-0.21194	S3E0N...5-..	2.36239	0.1149	0.30366
(...C...(...	0.44208	1.31569	0.59368	N...C.....	0.04523	0.11312	0.66355	P4E0O...3-..	0.11364	1.04375	0.22232	S3E0N...7-..	-0.83239	0.20229	0.36074
(...N...(...	0.35219	-0.42753	-0.18406	N...C...C...	2.54962	5.64337	1.5602	P4E0O...4-..	0.25402	-1.9477	-2.10702	S3E0N...9-..	1.27744	1.2502	2.40229
(...O...(...	0.58124	0.12107	0.18471	N...H.....	0.17781	0.36697	2.03444	P4E0O...7-..	0.20759	0.12769	-0.77148	S3E0O...1-..	0.08051	0.03254	1.30417
(...c...(...	-0.74909	1.1336	0.38208	N...N...(...	-0.74921	1.90765	1.06904	NNE0C...100-	0.33163	1.96189	2.73753	S3E0O...10-.	1.65975	0.83388	4.82981
++++N---B2==	2.884	-1.12433	1.23261	N...N.....	2.36322	0.27845	0.76533	NNE0C...109-	2.46283	0.27087	1.07988	S3E0O...3-..	-0.53022	-0.55796	-0.5503
++++N---O===	1.03622	8.31279	9.88303	N...N...=...	2.50616	0.01096	0.92738	NNE0C...209-	-0.62128	-0.59857	0.31681	S3E0O...4-..	0.08073	0.28367	0.84868
++++O---B2==	0.95908	1.59837	1.44566	O...(.....	1.97083	0.48079	1.00419	NNE0C...218-	-0.40681	0.17087	-0.06721	S3E0O...5-..	0.14141	0.82546	2.79373
1...(.....	-1.49336	-1.36518	-1.14697	O...(...C...	-0.53964	1.17788	0.4236	NNE0C...300-	0.21386	0.70206	1.27845	S3E0O...7-..	2.06933	-0.96112	-0.68826
1.....	-0.41821	-1.16055	-0.20016	O...(...N...	0.03976	0.0827	3.5987	NNE0C...309-	0.39338	-0.17749	1.49791	S3E0O...9-..	-0.10598	2.08115	-0.18188
1...C...(...	0.3748	-0.73544	0.44721	O...(...O...	0.4955	1.21035	0.29777	NNE0C...318-	-0.97419	0.74333	0.43909	Nmax.0.....	1.25404	-0.08787	0.38872
1...N...(...	-0.54852	-0.5771	0.10741	O.....	0.34916	0.39242	0.34532	NNE0C...327-	-0.11937	-0.56352	-0.62659	Nmax.1.....	0.26869	0.43185	0.1897
1...c...(...	-0.98231	-0.55175	-1.05962	O...=...(...	0.00415	0.14079	0.38391	NNE0C...427-	-0.66271	-2.87665	0.24384	Nmax.4.....	-0.02744	0.05736	0.02114
1...c...1...	2.33586	0.4091	0.09163	O...=.....	-0.3284	-0.60173	-0.23845	NNE0N...200-	0.36899	2.10058	0.72725	Omax.1.....	0.32734	0.5422	0.3203
1...n...(...	0.56988	0.74836	0.91174	O...=...1...	-0.35187	0.17998	-0.14613	NNE0N...209-	-0.1308	0.65726	0.56803	Omax.2.....	-0.80813	0.27495	0.14011
2...(.....	-0.71278	-0.6707	0.24203	O...=...C...	1.03648	0.06551	0.47791	NNE0N...218-	-0.13105	0.39656	0.87468	Omax.3.....	0.73644	0.02312	0.29613
2.....	-0.05951	-0.31446	-0.15578	O...C...(...	0.96648	0.3751	0.33236	NNE0N...318-	-0.04732	0.09675	0.12331	Omax.4.....	-0.21454	-0.61073	-0.20548
2...c...(...	-1.81634	-1.29448	0.63109	O...C.....	0.10397	0.07248	-0.67163	NNE0N...327-	4.62076	5.1181	5.93128	Omax.5.....	2.11071	-0.53031	2.37093
=...(.....	0.34128	0.22031	-0.10941	O...C...C...	-1.39532	0.56371	-0.31774	NNE0O...109-	0.7151	0.56691	0.1294	Smax.0.....	5.60235	3.94877	2.52951
=.....	0.05546	0.05878	0.12412	P2E0C...0-..	0.05176	-0.91745	0.33398	NNE0O...218-	0.22907	0.33797	-0.63882	[.....	0.16989	0.05071	0.39835
=...1.....	1.08381	-1.21586	2.28779	P2E0C...1-..	0.21508	-0.24881	0.3518	NOSP01000000	0.05744	0.40933	0.39209	[...1...(...	2.32256	-1.11143	0.57144
=...C...(...	-0.27292	3.92459	-0.54374	P2E0C...2-..	-0.15381	-0.84473	-0.63893	NOSP11000000	0.45543	-1.03893	2.27268	[...1.....	0.16202	-0.33643	-0.75556
=...N...1...	2.25505	0.76502	-1.17807	P2E0C...3-..	1.35868	-0.07401	-0.48209	S2E0C...0-..	2.38352	0.295	2.36408	[...H.....	0.33439	0.73996	0.08617
=...O...(...	0.09903	0.61651	-0.63162	P2E0N...0-..	2.20458	0.05884	0.37436	S2E0C...1-..	-0.72495	-0.47956	-0.73546	[...H...N...	0.70593	0.06182	0.62549
C...(...(...	0.63829	2.3092	0.59378	P2E0N...1-..	-0.14788	0.45669	0.15585	S2E0C...10-.	-0.35003	1.07508	-0.11225	[...N.....	0.44356	0.12394	0.05506
C...(.....	0.22985	-0.61313	2.05222	P2E0N...2-..	-0.26787	-0.77067	-1.64795	S2E0C...11-.	-0.57976	2.07557	2.37622	[...N...H...	-0.24332	-0.26696	0.34184

C...(...1...	-2.31798	-2.57282	-1.93727	P2E0N...3-..	2.21486	1.47225	1.74967	S2E0C...2-..	-0.71272	0.13176	-0.31038	[...n...1...	-0.95229	0.05686	-0.5693
C...(...2...	-0.61289	1.80825	1.38069	P2E0O...0-..	0.27343	-0.16246	-1.90557	S2E0C...3-..	0.44796	0.40613	0.64996	c...(.....	-0.01046	-0.16031	-0.33615
C...(...=...	-0.99583	-0.58574	0.41642	P2E0O...1-..	0.12237	0.11805	0.31751	S2E0C...4-..	-1.49368	-0.42943	-1.52251	c...(...1...	0.24247	-0.89699	0.30287
C...(...C...	0.26605	0.32557	0.37422	P2E0O...2-..	-0.88943	0.75205	0.22301	S2E0C...5-..	-0.95323	-0.44629	-0.68431	c...(...C...	0.463	0.28202	0.6814
C.....	0.19844	0.42293	0.90505	P3E0C...0-..	-0.40618	0.14691	-0.97543	S2E0C...6-..	-0.50226	-0.51413	-0.2886	c...(...O...	1.03781	-0.95778	-0.23087
C...1.....	0.28403	0.40044	0.45363	P3E0C...1-..	-0.73894	-0.83101	-0.20963	S2E0C...7-..	0.26406	1.2398	1.44819	c...(...c...	1.33826	0.40981	1.4185
C...1...=...	-1.11639	0.10967	0.04558	P3E0C...2-..	-0.62064	-0.50577	-0.97282	S2E0C...8-..	0.00792	-0.73587	-0.77382	c.....	-0.41459	0.21361	-0.09949
C...=.....	-0.42688	-1.63586	-1.49619	P3E0C...3-..	2.44727	0.34148	2.24085	S2E0C...9-..	-2.56514	-2.69641	-4.57206	c...1...(...	0.03431	1.23047	0.19777
C...C...(...	2.08254	0.08109	0.37139	P3E0C...4-..	-0.75019	0.30344	0.23716	S2E0N...10-.	0.24024	-1.04133	-0.09969	c...1.....	-0.56116	-0.72717	-0.92703
C...C.....	0.39924	0.24594	0.25255	P3E0C...5-..	0.26848	-0.13197	-0.88592	S2E0N...11-.	1.77714	4.09411	2.0581	c...1...C...	-0.8805	0.38278	0.1189
C...C...1...	2.07879	-0.84435	-0.68477	P3E0N...0-..	2.42542	0.17107	0.21777	S2E0N...2-..	0.17723	0.97934	0.4452	c...1...N...	0.35636	0.33982	-0.21213
C...C...C...	0.91709	0.15062	-0.52688	P3E0N...1-..	-0.54709	0.16098	-0.63939	S2E0N...3-..	0.26692	0.47328	0.26568	c...1...c...	0.37119	-0.01932	0.12243
C...N...1...	0.19896	-0.07793	2.24169	P3E0N...2-..	-0.17361	2.47701	2.41979	S2E0N...5-..	0.98699	0.47511	0.15749	c...2...(...	0.90758	1.05968	-0.39853
C...O...(...	-0.69263	-0.93661	-0.52906	P3E0N...3-..	1.77675	0.93243	-1.08187	S2E0N...6-..	2.11719	2.55983	1.9716	c...2.....	0.11191	-0.36895	0.29476
C3.....0...	9.28284	1.05877	1.51821	P3E0N...4-..	1.04279	1.05678	2.3201	S2E0N...7-..	0.38417	1.2938	0.20589	c...2...c...	0.11962	-0.78404	0.27407
C4.....0...	4.08878	4.51195	4.28095	P3E0N...5-..	0.04337	0.20132	1.89234	S2E0N...8-..	-1.13724	-1.01777	-2.26651	c...C.....	1.61988	-0.64666	1.03938
C5....H.1...	0.02879	0.2011	0.4965	P3E0N...6-..	2.23	-0.31706	0.26436	S2E0N...9-..	0.33236	0.23799	0.11581	c...c...(...	0.39795	-0.12867	-0.88266
C5...AH.1...	2.44161	-0.82637	0.40506	P3E0O...0-..	0.25603	-0.91926	0.41908	S2E0O...2-..	-0.71146	0.2962	0.91385	c...c.....	0.03286	0.0004	-0.21154
C6...A..2...	-0.7052	-0.95853	0.42029	P3E0O...1-..	1.12883	0.28379	1.4432	S2E0O...3-..	1.23257	-0.73063	-0.5875	c...c...1...	-0.48936	0.45437	0.18974
C6...AH.3...	-0.18728	0.60854	-0.48772	P3E0O...2-..	-0.72507	-1.9454	-0.5186	S2E0O...4-..	0.33211	0.47139	0.60672	c...c...2...	-0.35226	-0.05494	-0.08743
C6...AH.4...	4.39143	4.33197	6.66957	P3E0O...3-..	1.47315	0.57345	0.01434	S2E0O...5-..	0.46559	0.2837	-0.3219	c...c...c...	0.34528	-0.37488	-0.54255
C7.....0...	4.25663	0.87218	8.19829	P4E0C...0-..	-0.41614	0.26423	0.1956	S3E0C...0-..	1.56126	2.10161	1.37293	c...n...(...	-0.07274	1.18844	1.54024
BOND10000000	-0.0634	-1.07638	1.7716	P4E0C...1-..	-0.7254	-1.25517	-0.86488	S3E0C...1-..	0.18909	0.38213	0.40928	n...(.....	0.42219	0.22836	0.1064
EC0-C...1...	0.15587	2.19253	-0.62014	P4E0C...10-.	0.34328	0.27037	-0.71764	S3E0C...10-.	0.0012	-0.65386	-0.16779	n...(...1...	2.19847	-0.34895	0.48289
EC0-C...2...	0.49223	0.29909	-0.50329	P4E0C...15-.	0.43284	0.95718	0.35662	S3E0C...11-.	2.31798	0.83759	1.73718	n...(...C...	2.44832	0.18682	0.43793
EC0-C...3...	-0.37771	-0.6142	-0.02636	P4E0C...2-..	-0.29457	-0.56016	0.24702	S3E0C...12-.	0.14432	0.31944	0.29629	n...(...c...	-2.43829	-3.32609	-6.96983
EC0-C...4...	0.09174	0.07398	0.48479	P4E0C...3-..	0.44732	-0.99654	0.10759	S3E0C...13-.	0.05379	0.76244	0.3684	n.....	0.26747	-0.24483	0.171
EC0-N...2...	0.4936	0.45048	0.12888	P4E0C...4-..	-0.70388	-0.11642	-0.83729	S3E0C...14-.	-0.37463	-1.64118	-0.73391	n...1.....	-0.68876	0.45191	-0.0595
EC0-N...3...	0.72657	-0.4164	0.22357	P4E0C...5-..	0.69099	0.16692	1.13301	S3E0C...15-.	-1.0986	-0.15967	0.00746	n...1...c...	0.4059	-0.11456	0.23757
EC0-O...1...	1.42151	-0.31618	0.30185	P4E0C...6-..	0.40214	-0.97984	0.08763	S3E0C...2-..	-1.70065	-2.07478	-0.84601	n...[.....	-0.79156	-0.83715	-0.52579
EC0-O...2...	-0.50618	0.44263	0.20981	P4E0C...7-..	0.61353	1.37115	0.23856	S3E0C...3-..	-0.77105	-1.18978	-0.39089	n...[...H...	0.42002	0.08674	1.49114
H.....	0.29866	0.06851	2.17577	P4E0C...8-..	0.0275	-0.54045	-0.38546	S3E0C...4-..	0.35629	0.08879	-0.01609	n...[...N...	0.29468	-0.94431	0.01127
H...[...1...	0.34519	0.17683	0.38056	P4E0C...9-..	2.21089	2.19774	2.23628	S3E0C...5-..	-0.6688	0.26357	-0.95006	n...c...(...	-0.01053	0.46209	0.17126
Cmax.1.....	-0.33712	-0.98892	-0.4456	P4E0N...0-..	0.49816	0.18879	0.29721	S3E0C...6-..	-0.32367	0.03147	-0.07364	n...c.....	2.49155	-0.17754	0.22216
Cmax.2.....	5.58331	3.43285	4.07161	P4E0N...11-.	0.27873	-0.93878	-1.41686	S3E0C...7-..	0.36894	0.7453	0.74868	n...c...1...	0.48254	0.10791	-0.08892

HALO00000000	-2.31765	-2.22726	-5.58357	P4E0N...16-.	1.94035	-0.91011	2.26129	S3E0C...8-..	1.29915	-0.03101	0.01998	n...n.....	0.17361	0.04579	0.17752
N...(.....	0.32853	0.73368	0.34017	P4E0N...3-..	0.78557	0.12408	0.1555	S3E0C...9-..	0.16622	0.35769	0.42114	n...n...1...	0.2836	0.57213	1.00785
N...(...C...	0.03258	0.48481	0.15934	P4E0N...4-..	0.45158	0.06161	0.38437	S3E0N...10-.	0.19551	-1.26551	0.36911	n...n...[...	0.34753	-0.10564	0.34394
N.....	0.81823	0.09649	0.29706	P4E0N...5-..	0.12772	0.41147	-0.8407	S3E0N...11-.	1.37369	-0.71558	2.32144	n...n...n...	0.11804	0.4636	0.79667
N...1.....	-0.23542	-0.80148	0.12611	P4E0N...6-..	1.1164	1.91224	-0.92012	S3E0N...12-.	2.26507	0.74976	2.22559				
N...1...N...	0.18979	-0.29986	-0.11304	P4E0N...7-..	0.3622	0.48118	0.82364	S3E0N...13-.	-0.05137	-1.25911	-1.57031				

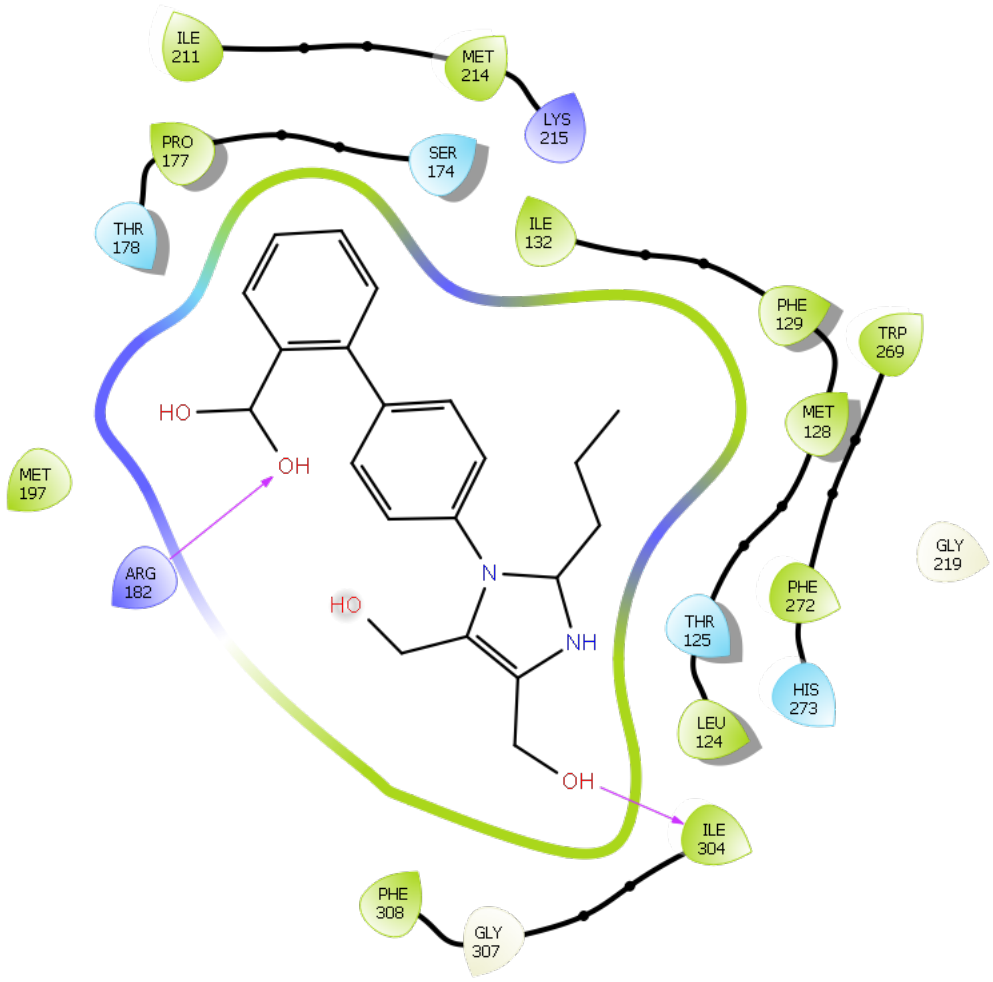

Figure S1. Two-dimensional representation of the interaction between molecule A and amino acids inside angiotensin II type 2 receptoror binding pocket.

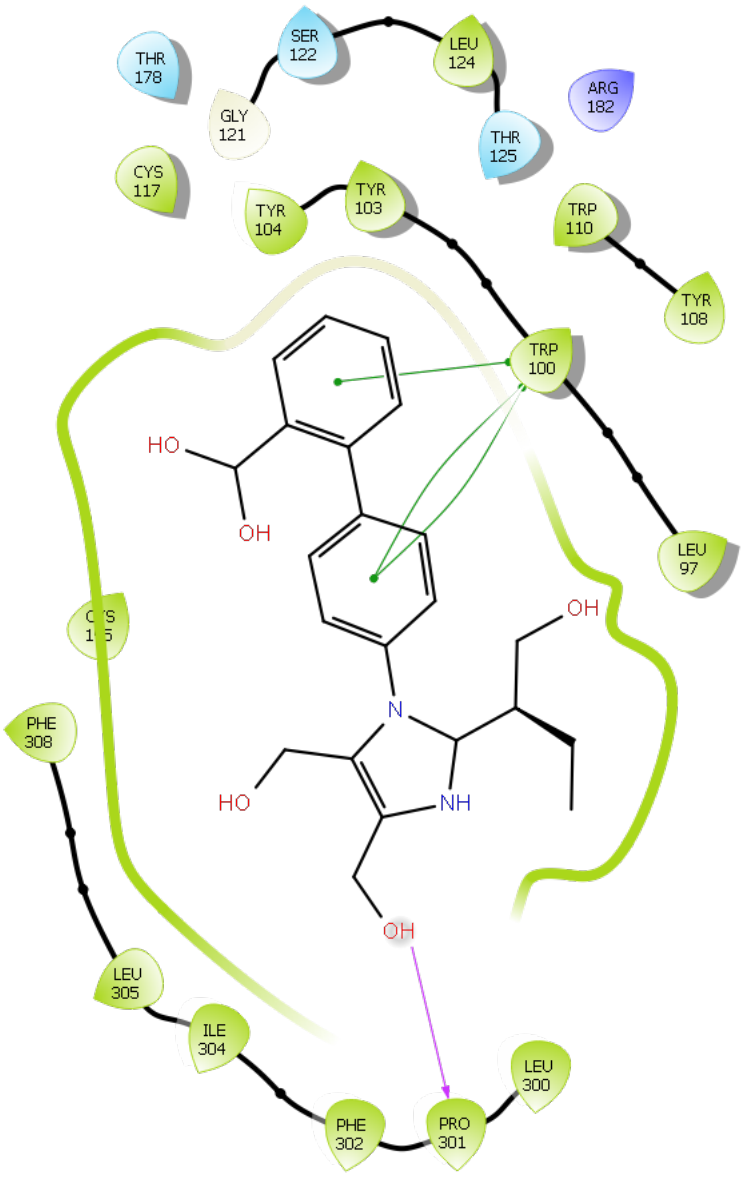

Figure S2. Two-dimensional representation of the interaction between molecule A1 and amino acids inside angiotensin II type 2 receptoror binding pocket.

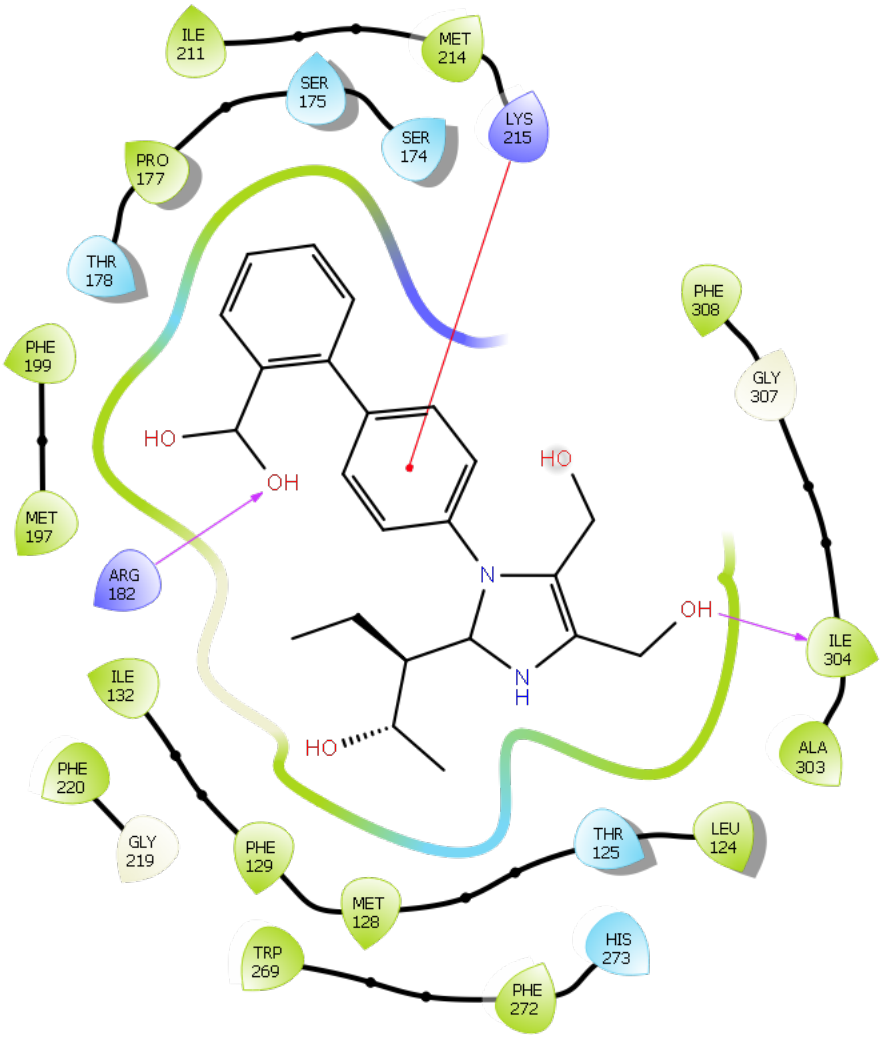

Figure S3. Two-dimensional representation of the interaction between molecule A2 and amino acids inside angiotensin II type 2 receptoror binding pocket.

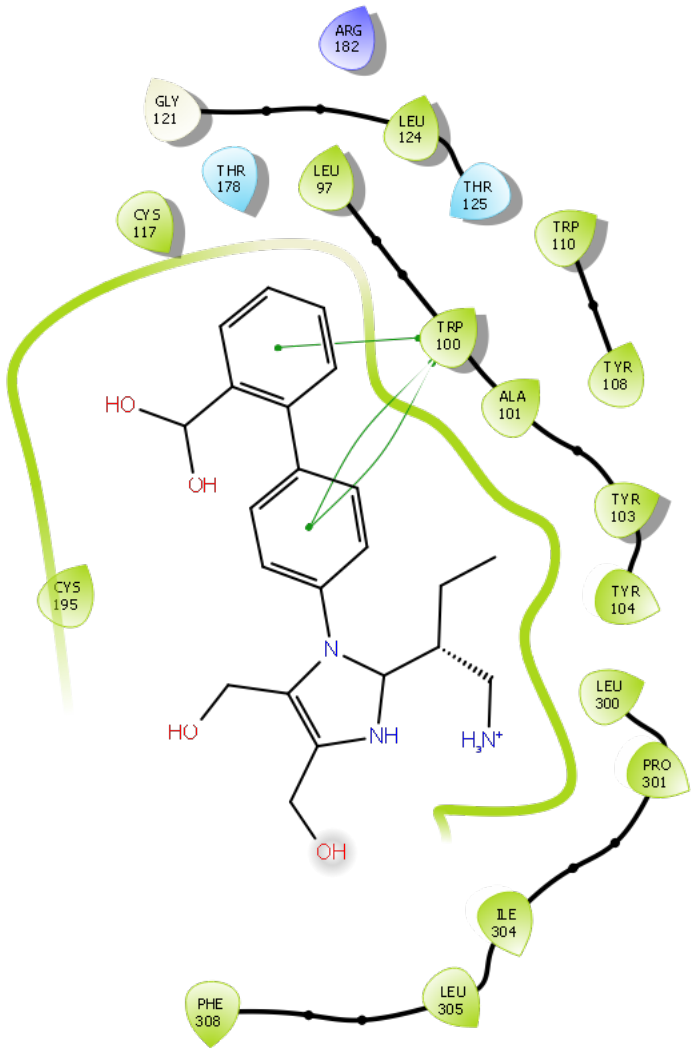

Figure S4. Two-dimensional representation of the interaction between molecule A3 and amino acids inside angiotensin II type 2 receptoror binding pocket.

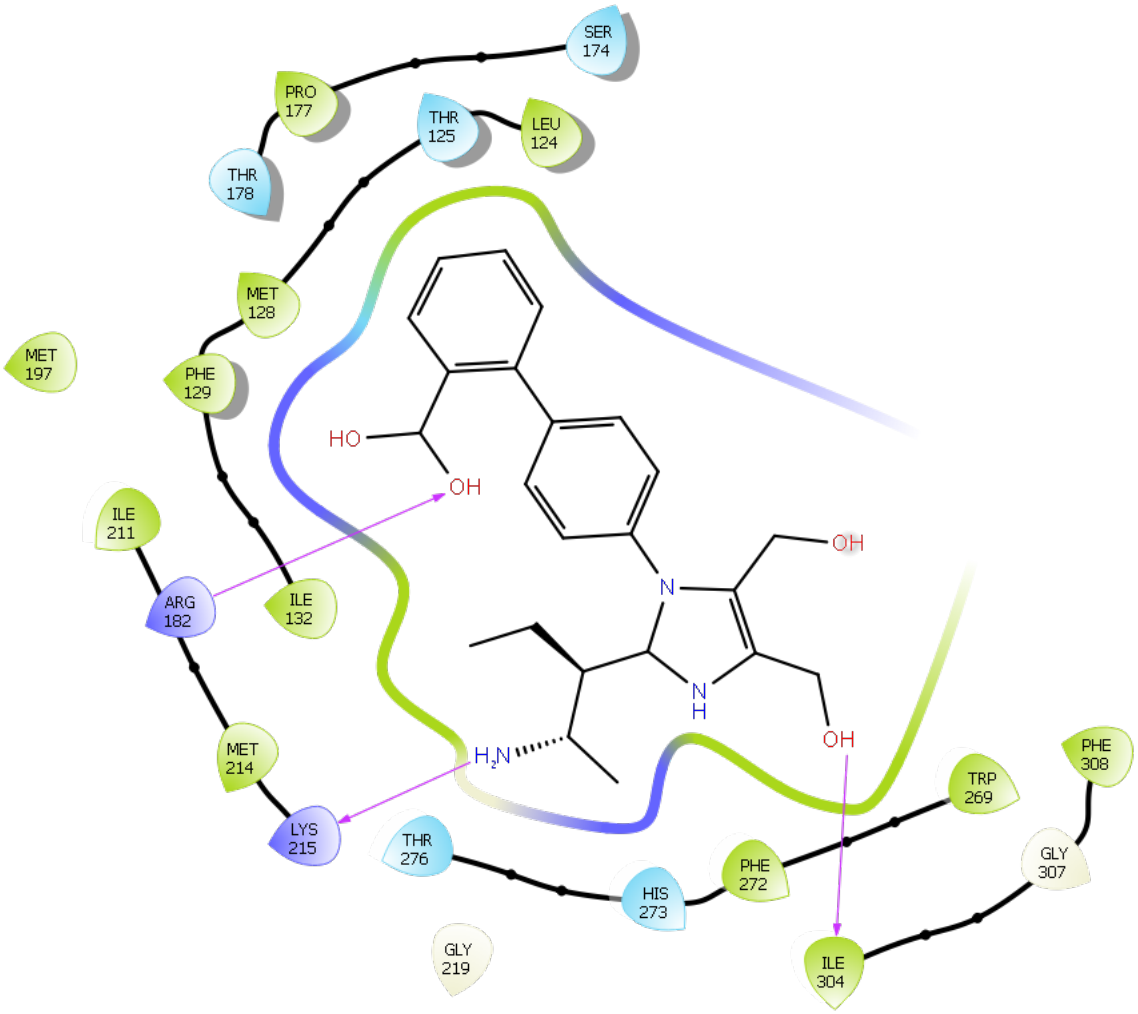

Figure S5. Two-dimensional representation of the interaction between molecule A4 and amino acids inside angiotensin II type 2 receptoror binding pocket.

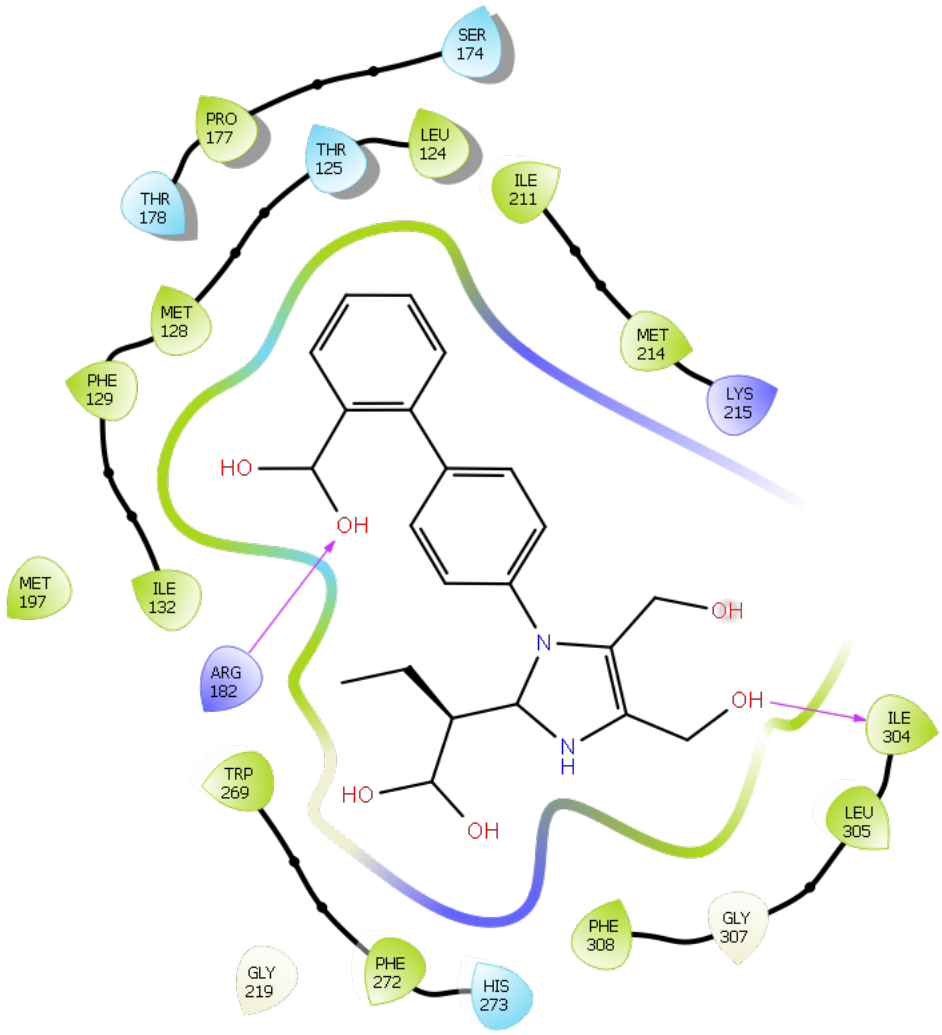

Figure S6. Two-dimensional representation of the interaction between molecule A5 and amino acids inside angiotensin II type 2 receptoror binding pocket.