Supplementary Information

Development of novel therapeutics for the treatment of glaucoma based on actin-binding kinases inhibition – *In silico* approach

Maja Zivkovic, Marko Zlatanovic, Nevena Zlatanovic, Jasmina Djordjevic Jocic, Mladjan Golubović, Aleksandar M. Veselinović

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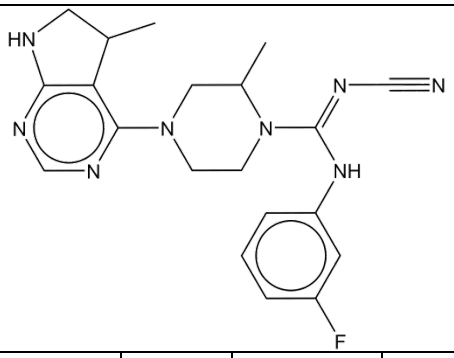
Table S1. The SMILES notation of the studied molecules, calculated values for the DCW, experimental data (Ac) – expr, the values of Ac calculated with the application of CORAL software – calc, the difference between expr and calc – diff for the built QSPR model

	SMILES notation	Ac(expr)	Split 1				Split 2				Split 3			
			DCW	Ac(calc)	Diff	Set	DCW	Ac(calc)	Diff	Set	DCW	Ac(calc)	Diff	Set
1	O=C(C1CCN(CC1)c1ncnc2c1C(C)CN2)Nc1ccccc1	6.1	81.46787	5.7189	0.3811	Tr	89.22062	5.7477	0.3523	Tr	131.537	6.0333	0.0667	Tr
2	Cc1ccccc1NC(=O)C1CCN(CC1)c1ncnc2[NH]cc(C)c12	4.94	79.64905	5.6277	-0.6877	Tr	87.48562	5.6533	-0.7133	Tr	117.7608	5.2203	-0.2803	Ts
3	Cc1cc(ccc1)NC(=O)C1CCN(CC1)c1ncnc2[NH]cc(C)c12	6.19	86.27193	5.9597	0.2303	Tr	94.36155	6.0274	0.1626	Tr	133.1602	6.1291	0.0609	Tr
4	Cc1ccc(cc1)NC(=O)C1CCN(CC1)c1ncnc2[NH]cc(C)c12	5.89	82.45998	5.7686	0.1214	Tr	85.02449	5.5194	0.3706	Tr	129.5334	5.9151	-0.0251	Tr
5	COc1cccc(c1)NC(=O)C1CCN(CC1)c1ncnc2[NH]cc(C)c12	6.28	97.07177	6.501	-0.221	Tr	96.34988	6.1356	0.1444	Tr	132.5929	6.0956	0.1844	Tr
6	COc1ccc(cc1)NC(=O)C1CCN(CC1)c1ncnc2[NH]cc(C)c12	5.82	90.13402	6.1532	-0.3332	Ts	96.00507	6.1168	-0.2968	Tr	131.9221	6.056	-0.236	Tr
7	O=C(C1CCN(CC1)c1ncnc2c1C(C)CN2)Nc1cccc(c1)Oc1ccccc1	7.19	107.6583	7.0316	0.1584	Tr	112.3171	7.0044	0.1856	Ts	153.3137	7.3185	-0.1285	Ts
8	Brc1cccc(c1)NC(=O)C1CCN(CC1)c1ncnc2[NH]cc(C)c12	6.52	92.72994	6.2834	0.2366	Tr	96.24135	6.1297	0.3903	Tr	133.6192	6.1562	0.3638	Tr
9	O=C(Nc1cc(C)ccc1)N1CCN(CC1)c1ncnc2[NH]cc(C)c12	7.04	101.8741	6.7417	0.2983	Tr	111.3363	6.951	0.089	Ts	152.2328	7.2547	-0.2147	Ts
10	O=C(Nc1cccc(OC)c1)N1CCN(CC1)c1ncnc2[NH]cc(C)c12	6.85	112.7968	7.2891	-0.4391	Tr	116.1335	7.212	-0.362	Tr	152.048	7.2438	-0.3938	Tr
11	O=C(Nc1cccc(Br)c1)N1CCN(CC1)c1ncnc2[NH]cc(C)c12	7.42	111.8894	7.2436	0.1764	Ts	114.9782	7.1492	0.2708	Tr	149.5764	7.0979	0.3221	Tr
12	N#CN=C(N1CCN(CC1)c1ncnc2c1C(C)CN2)Nc1cccc(c1)Br	7.96	133.5689	8.3302	-0.3702	Tr	127.2402	7.8163	0.1437	Ts	163.6078	7.926	0.034	Tr
13	O=C(Nc1cccc(Br)c1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.41	135.7538	8.4397	-0.0297	Tr	139.7067	8.4946	-0.0846	Tr	167.0904	8.1315	0.2785	Ts
14	N#CN=C(N1CCN(CC1C)c1ncnc2c1C(C)CN2)Nc1cccc(c1)Br	9.05	144.0904	8.8576	0.1924	Ts	148.6898	8.9834	0.0666	Ts	179.9821	8.8923	0.1577	Tr
15	O=C(Nc1cccc(Br)c1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	7.43	135.7538	8.4397	-1.0097	Tr	139.7067	8.4946	-1.0646	Tr	167.0904	8.1315	-0.7015	Tr
16	CC(C)C1CN(CCN1C(\Nc1cccc(Br)c1)=N\C#N)c1ncnc2[NH]cc(C)c21	8.38	137.6286	8.5337	-0.1537	Ts	140.7712	8.5526	-0.1726	Tr	166.6068	8.103	0.277	Tr
17	CC1CNc2ncnc(N3CC(C)N(CC3C)C(\Nc3cccc(Br)c3)=N\C#N)c12	8.41	131.1188	8.2074	0.2026	Ts	136.1218	8.2996	0.1104	Tr	172.3749	8.4434	-0.0334	Tr
18	CC1CN(CC(C)N1C(=O)Nc1cccc(Br)c1)c1ncnc2[NH]cc(C)c21	6.88	119.9478	7.6475	-0.7675	Tr	115.5754	7.1816	-0.3016	Tr	144.8783	6.8206	0.0594	Tr
19	Brc1cccc(c1)NC(=O)N1C2CCCC1CN(C2)c1ncnc2[NH]cc(C)c21	7.12	115.0208	7.4006	-0.2806	Tr	112.7196	7.0263	0.0937	Tr	148.403	7.0287	0.0913	Tr
20	Brc1cccc(c1)NC(=O)N1CC2CCC1CN2c1ncnc2[NH]cc(C)c21	7.12	112.3692	7.2677	-0.1477	Tr	117.708	7.2977	-0.1777	Tr	152.3688	7.2627	-0.1427	Tr
21	Cc1c[NH]c2ncnc(N3CC(C)N(CC3)C(\Nc3cccc(Br)c3)=N\C#N)c12	8.09	128.8614	8.0943	-0.0043	Ts	132.2797	8.0905	-0.0005	Ts	167.7117	8.1682	-0.0782	Tr
22	N#CN=C(N1CCN(CC1C)c1ncnc2c1C(Cl)CN2)Nc1cccc(c1)Br	8.92	144.3075	8.8684	0.0516	Ts	146.0148	8.8379	0.0821	Tr	181.8458	9.0023	-0.0823	Tr
23	Cc1cc2c([NH]1)ncnc2N1CC(C)N(CC1)C(\Nc1cccc(Br)c1)=N\C#N	8.38	135.5841	8.4312	-0.0512	Tr	140.3216	8.5281	-0.1481	Tr	174.9435	8.595	-0.215	Ts
24	CS(=O)(=O)/N=C(\Nc1ccccc1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c21	8.17	119.6083	7.6305	0.5395	Tr	131.453	8.0455	0.1245	Ts	163.2384	7.9042	0.2658	Ts
25	N#CN=C(N1CCN(CC1C)c1ncnc2c1C(C)CN2)Nc1cccc(c1)Cl	8.8	137.6799	8.5363	0.2637	Tr	145.3364	8.8009	-0.0009	Tr	182.5951	9.0465	-0.2465	Tr
26	O=C(Nc1cccc(Cl)c1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.64	126.6156	7.9817	0.6583	Tr	136.0721	8.2969	0.3431	Ts	172.548	8.4536	0.1864	Ts
27	N#CN=C(N1CCN(CC1C)c1ncnc2c1C(C)CN2)Nc1cccc(c1)F	8.74	139.5282	8.6289	0.1111	Tr	145.3364	8.8009	-0.0609	Ts	174.088	8.5445	0.1955	Ts
28	N#CN=C(N1CCN(CC1C)c1ncnc2c1C(C)CN2)Nc1ccc(c(c1)Br)F	8.82	147.6065	9.0338	-0.2138	Tr	145.5702	8.8137	0.0063	Tr	176.8934	8.71	0.11	Ts
29	O=C(Nc1ccc(F)c(Br)c1)N1CCN(CC1C)c1ncnc2[NH]c(C)cc12	8.49	140.0359	8.6543	-0.1643	Tr	137.0448	8.3498	0.1402	Tr	176.4429	8.6834	-0.1934	Tr

30	FC(F)(F)c1cc(N/C(=N\C#N)N2CCN(CC2C)c2ncnc3[NH]cc(C)c32)ccc1	8.72	139.4372	8.6243	0.0957	Tr	137.7191	8.3865	0.3335	Tr	172.2701	8.4372	0.2828	Ts
31	N#CN=C(N1CCN(CC1C)c1ncnc2c1C(C)CN2)Nc1cccc(c1)C#N	8.92	146.6243	8.9846	-0.0646	Tr	149.1078	9.0062	-0.0862	Tr	179.7481	8.8785	0.0415	Tr
32	CC(C)(C)c1cc(N/C(=N\C#N)N2CCN(CC2C)c2ncnc3[NH]cc(C)c32)ccc1	8.96	147.4606	9.0265	-0.0665	Tr	149.0787	9.0046	-0.0446	Tr	181.4725	8.9803	-0.0203	Tr
33	O=C(Nc1cccc(OC(=O)N(C)C)c1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.92	134.8932	8.3966	0.5234	Ts	137.6691	8.3838	0.5362	Tr	173.8831	8.5324	0.3876	Tr
34	CC(C)NC(=O)c1cc(N/C(=N\C#N)N2CCN(CC2C)c2ncnc3[NH]cc(C)c32)ccc1	8.46	137.54	8.5293	-0.0693	Tr	138.5752	8.4331	0.0269	Tr	176.0816	8.6621	-0.2021	Tr
35	O=C(Nc1cc(ccc1)C(=O)NC(C)C)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.26	134.218	8.3628	-0.1028	Tr	134.8113	8.2283	0.0317	Tr	170.2957	8.3207	-0.0607	Tr
36	OCCNC(=O)c1cc(N\C(=N\C#N)N2CCN(CC2C)c2ncnc3[NH]cc(C)c32)ccc1	9.1	139.3641	8.6207	0.4793	Tr	143.8449	8.7198	0.3802	Ts	176.5981	8.6926	0.4074	Tr
37	O=C(Nc1cc(ccc1)C(=O)NCCO)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.52	134.8871	8.3963	0.1237	Ts	141.9671	8.6176	-0.0976	Tr	172.2942	8.4386	0.0814	Tr
38	O=C(Nc1cc(ccc1)C(=O)NC(CO)CO)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.52	135.8172	8.4429	0.0771	Ts	140.4758	8.5365	-0.0165	Tr	173.8169	8.5285	-0.0085	Tr
39	CN(C)CCNC(=O)c1cc(N/C(=N\C#N)N2CCN(CC2C)c2ncnc3[NH]cc(C)c32)ccc1	8.47	137.0331	8.5038	-0.0338	Tr	142.2287	8.6319	-0.1619	Tr	179.5604	8.8674	-0.3974	Tr
40	CC(C)NS(=O)(=O)c1cccc(N/C(=N\C#N)N2CCN(CC2C)c2ncnc3[NH]cc(C)c32)c1	8.77	142.5832	8.782	-0.012	Tr	144.4885	8.7548	0.0152	Tr	174.671	8.5789	0.1911	Tr
41	OCCNS(=O)(=O)c1cccc(N\C(=N\C#N)N2CCN(CC2C)c2ncnc3[NH]cc(C)c32)c1	8.54	141.4753	8.7265	-0.1865	Tr	143.3197	8.6912	-0.1512	Tr	175.4298	8.6237	-0.0837	Tr
42	O=C(Nc1cccc(OC(=O)N(C)C)c1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.92	134.8932	8.3966	0.5234	Tr	137.6691	8.3838	0.5362	Tr	173.8831	8.5324	0.3876	Tr
43	O=C(Nc1cccc(OC(=O)NC(C)C)c1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.26	138.7343	8.5891	-0.3291	Tr	142.5679	8.6503	-0.3903	Ts	175.4436	8.6245	-0.3645	Tr
44	O=C(Nc1cccc(OC)c1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.57	136.6613	8.4852	0.0848	Ts	140.862	8.5575	0.0125	Tr	169.562	8.2774	0.2926	Tr
45	O=C(Nc1ccccc1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.92	120.8906	7.6948	1.2252	Tr	130.6029	7.9993	0.9207	Ts	162.1893	7.8423	1.0777	Tr
46	O=C(Cc1ccccc1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	6.18	110.1019	7.154	-0.974	Tr	115.6736	7.187	-1.007	Tr	148.0471	7.0077	-0.8277	Tr
47	O=C(Nc1cccc(OC(=O)N(C)C)c1)N1CCN(CC1C)c1ncnc2[NH]cc(C)c12	8.92	134.8932	8.3966	0.5234	Tr	137.6691	8.3838	0.5362	Tr	173.8831	8.5324	0.3876	Tr
48	O=C(Nc1cccc(OC(=O)N(C)C)c1)N1CCC(CC1)c1ncnc2[NH]cc(C)c12	6.66	105.3901	6.9179	-0.2579	Tr	110.864	6.9253	-0.2653	Tr	149.1726	7.0741	-0.4141	Tr
49	O=C(Nc1cccc(OC(=O)N(C)C)c1)N1CCN(CC1C(C)(C)C)c1ncnc2[NH]cc(C)c12	7.59	131.5041	8.2267	-0.6367	Tr	123.1351	7.593	-0.003	Tr	166.0359	8.0693	-0.4793	Ts
50	CC(C)Oc1cccc(c1)NC(=O)C1CCN(CC1)c1ncnc2[NH]cc(C)c12	6.48	92.59698	6.2767	0.2033	Tr	102.3448	6.4618	0.0182	Ts	134.6986	6.2199	0.2601	Tr
51	Clc1cccc(c1)NC(=O)C1(CCN(CC1)c1ncnc2[NH]cc(C)c12)CC=C	8.72	128.2389	8.0631	0.6569	Tr	138.1621	8.4106	0.3094	Tr	175.7928	8.6451	0.0749	Tr
52	CC(C)(C)c1cc(ccc1)NC(=O)C1(C)CCN(CC1)c1ncnc2[NH]cc(C)c12	8.5	129.3613	8.1193	0.3807	Tr	135.6743	8.2752	0.2248	Ts	172.2306	8.4349	0.0651	Ts
53	CN(C)C(=O)Oc1cccc(c1)NC(=O)C1(CCN(CC1)c1ncnc2[NH]cc(C)c12)CC=C	8.66	136.6331	8.4838	0.1762	Ts	140.365	8.5304	0.1296	Ts	173.076	8.4847	0.1753	Tr
54	CN(C)C(=O)Oc1cccc(c1)NC(=O)C1(C)CCN(CC1)c1ncnc2[NH]cc(C)c12	8.32	121.2495	7.7128	0.6072	Tr	123.1307	7.5927	0.7273	Tr	159.7439	7.6979	0.6221	Ts
55	CN(C)C(=O)Oc1cccc(c1)NC(=O)C1(O)CCN(CC1)c1ncnc2[NH]cc(C)c12	6.86	114.7349	7.3863	-0.5263	Tr	118.9103	7.3631	-0.5031	Ts	156.5331	7.5085	-0.6485	Tr
56	CN(C)C(=O)Oc1cccc(c1)NC(=O)C1(CCN(CC1)c1ncnc2[NH]cc(C)c12)N(C)C	8.29	130.4024	8.1715	0.1185	Ts	132.2716	8.0901	0.1999	Tr	171.1649	8.372	-0.082	Tr
57	CN(C)C(=O)Oc1cccc(c1)NC(=O)C1(CCN(CC1)c1ncnc2[NH]cc(C)c12)COCOOC	8.57	139.0004	8.6025	-0.0325	Tr	143.0826	8.6783	-0.1083	Tr	172.7932	8.4681	0.1019	Ts
58	CN(C)C(=O)Oc1cccc(c1)NC(=O)C1(CCN(CC1)c1ncnc2[NH]cc(C)c12)Cc1ncc[NH]1	9	146.9379	9.0003	-0.0003	Ts	149.4454	9.0245	-0.0245	Tr	183.5368	9.1021	-0.1021	Tr
59	CN(C)C(=O)Oc1cccc(c1)NC(=O)C1(CCN(CC1)c1ncnc2[NH]cc(C)c12)CCNC	8.14	137.19	8.5117	-0.3717	Ts	140.2995	8.5269	-0.3869	Tr	168.7283	8.2282	-0.0882	Ts
60	CN(C)C(=O)Oc1cccc(c1)NC(=O)C1(CCN(CC1)c1ncnc2[NH]cc(C)c12)CN	8.37	134.7533	8.3896	-0.0196	Tr	132.1605	8.084	0.286	Tr	171.7738	8.4079	-0.0379	Tr

Table S2. The example of DCW(2,15) calculation



SMILES notation:
N#C/N=C(/N1CCN(CC1C)c1ncnc2c1C(C)CN2)\Nc1cccc(c1)F
DCW = 170.86417
pIC_{50}(calc.) = 8.3542

SA_k	$CW(SA_k)$	SA_k	$CW(SA_k)$	SA_k	$CW(SA_k)$	SA_k	$CW(SA_k)$	SA_k	$CW(SA_k)$
EC0-N...1...	0.0286	PT4-N...9...	0.2243	P2E0C...1-..	0.2059	S2E0C...2-..	0.3083	F.....	0
EC0-C...2...	0.1576	PT4-N...7...	0.0429	P2E0N...1-..	0.3356	S2E0C...5-..	0.3441	N...#.....	0.1221
EC0-N...2...	0.6214	PT4-C...9...	0.074	P2E0C...2-..	0.2071	S2E0F...3-..	0	C...#.....	0.2617
EC0-C...3...	0.2223	PT4-C...3...	0.1736	P2E0C...0-..	0.2438	S3E0N...2-..	1.9129	N...C.....	-0.7731
EC0-N...3...	0.0789	PT4-C...8...	0.2646	P2E0C...1-..	0.2059	S3E0C...3-..	0.472	N...=.....	6.1748
EC0-C...2...	0.1576	PT4-C...2...	2.3543	P2E0C...2-..	0.2071	S3E0N...6-..	0.1568	C...=.....	1.6108
EC0-C...2...	0.1576	PT4-C...5...	0.3547	P2E0N...1-..	0.3356	S3E0C...7-..	0.1042	C...(.....	0.4483
EC0-N...3...	0.0789	PT4-C...3...	0.1736	P2E0C...0-..	0.2438	S3E0N...8-..	0.126	N...(.....	0.3334
EC0-C...2...	0.1576	PT4-F...2...	0	P2E0N...1-..	0.3356	S3E0C...10-.	0.1914	N...1.....	0.5162
EC0-C...3...	0.2223	VS2-N...2...	-3.4674	P2E0C...1-..	0.2059	S3E0C...12-.	-0.623	C...1.....	0.1841
EC0-C...1...	0.3861	VS2-C...3...	0.4143	P2E0C...3-..	-4.7956	S3E0N...12-.	2.2406	C...C.....	0.282
EC0-C...3...	0.2223	VS2-N...6...	0.1379	P2E0C...0-..	0.2438	S3E0C...10-.	0.1914	N...C.....	-0.7731
EC0-N...2...	0.6214	VS2-C...10..	0.1316	P2E0C...1-..	0.2059	S3E0C...8-..	-0.2491	N...(.....	0.3334
EC0-C...2...	0.1576	VS2-N...9...	0.335	P2E0C...1-..	0.2059	S3E0C...7-..	0.1042	C...(.....	0.4483
EC0-N...2...	0.6214	VS2-C...9...	0.1363	P2E0N...1-..	0.3356	S3E0C...11-.	0.1816	C...C.....	0.282
EC0-C...3...	0.2223	VS2-C...8...	0.4188	P2E0N...2-..	2.2812	S3E0N...11-.	0.1768	C...1.....	0.1841
EC0-C...3...	0.2223	VS2-N...10..	0.4177	P2E0C...0-..	0.2438	S3E0C...9-..	0.1102	C...1.....	0.1841
EC0-C...3...	0.2223	VS2-C...9...	0.1363	P2E0C...1-..	0.2059	S3E0N...9-..	0.3945	C...(.....	0.4483
EC0-C...1...	0.3861	VS2-C...8...	0.4188	P2E0C...0-..	0.2438	S3E0C...10-.	0.1914	c...(.....	0.0022
EC0-C...2...	0.1576	VS2-C...5...	0.4156	P2E0C...1-..	0.2059	S3E0C...9-..	0.1102	c...1.....	0.3779
EC0-N...2...	0.6214	VS2-C...12..	0.194	P2E0C...1-..	0.2059	S3E0C...9-..	0.1102	n...1.....	0.4603
EC0-N...2...	0.6214	VS2-N...8...	0.5662	P2E0C...2-..	0.2071	S3E0C...7-..	0.1042	n...c.....	0.2834
EC0-C...3...	0.2223	VS2-C...6...	0.0278	P2E0F...1-..	0	S3E0C...9-..	0.1102	n...c.....	0.2834
EC0-C...2...	0.1576	VS2-N...7...	-0.897	P3E0N...0-..	0.3707	S3E0N...10-.	-1.3748	n...c.....	0.2834
EC0-C...2...	0.1576	VS2-C...10..	0.1316	P3E0C...0-..	-0.0974	S3E0N...10-.	-1.3748	c...2.....	0.3801
EC0-C...2...	0.1576	VS2-C...12..	0.194	P3E0N...1-..	-0.5303	S3E0C...7-..	0.1042	c...2.....	0.3801
EC0-C...3...	0.2223	VS2-C...8...	0.4188	P3E0C...3-..	0.0367	S3E0C...7-..	0.1042	c...1.....	0.3779
EC0-C...2...	0.1576	VS2-C...5...	0.4156	P3E0N...1-..	-0.5303	S3E0C...5-..	0.3855	C...1.....	0.1841
EC0-F...1...	0	VS2-C...7...	-0.4546	P3E0C...4-..	0.0155	S3E0C...4-..	0.2324	C...(.....	0.4483
PT2-N...1...	0.36	VS2-N...8...	0.5662	P3E0C...3-..	0.0367	S3E0C...3-..	0.472	C...(.....	0.4483
PT2-C...1...	0.2704	VS2-N...9...	0.335	P3E0N...3-..	0.1673	S3E0C...5-..	0.3855	C...(.....	0.4483
PT2-N...3...	0.0188	VS2-C...8...	0.4188	P3E0C...3-..	0.0367	S3E0F...4-..	0	C...(.....	0.4483
PT2-C...4...	0.2017	VS2-C...6...	0.0278	P3E0C...2-..	0.0255	NNE0N...109-	0.0205	N...C.....	-0.7731
PT2-N...5...	0.3753	VS2-C...6...	0.0278	P3E0C...2-..	0.0255	NNE0C...200-	-2.1176	N...2.....	0.3576
PT2-C...3...	0.0896	VS2-C...5...	0.4156	P3E0C...4-..	0.0155	NNE0N...218-	0.193	2...(.....	4.1134
PT2-C...3...	0.0896	VS2-C...5...	0.4156	P3E0N...3-..	0.1673	NNE0C...300-	0.3838	N...(.....	0.3334

PT2-N...4...	-0.4989	VS2-C...7...	-0.4546	P3E0C...2-..	0.0255	NNE0N...327-	0.4929	c...N.....	0.467
PT2-C...4...	0.2017	VS2-F...4...	0	P3E0N...2-..	0.4778	NNE0C...209-	0.0137	c...1.....	0.3779
PT2-C...3...	0.0896	VS3-N...3...	-3.1771	P3E0C...3-..	0.0367	NNE0C...209-	0.0137	c...1.....	0.3779
PT2-C...2...	0.3307	VS3-C...5...	0.2796	P3E0C...3-..	0.0367	NNE0N...327-	0.4929	c...c.....	0.3238
PT2-C...5...	2.418	VS3-N...8...	0.3274	P3E0C...2-..	0.0255	NNE0C...209-	0.0137	c...c.....	0.3238
PT2-N...3...	0.0188	VS3-C...10..	0.3796	P3E0C...2-..	0.0255	NNE0C...318-	0.2633	c...c.....	0.3238
PT2-C...2...	0.3307	VS3-N...11..	0.2381	P3E0C...2-..	0.0255	NNE0C...109-	0.0792	c...(.....	0.0022
PT2-N...3...	0.0188	VS3-C...12..	-0.1151	P3E0N...3-..	0.1673	NNE0C...309-	-0.0699	c...(.....	0.0022
PT2-C...4...	0.2017	VS3-C...14..	0.2175	P3E0N...3-..	0.1673	NNE0N...218-	0.193	c...1.....	0.3779
PT2-C...6...	-1.0902	VS3-N...15..	0.0911	P3E0C...2-..	0.0255	NNE0C...200-	-2.1176	1...(.....	0.1365
PT2-C...3...	0.0896	VS3-C...12..	-0.1151	P3E0C...1-..	0.2185	NNE0N...218-	0.193	F...(.....	0
PT2-C...2...	0.3307	VS3-C...11..	0.4426	P3E0C...2-..	0.0255	NNE0C...309-	-0.0699	N...#...C...	0.2243
PT2-C...3...	0.0896	VS3-C...8...	0.2334	P3E0C...0-..	-0.0974	NNE0C...327-	-0.2912	N...C...#...	2.006
PT2-N...3...	0.0188	VS3-C...14..	0.2175	P3E0C...0-..	-0.0974	NNE0C...327-	-0.2912	C...N...=...	0.6689
PT2-N...4...	-0.4989	VS3-N...13..	-0.9967	P3E0C...1-..	0.2185	NNE0C...109-	0.0792	N...=...C...	0.4845
PT2-C...3...	0.0896	VS3-C...11..	0.4426	P3E0F...1-..	0	NNE0C...209-	0.0137	=...C...(...	2.1771
PT2-C...3...	0.0896	VS3-N...11..	0.2381	P4E0N...0-..	0.0725	NNE0N...218-	0.193	N...(...C...	3.2423
PT2-C...2...	0.3307	VS3-C...13..	0.185	P4E0C...2-..	1.315	NNE0N...218-	0.193	1...N...(...	0.3247
PT2-C...3...	0.0896	VS3-C...12..	-0.1151	P4E0N...3-..	2.282	NNE0C...318-	0.2633	N...1...C...	-5.1167
PT2-C...2...	0.3307	VS3-C...12..	-0.1151	P4E0C...7-..	0.1755	NNE0C...218-	0.1389	C...C...1...	0.3636
PT2-C...4...	0.2017	VS3-C...8...	0.2334	P4E0N...1-..	0.0108	NNE0C...218-	0.1389	N...C...C...	0.3251
PT2-F...2...	0	VS3-C...11..	0.4426	P4E0C...10-.	0.4534	NNE0C...218-	0.1389	C...N...(...	0.2301
PT3-N...1...	0.1551	VS3-N...12..	-0.028	P4E0C...7-..	0.1755	NNE0C...318-	0.2633	N...(...C...	3.2423
PT3-C...2...	0.1335	VS3-N...12..	-0.028	P4E0N...7-..	0.2641	NNE0C...218-	0.1389	C...C...(...	0.452
PT3-N...3...	0.2728	VS3-C...10..	0.3796	P4E0C...7-..	0.1755	NNE0F...109-	0	C...C...1...	0.3636
PT3-C...6...	1.4429	VS3-C...9...	0.4197	P4E0C...6-..	0.0656	N..........	0.3653	C...1...C...	0.3798
PT3-N...4...	0.1858	VS3-C...7...	0.2346	P4E0C...4-..	0.0119	#..........	0.4874	1...C...(...	0.4776
PT3-C...6...	1.4429	VS3-C...6...	0.218	P4E0C...8-..	0.0041	C..........	0.4163	c...(...C...	0.3025
PT3-C...5...	-0.3344	VS3-C...6...	0.218	P4E0N...7-..	0.2641	N..........	0.3653	1...c...(...	0.0432
PT3-N...6...	-0.5241	VS3-C...7...	0.2346	P4E0C...6-..	0.0656	=..........	0.2201	n...1...c...	-1.0069
PT3-C...5...	-0.3344	VS3-F...5...	0	P4E0N...4-..	0.2159	C..........	0.4163	c...n...1...	-0.0704
PT3-C...5...	-0.3344	NNC-N...110.	0.3385	P4E0C...7-..	0.1755	(..........	0.4577	n...c...n...	6.9767
PT3-C...3...	0.1487	NNC-C...202.	-0.9498	P4E0C...5-..	0.3162	N..........	0.3653	c...n...c...	6.2806
PT3-C...7...	0.2217	NNC-N...220.	0.1411	P4E0C...6-..	0.0656	1..........	0.1317	n...c...2...	-0.5959
PT3-N...5...	1.1435	NNC-C...303.	0.2362	P4E0C...4-..	0.0119	C..........	0.4163	c...2...c...	0.4037
PT3-C...4...	0.2734	NNC-N...330.	0.2638	P4E0C...6-..	0.0656	C..........	0.4163	2...c...1...	0.6481
PT3-N...4...	0.1858	NNC-C...211.	2.2033	P4E0N...7-..	0.2641	N..........	0.3653	c...1...C...	0.1437
PT3-C...6...	1.4429	NNC-C...211.	2.2033	P4E0N...5-..	0.0189	(..........	0.4577	1...C...(...	0.4776
PT3-C...6...	1.4429	NNC-N...330.	0.2638	P4E0C...6-..	0.0656	C..........	0.4163	C...(...C...	0.264
PT3-C...5...	-0.3344	NNC-C...211.	2.2033	P4E0C...1-..	0.358	C..........	0.4163	(...C...(...	-0.794
PT3-C...3...	0.1487	NNC-C...321.	0.4714	P4E0C...6-..	0.0656	1..........	0.1317	C...(...C...	0.264
PT3-C...4...	0.2734	NNC-C...110.	0.3021	P4E0C...0-..	-0.9513	C..........	0.4163	N...C...(...	0.282
PT3-N...5...	1.1435	NNC-C...312.	-0.184	P4E0C...2-..	1.315	(..........	0.4577	C...N...2...	0.0573
PT3-N...5...	1.1435	NNC-N...220.	0.1411	P4E0C...1-..	0.358	c..........	0.3688	N...2...(...	2.0213
PT3-C...5...	-0.3344	NNC-C...202.	-0.9498	P4E0F...1-..	0	1..........	0.1317	N...(...2...	-0.0831
PT3-C...3...	0.1487	NNC-N...220.	0.1411	S2E0N...1-..	0.3437	n..........	-0.056	c...N...(...	2.0713
PT3-C...4...	0.2734	NNC-C...312.	-0.184	S2E0C...1-..	0.1063	c..........	0.3688	N...c...1...	1.1702

PT3-C...2...	0.1335	NNC-C...330.	0.251	S2E0N...4-..	0.1289	n.....	-0.056	c...1...c...	0.4611
PT3-C...3...	0.1487	NNC-C...330.	0.251	S2E0C...7-..	2.1705	c.....	0.3688	c...c...1...	0.1309
PT3-C...3...	0.1487	NNC-C...110.	0.3021	S2E0N...6-..	0.1176	2.....	-0.9023	c...c...c...	0.1879
PT3-F...2...	0	NNC-C...211.	2.2033	S2E0C...7-..	2.1705	c.....	0.3688	c...c...c...	0.1879
PT4-N...1...	0.0125	NNC-N...220.	0.1411	S2E0C...6-..	-0.87	1.....	0.1317	c...c...(...	0.4043
PT4-C...4...	0.4389	NNC-N...220.	0.1411	S2E0N...7-..	0.5201	C.....	0.4163	c...(...c...	0.4636
PT4-N...5...	0.3972	NNC-C...321.	0.4714	S2E0C...7-..	2.1705	(.....	0.4577	1...c...(...	0.0432
PT4-C...10..	0.6786	NNC-C...220.	0.0933	S2E0C...5-..	0.3441	C.....	0.4163	c...1...(...	2.2709
PT4-N...4...	0.353	NNC-C...220.	0.0933	S2E0C...4-..	-1.1756	(.....	0.4577	F...(...1...	0
PT4-C...12..	0.3842	NNC-C...220.	0.0933	S2E0C...9-..	0.1074	C.....	0.4163	Cmax.2.....	0.4692
PT4-C...9...	0.074	NNC-C...321.	0.4714	S2E0N...6-..	0.1176	N.....	0.3653	Nmax.6.....	0.3261
PT4-N...10..	0.0972	NNC-C...220.	0.0933	S2E0C...4-..	-1.1756	2.....	-0.9023	Omax.0.....	0.4253
PT4-C...9...	0.074	NNC-F...110.	0	S2E0N...5-..	0.1705	(.....	0.4577	Smax.0.....	2.1015
PT4-C...9...	0.074	C7.....0...	5.8174	S2E0C...7-..	2.1705	N.....	0.3653	NOSP10000000	0.4366
PT4-C...5...	0.3547	C6...AH.3...	-0.0008	S2E0C...9-..	0.1074	c.....	0.3688	BOND11000000	0.2034
PT4-C...11..	1.3977	C5...AH.1...	0.317	S2E0C...5-..	0.3441	1.....	0.1317	++++F---N===	0
PT4-N...9...	0.2243	C4.....0...	8.4462	S2E0C...4-..	-1.1756	c.....	0.3688	++++F---B2==	0
PT4-C...8...	0.2646	C3.....0...	6.0724	S2E0C...5-..	0.3441	c.....	0.3688	++++F---B3==	0
PT4-N...6...	0.2569	P2E0N...0-..	0.3058	S2E0N...6-..	0.1176	c.....	0.3688	++++N---B2==	10.0858
PT4-C...10..	0.6786	P2E0C...1-..	0.2059	S2E0N...7-..	0.5201	c.....	0.3688	++++N---B3==	0.225
PT4-C...8...	0.2646	P2E0N...1-..	0.3356	S2E0C...5-..	0.3441	(.....	0.4577	++++B2--B3==	-0.0024
PT4-C...9...	0.074	P2E0C...1-..	0.2059	S2E0C...4-..	-1.1756	c.....	0.3688		
PT4-C...5...	0.3547	P2E0N...2-..	2.2812	S2E0C...4-..	-1.1756	1.....	0.1317		
PT4-C...8...	0.2646	P2E0C...1-..	0.2059	S2E0C...3-..	0.0092	(.....	0.4577		

Table S3. The list of SA_ks together with their correlation weights for the three runs of the Monte Carlo optimization

SA_k	$CW(SA_k)$			SA_k	$CW(SA_k)$			SA_k	$CW(SA_k)$			SA_k	$CW(SA_k)$		
	Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3		Run 1	Run 2	Run 3
#.....	0.32946	0.48737	2.38191	N...C.....	-0.13565	-0.77313	0.11324	S2E0C...6-..	-0.06275	-0.86997	-0.73327	VS2-C...10..	0.15648	0.13163	1.10461
$10011000000	0.1944	0.2978	-0.32973	N...C...1...	2.13545	0.23208	0.0102	S2E0C...7-..	0.47941	2.17047	1.34843	VS2-C...11..	-1.24519	-0.11844	0.22305
$10011000010	0.14153	0.31469	0.11874	N...C...C...	0.14729	0.32515	1.3843	S2E0C...8-..	0.48772	0.1889	-0.2135	VS2-C...12..	0.22925	0.19402	0.03171
$11010000000	0.11132	0.13777	-0.03588	N...H.....	0.16071	0.18982	0.01462	S2E0C...9-..	0.47568	0.10744	-0.50569	VS2-C...13..	0.09418	1.05171	0.48726
$11010000010	0.0967	2.07687	-0.00348	N...S...(...	0.37336	0.08092	0.2816	S2E0Br..3-..	0.17877	0.47585	0.40341	VS2-C...2...	0.60139	0.22828	0.15873
$11011000000	0.14275	0.20016	-0.83225	N...[...2...	0.38541	-0.09818	-0.30319	S2E0Cl..3-..	1.38222	-0.33276	0.15061	VS2-C...3...	0.22413	0.41434	0.03527
$11011100000	0.4342	0.22978	-0.94774	N...[...3...	-0.88194	0.45368	0.07139	S2E0N...0-..	0.12971	-0.53894	0.30654	VS2-C...4...	0.38894	0.23977	0.48333
(...(.....	0.23143	0.77079	0.58641	N...\...(...	0.03755	0.36019	-0.31936	S2E0N...1-..	0.37408	0.34366	-0.09567	VS2-C...5...	0.30817	0.41557	0.31929
(.....	0.11498	0.45774	0.23651	N...\...C...	0.25674	0.68562	2.19699	S2E0N...3-..	0.48462	0.42871	1.09018	VS2-C...6...	0.17167	0.02775	0.22804
(...C...(...	0.05513	0.794	0.45524	N...c...1...	0.293	1.17016	0.65727	S2E0N...4-..	0.30228	0.12893	-0.16093	VS2-C...7...	-1.21082	-0.45465	0.31108
(...Br..(...	2.10116	0.14235	-0.27048	N...c...3...	0.24262	2.23557	-0.00452	S2E0N...5-..	0.10922	0.17054	0.35939	VS2-C...8...	0.15647	0.41877	0.48821
(...N...#...	0.25303	0.34576	0.49898	O...(...(...	-1.48266	-0.97341	-0.04956	S2E0N...6-..	0.15507	0.11763	2.01639	VS2-C...9...	0.13427	0.13628	0.2101
(...N...(...	0.03105	-1.24206	-0.9964	O...(.....	0.19651	-0.08424	-1.08045	S2E0N...7-..	2.27846	0.52006	0.44361	VS2-Br..4...	0.02645	0.0105	0.29197
++++B2--B3==	0.30782	-0.0024	0.07393	O...(...C...	-2.08071	-1.98211	-0.65607	S2E0N...8-..	-1.06556	-0.78966	-0.89021	VS2-Cl..4...	0.46471	-0.39184	-0.43522
++++CL--N===	0.11611	1.64146	1.02437	O...(...N...	0.43306	0.20001	0.26434	S2E0O...1-..	-0.83093	-0.6051	-0.45383	VS2-N...10..	0.09782	0.41771	0.30405
++++Br--B2==	0.23044	0.15858	0.26571	O...(...O...	0.32043	-0.03137	0.12623	S2E0O...2-..	0.01481	0.46497	0.11562	VS2-N...11..	-2.25211	-0.91478	-0.63561
++++Br--B3==	-0.29204	-1.07435	1.72553	O.....	1.31963	0.69123	0.17923	S2E0O...4-..	0.19954	0.14415	0.2206	VS2-N...2...	0.32618	-3.46738	-5.24173
++++Br--N===	0.27215	0.09146	0.50591	O...=...(...	-0.92865	-1.12335	-0.16063	S2E0O...5-..	1.74544	-0.08768	0.02517	VS2-N...3...	0.08417	-0.09413	0.14119
++++Br--O===	0.38937	0.02276	0.07665	O...=.....	0.23694	0.08863	0.61552	S2E0O...6-..	0.4241	0.2165	0.17128	VS2-N...5...	0.30946	0.06228	0.1483
++++Cl--B2==	0.05023	1.79694	-0.12467	O...=...C...	2.23599	1.40581	1.35881	S3E0C...1-..	0.0956	0.05446	-0.51382	VS2-N...6...	1.37035	0.13795	0.10851
++++Cl--B3==	0.17249	-0.04505	0.46992	O...C...(...	0.24877	0.54367	2.23245	S3E0C...10-.	0.38178	0.19135	0.3527	VS2-N...7...	0.4469	-0.897	0.32728
++++N---B2==	3.61673	10.08577	8.26465	O...C.....	0.56341	1.09501	0.02571	S3E0C...11-.	0.41083	0.18159	0.39485	VS2-N...8...	0.40719	0.5662	0.41762
++++N---B3==	0.95092	0.22495	-0.08067	O...C...C...	0.56524	0.16685	1.44368	S3E0C...12-.	-0.35495	-0.62303	-1.28797	VS2-N...9...	0.34436	0.335	0.01651
++++N---O===	0.06476	0.68371	0.29106	O...c...1...	0.1024	0.24977	-0.18713	S3E0C...13-.	-0.85024	-1.72571	-1.11698	VS2-O...2...	0.51725	3.27547	-0.17923
++++N---S===	0.04581	0.83305	0.26807	P2E0C...0-..	0.5689	0.24384	0.62422	S3E0C...14-.	-1.0367	0.17109	-0.48051	VS2-O...4...	-0.05508	-0.56118	2.15812
++++O---B2==	0.43002	0.45828	0.30039	P2E0C...1-..	0.47456	0.20587	0.03326	S3E0C...2-..	0.19592	0.36911	-0.04748	VS2-O...5...	0.1838	0.28867	0.23929
++++O---B3==	-0.09423	0.46905	-0.60241	P2E0C...2-..	0.45923	0.20708	0.2841	S3E0C...3-..	1.02142	0.47201	0.09408	VS2-O...6...	0.35656	0.1445	1.48642
++++O---S===	0.00195	0.28085	-0.26679	P2E0C...3-..	-7.64762	-4.79561	-3.27559	S3E0C...4-..	0.64911	0.23242	-0.17332	VS2-O...7...	0.14229	1.35481	0.47404
++++S---B2==	-0.26568	-0.44694	-0.27422	P2E0Br..1-..	0.30335	0.43932	0.43055	S3E0C...5-..	0.35472	0.38551	0.37562	VS2-O...8...	0.0084	0.07172	0.34956
++++S---B3==	-0.97995	-0.5982	0.06808	P2E0Cl..1-..	-0.16738	-0.32136	0.26514	S3E0C...6-..	0.17425	0.45982	-0.26633	VS3-C...10..	0.36568	0.37958	0.19947
/.....	0.05541	2.00888	0.16705	P2E0N...0-..	0.72435	0.30577	0.09066	S3E0C...7-..	0.24164	0.10422	0.22207	VS3-C...11..	0.19171	0.44265	0.32155

/...C...(...	1.49955	0.11141	0.04012	P2E0N...1-..	0.19657	0.33561	2.29845	S3E0C...8-..	0.24363	-0.2491	0.45554	VS3-C...12..	0.33837	-0.11511	0.33521
/...N...(...	0.45432	-0.54173	-0.02883	P2E0N...2-..	0.18491	2.28115	0.73084	S3E0C...9-..	0.11024	0.11019	0.19351	VS3-C...13..	0.42308	0.18499	-0.21845
1...(.....	0.06707	0.13647	-0.0665	P2E0N...3-..	1.06551	0.68539	-0.59582	S3E0Br..4-..	0.24432	0.54509	0.05961	VS3-C...14..	-0.07263	0.21751	0.20856
1.....	0.09754	0.13174	0.25502	P2E0O...0-..	0.07999	-0.87984	-0.0405	S3E0Cl..4-..	-0.32643	0.91379	2.51528	VS3-C...15..	-1.07965	0.26501	-0.83939
1...2...(...	0.41779	2.2219	0.09354	P2E0O...1-..	-0.03893	-0.07769	-0.92606	S3E0N...0-..	0.3967	0.1943	-0.49454	VS3-C...16..	-0.61614	0.92631	0.41129
1...C...(...	0.08883	0.47765	0.80083	P2E0O...2-..	0.28658	0.49495	0.44083	S3E0N...1-..	-0.33959	0.06936	0.24137	VS3-C...3...	0.17723	-0.18667	-1.9945
1...N...(...	0.05337	0.32468	0.29071	P2E0S...1-..	0.10423	0.38297	-0.41976	S3E0N...10-.	0.32377	-1.37483	0.5811	VS3-C...4...	0.26708	0.15917	0.03344
1...c...(...	1.15114	0.04325	-0.49654	P3E0C...0-..	-0.8437	-0.0974	0.18248	S3E0N...11-.	0.24006	0.17675	0.1288	VS3-C...5...	0.08598	0.27962	0.21333
2...(.....	4.01411	4.1134	0.86075	P3E0C...1-..	0.32494	0.21846	0.21054	S3E0N...12-.	0.03196	2.24059	0.04896	VS3-C...6...	0.22348	0.21798	0.16061
2.....	0.34589	-0.90226	0.32706	P3E0C...2-..	0.42625	0.02551	0.34005	S3E0N...13-.	0.03791	0.129	0.35755	VS3-C...7...	2.17472	0.23459	0.00533
2...1.....	0.41299	-0.2052	0.41975	P3E0C...3-..	-0.7988	0.03673	-0.38615	S3E0N...15-.	0.04224	-0.09893	-0.65237	VS3-C...8...	0.11352	0.23339	-0.30598
2...C...(...	0.15685	0.46371	-0.81381	P3E0C...4-..	0.44325	0.01553	0.49642	S3E0N...2-..	0.87942	1.91285	0.17063	VS3-C...9...	0.39896	0.41969	-0.54472
2...N...(...	0.4223	0.1067	-0.06664	P3E0C...5-..	0.3169	0.10017	0.13154	S3E0N...3-..	0.11181	0.11775	0.16537	VS3-Br..5...	0.74652	0.16972	0.02335
2...c...(...	0.43456	0.25448	-0.87266	P3E0Br..1-..	2.00261	0.29773	0.30387	S3E0N...4-..	0.49386	0.07921	0.12833	VS3-Cl..5...	1.50737	0.42821	0.57307
2...c...1...	0.31847	0.64813	0.41264	P3E0Cl..1-..	-0.15823	0.16702	1.21896	S3E0N...5-..	-0.5149	0.42841	0.51583	VS3-N...10..	2.35389	0.38038	0.27591
3...(.....	0.33169	0.43563	0.24998	P3E0N...0-..	0.15642	0.37071	0.15074	S3E0N...6-..	0.35318	0.15685	0.05093	VS3-N...11..	0.29584	0.23807	0.48885
3.....	0.23099	0.15106	-0.64067	P3E0N...1-..	-1.31304	-0.53027	-0.54804	S3E0N...7-..	0.28842	1.23677	0.77205	VS3-N...12..	0.14608	-0.02803	-0.32827
3...2...(...	-0.17279	-0.06114	2.11127	P3E0N...2-..	0.4558	0.47778	-0.89357	S3E0N...8-..	0.36592	0.12603	0.0623	VS3-N...13..	0.25153	-0.99666	-0.74343
3...2.....	0.32204	0.09101	-0.89292	P3E0N...3-..	0.11709	0.16729	0.15153	S3E0N...9-..	-0.64501	0.39446	0.30448	VS3-N...14..	-1.09252	-0.40347	0.1804
3...N...(...	2.10973	0.23792	-0.09032	P3E0N...4-..	0.06905	0.18018	0.14591	S3E0O...1-..	0.22873	0.80331	2.2152	VS3-N...15..	0.11649	0.0911	0.56915
3...c...(...	-0.82652	0.17299	0.08687	P3E0O...0-..	0.05759	0.41736	0.73744	S3E0O...3-..	0.30249	0.43721	0.15438	VS3-N...16..	0.01272	0.19012	0.49845
=...(...(...	-0.87501	0.82909	-0.6894	P3E0O...1-..	0.43918	-1.22559	0.41885	S3E0O...4-..	0.41681	0.27418	0.46227	VS3-N...18..	-0.09301	-0.22523	-0.1193
=...(.....	0.27927	0.23788	0.17574	P3E0O...2-..	0.4601	-1.24481	-0.92661	S3E0O...5-..	0.2078	-0.14483	-0.28427	VS3-N...3...	-3.34381	-3.17708	-1.68203
=...(...3...	0.14025	0.43519	-0.21217	P3E0O...3-..	-0.4988	0.31371	0.72684	S3E0O...6-..	0.4234	0.43034	0.25262	VS3-N...4...	-0.97355	-3.16565	-1.78109
=.....	0.10972	0.22008	-0.65747	P4E0C...0-..	-0.48378	-0.95133	-0.2719	S3E0O...7-..	0.39936	0.39399	2.37876	VS3-N...5...	0.44664	0.12344	0.26177
=...C...(...	0.00698	2.17709	0.27308	P4E0C...1-..	0.4549	0.35804	0.04738	S3E0O...8-..	-1.69554	-0.60074	0.56023	VS3-N...6...	0.00442	0.10504	0.41697
=...O...(...	-0.80754	-0.2423	-0.62043	P4E0C...10-.	0.25766	0.45344	0.09047	S3E0S...3-..	0.16123	0.08027	-0.58835	VS3-N...7...	0.10975	0.31897	1.23354
C...#.....	0.31343	0.26173	0.42438	P4E0C...11-.	0.17069	0.27522	0.07429	PT2-C...1...	-0.22953	0.27042	0.47852	VS3-N...8...	1.36786	0.32743	-0.26879
C...(.....	0.21772	0.44829	0.35782	P4E0C...12-.	1.1632	0.22889	0.38355	PT2-C...2...	0.2877	0.33069	0.36664	VS3-N...9...	-0.93317	0.40609	0.31601
C...(...1...	1.08394	0.30232	0.0066	P4E0C...2-..	0.30419	1.31503	0.30479	PT2-C...3...	0.48378	0.08956	-0.51376	VS3-O...2...	0.12593	0.22579	1.41717
C...(...2...	0.26129	0.01568	0.35015	P4E0C...3-..	-0.72289	0.30968	0.02901	PT2-C...4...	0.13486	0.20167	0.38332	VS3-O...4...	-0.67975	0.07097	1.06823
C...(...=...	0.03112	-0.49494	0.02044	P4E0C...4-..	0.07894	0.0119	0.27475	PT2-C...5...	2.36311	2.41797	0.15748	VS3-O...5...	1.47746	0.14153	-0.79104
C...(...C...	0.13926	0.26403	0.2008	P4E0C...5-..	0.35038	0.31615	0.41098	PT2-C...6...	-2.52043	-1.09018	-5.19311	VS3-O...6...	0.29737	-0.8501	0.33058
C.....	0.01883	0.41631	0.31169	P4E0C...6-..	0.1942	0.0656	0.00635	PT2-Br..2...	0.20062	0.47003	0.18967	VS3-O...7...	0.04141	-0.00002	-0.50708
C.../.....	0.41153	0.29456	0.69587	P4E0C...7-..	0.46444	0.17545	0.28842	PT2-Cl..2...	-0.15414	0.31983	0.39862	VS3-O...8...	2.11067	0.41834	0.20431

C...1...(...	0.28698	-0.06602	0.47671	P4E0C...8-..	-0.24374	0.0041	1.33209	PT2-N...1...	0.0172	0.36004	0.1781	VS3-O...9...	0.21109	0.27144	0.47186
C...1.....	2.44644	0.18411	1.18663	P4E0C...9-..	0.01075	0.25452	-0.99707	PT2-N...2...	0.47969	-0.60099	0.23827	VS3-S...7...	0.49356	0.21135	0.1135
C...1...C...	0.27609	0.37979	0.07966	P4E0Br..1-..	0.14441	0.32307	0.28162	PT2-N...3...	0.21724	0.01877	0.47569	Smax.0.....	0.74627	2.10145	0.42931
C...2.....	0.26688	-0.15329	0.25151	P4E0Cl..1-..	1.1571	1.86831	-0.08554	PT2-N...4...	0.47555	-0.49893	-0.1221	Smax.1.....	0.14372	0.3172	0.4708
C...2...C...	0.2888	0.24513	0.38791	P4E0N...0-..	0.15624	0.07248	0.34169	PT2-N...5...	0.7306	0.37532	0.06725	[.....	0.00059	0.14549	0.00159
C...3.....	0.12557	0.32699	0.2429	P4E0N...1-..	0.45242	0.0108	0.2628	PT2-N...6...	0.17028	0.03627	0.48734	[...2.....	1.43148	0.90421	-1.59015
C...=.....	2.46534	1.61077	2.24359	P4E0N...10-.	0.13381	0.28946	0.18355	PT2-O...1...	0.0587	-0.16848	0.2616	[...3.....	0.1546	0.3445	0.13388
C...=...C...	0.47665	0.25062	0.28226	P4E0N...2-..	-1.20057	-1.98746	0.52752	PT2-O...2...	-0.82489	0.13718	-0.70849	[...H.....	0.06239	0.33066	0.16526
C...C...(...	0.40757	0.45197	0.04767	P4E0N...3-..	0.4182	2.28195	-0.06401	PT2-O...3...	-1.77439	-1.47942	-0.85554	[...H...N...	0.04605	0.16058	0.48319
C...C.....	0.33842	0.28198	0.33169	P4E0N...4-..	0.19258	0.21589	-0.56307	PT2-O...4...	0.08577	0.06907	0.16184	[...N.....	0.22734	-0.0054	1.48698
C...C...1...	0.47944	0.3636	0.33266	P4E0N...5-..	2.0657	0.01891	0.07131	PT2-S...3...	0.32289	0.25293	-0.97217	[...N...H...	0.02014	0.05997	0.0174
C...C...2...	0.39719	0.08831	0.42369	P4E0N...6-..	0.34403	0.44557	-0.646	PT3-C...1...	0.46163	0.28099	-0.12475	\...(.....	0.01564	-0.09799	0.24185
C...C...3...	0.19171	-0.51317	2.29022	P4E0N...7-..	0.0503	0.26406	0.73586	PT3-C...2...	0.48326	0.1335	0.27982	\...(...C...	0.57798	0.08036	0.35944
C...C...=...	0.15742	0.25513	0.09303	P4E0N...8-..	0.1944	0.47002	-1.08275	PT3-C...3...	0.10015	0.14873	0.33426	\.....	0.01273	0.28718	0.82846
C...C...C...	0.02202	2.46509	0.98626	P4E0N...9-..	0.20475	0.21436	0.08427	PT3-C...4...	-0.31023	0.27343	-0.88704	\...C...#...	0.2711	-0.88842	-0.02744
C...N...(...	0.12816	0.23005	-0.03282	P4E0O...0-..	0.57981	0.01051	0.15701	PT3-C...5...	-0.71909	-0.33439	-0.14607	\...C...(...	-0.71516	0.43186	0.11835
C...N...2...	0.14159	0.05734	0.12881	P4E0O...4-..	-0.86749	0.44253	-0.31087	PT3-C...6...	1.47793	1.44286	0.04636	\...C.....	0.23875	0.35255	0.12396
C...N...=...	3.14488	0.66886	0.32574	P4E0O...9-..	0.18301	0.01601	0.40059	PT3-C...7...	0.41341	0.22166	0.52952	\...N...(...	0.49617	0.23616	0.55633
C...N...C...	0.25275	-0.8166	-0.20608	NNC-C...101.	0.01584	0.16402	0.32156	PT3-C...8...	0.29086	0.35414	0.44836	\...N.....	0.4687	0.02584	0.39484
C...O...(...	0.38272	-0.02627	-0.20617	NNC-C...110.	0.12836	0.3021	0.27421	PT3-Br..2...	0.30904	0.17408	0.06934	\...N...=...	0.25858	0.10997	-0.70813
C...c...1...	0.26751	-0.64702	-0.02873	NNC-C...202.	2.01989	-0.9498	-1.32226	PT3-Cl..2...	2.11155	-0.37219	1.04435	c...(.....	0.18518	0.00223	0.18374
C3.....0...	3.43042	6.07245	3.24392	NNC-C...211.	2.05549	2.20332	0.43889	PT3-N...1...	-0.58767	0.15512	-0.7275	c...(...1...	0.02533	0.37079	-0.00388
C4.....0...	2.02107	8.44617	6.04264	NNC-C...220.	0.15528	0.09332	-0.6283	PT3-N...2...	0.02842	0.4137	0.22241	c...(...2...	0.20071	-0.11716	0.12042
C5.....0...	0.10643	0.47777	0.57879	NNC-C...303.	0.26279	0.23619	0.32344	PT3-N...3...	0.07773	0.27279	0.46233	c...(...C...	2.32343	0.3025	1.18845
C5...AH.1...	0.36897	0.317	-0.47008	NNC-C...312.	-0.21689	-0.18396	0.00843	PT3-N...4...	0.30115	0.18583	0.28771	c...(...Br..	-0.8029	0.48324	0.98768
C6...AH.3...	2.44082	-0.00083	0.02565	NNC-C...321.	0.31087	0.4714	0.29642	PT3-N...5...	-0.78976	1.14347	0.1991	c...(...N...	0.24138	0.15891	0.47894
C6...AH.4...	0.15856	0.3686	-0.51468	NNC-C...330.	0.34653	0.25099	0.11494	PT3-N...6...	-0.18457	-0.52409	-1.81585	c...(...O...	0.07753	0.47983	0.48228
C6...AH.5...	0.04782	0.04935	-0.08429	NNC-C...431.	0.1892	0.41227	1.38023	PT3-N...7...	0.32103	-0.7165	0.472	c...(...c...	0.36584	0.46362	2.54689
C7.....0...	4.47615	5.81739	6.21642	NNC-C...440.	0.14142	0.15901	-0.01867	PT3-O...1...	0.58327	0.15276	0.23065	c.....	0.24789	0.36876	-0.95711
BOND10000000	0.0947	0.20708	0.48934	NNC-Br..110.	0.24852	0.10403	0.12934	PT3-O...2...	0.1167	0.06936	0.13726	c...1...(...	0.67951	2.27091	2.29314
BOND11000000	0.09195	0.20343	1.42165	NNC-Cl..110.	0.18049	1.32182	0.6086	PT3-O...3...	0.47683	0.16928	0.24801	c...1.....	0.28067	0.37792	0.44293
EC0-C...1...	0.39844	0.38611	0.30899	NNC-N...110.	0.72668	0.33852	0.45335	PT3-O...4...	0.35116	0.10155	0.26476	c...1...2...	0.65041	0.13492	-0.87204
EC0-C...2...	0.36222	0.15756	-0.09071	NNC-N...211.	0.18188	-0.98283	0.4638	PT4-C...1...	0.29492	0.34283	-0.54495	c...1...C...	0.28489	0.14375	0.08277
EC0-C...3...	0.44324	0.2223	0.13148	NNC-N...220.	0.47253	0.14115	0.42017	PT4-C...10..	0.38093	0.6786	0.28802	c...1...c...	0.07217	0.46107	0.11666
EC0-C...4...	0.15014	0.1363	0.09523	NNC-N...330.	0.04555	0.26378	-0.1723	PT4-C...11..	0.17336	1.39766	0.09039	c...2.....	0.15323	0.38012	0.49357

EC0-Br..1...	0.38613	0.1857	0.4249	NNC-O...101.	0.03285	0.54919	-0.76712	PT4-C...12..	2.42516	0.38424	0.25557	c...2...1...	0.00889	-0.27665	0.37941
EC0-Cl..1...	2.15395	0.02506	-0.48192	NNC-O...110.	-0.00911	0.17043	-0.90832	PT4-C...13..	0.39976	0.05337	0.24989	c...2...[...	0.53082	0.1274	0.70847
EC0-N...1...	0.15791	0.02856	2.27149	NNC-O...220.	0.38314	0.15568	0.43839	PT4-C...14..	0.33079	0.66525	0.05084	c...2...c...	0.26295	0.4037	0.12686
EC0-N...2...	0.41353	0.62141	0.33826	NNC-S...413.	0.55412	0.98662	0.11139	PT4-C...2...	0.21689	2.35433	0.03486	c...3...(...	0.36046	0.07441	0.13861
EC0-N...3...	0.13154	0.07887	0.33148	NNE0C...100-	0.33861	0.15344	0.20507	PT4-C...3...	0.11045	0.1736	0.10845	c...3.....	0.10289	0.19595	0.36286
EC0-O...1...	0.41258	-0.6092	0.02379	NNE0C...109-	0.02186	0.07924	0.78649	PT4-C...4...	0.01774	0.43892	0.37802	c...3...2...	0.15095	0.20793	0.33554
EC0-O...2...	0.22276	0.18714	0.48616	NNE0C...200-	-0.44246	-2.11764	-0.75813	PT4-C...5...	0.24115	0.35472	0.07726	c...3...[...	0.35227	0.36792	0.38348
EC0-S...4...	0.55994	0.25936	0.15734	NNE0C...209-	0.03389	0.0137	0.10251	PT4-C...6...	0.09063	0.10044	-0.09419	c...3...c...	0.10671	-1.03252	-0.16597
H.....	0.29897	-0.1356	0.18505	NNE0C...218-	0.03505	0.13889	0.47659	PT4-C...7...	0.14945	-0.11653	0.24441	c...C...(...	0.20174	0.03618	0.1672
Br..(.....	-0.72178	-1.16113	-1.17056	NNE0C...300-	0.03615	0.38378	0.33599	PT4-C...8...	0.21445	0.26465	0.06781	c...C.....	0.07144	0.2066	-0.88998
Br..(...1...	1.27762	1.75292	0.51295	NNE0C...309-	0.49108	-0.06989	-0.09437	PT4-C...9...	0.38592	0.07399	0.48843	c...Br.....	0.45473	0.30542	-0.34123
Br.....	0.1176	0.41337	-0.33082	NNE0C...318-	0.28919	0.26334	-0.025	PT4-Br..2...	0.14934	0.41882	0.07213	c...N...(...	2.61086	2.07128	-0.16789
Br..c...1...	0.37846	0.44858	0.41225	NNE0C...327-	0.29662	-0.29119	-0.71918	PT4-Cl..2...	-0.58628	-0.06776	1.70144	c...N.....	0.158	0.46702	-0.08413
Cl..(.....	0.41253	0.32934	0.46514	NNE0C...427-	0.21255	0.87578	-0.18389	PT4-N...1...	-0.28657	0.01247	0.4172	c...N...\...	0.41856	0.0987	0.40374
Cl.....	0.03162	1.16957	-0.22598	NNE0C...436-	0.24878	0.04375	0.1354	PT4-N...10..	-0.16413	0.09716	0.34058	c...O...(...	0.0678	-0.53617	0.34202
Cmax.2.....	0.3279	0.46915	0.28251	NNE0Br..109-	0.26396	0.02242	-0.05151	PT4-N...11..	0.0012	0.30545	0.35241	c...O.....	0.18388	-0.58738	0.18489
Cmax.3.....	0.06471	0.48518	0.29309	NNE0Cl..109-	1.5214	0.05664	0.43587	PT4-N...13..	0.01712	0.45595	0.31041	c...O...C...	0.38348	0.47086	0.00206
N...#.....	0.3872	0.12214	0.40403	NNE0N...109-	0.45168	0.02051	0.61273	PT4-N...3...	0.04968	0.21291	0.27491	c...[.....	0.07635	0.22233	0.27122
N...#...C...	0.41732	0.22434	0.37538	NNE0N...209-	0.00606	0.10597	0.08515	PT4-N...4...	0.51443	0.35305	0.43682	c...[...H...	-0.74056	0.32166	0.11499
N...(.....	0.32032	0.33336	2.32369	NNE0N...218-	1.28162	0.19301	0.02057	PT4-N...5...	0.49037	0.39724	0.4186	c...[...N...	0.24054	0.2169	-0.80053
N...(...1...	4.46569	8.05081	0.44099	NNE0N...327-	0.04946	0.4929	0.41174	PT4-N...6...	0.40749	0.25692	0.04448	c...c...(...	0.08393	0.4043	0.35623
N...(...2...	0.23574	-0.08308	0.11978	NNE0O...100-	0.21593	0.27353	0.37818	PT4-N...7...	0.22606	0.04286	0.43915	c...c.....	0.28834	0.32376	0.10297
N...(...C...	1.88365	3.24229	0.83165	NNE0O...109-	0.18627	-0.87865	0.1389	PT4-N...8...	0.17348	0.24139	0.45845	c...c...1...	0.01176	0.13088	-0.93791
N...(...N...	0.22948	-0.68257	0.14983	NNE0O...218-	0.25647	0.36923	0.48458	PT4-N...9...	0.72476	0.22427	0.00994	c...c...3...	0.24575	-0.05597	0.29779
N.....	0.48622	0.36526	0.29685	NNE0S...409-	0.13498	0.21804	-0.34943	PT4-O...1...	0.49159	0.12458	0.2791	c...c...[...	0.28764	0.02217	0.26201
N.../.....	0.12919	-0.22935	0.31583	NOSP10000000	0.44247	0.43657	-0.03389	PT4-O...10..	0.09435	0.22202	-0.47523	c...c...c...	0.29642	0.18786	0.37814
N.../...C...	0.27891	0.37225	0.39283	NOSP11000000	0.15554	0.04116	0.4635	PT4-O...2...	0.27016	0.06278	0.17795	c...n...1...	-0.66044	-0.07037	1.43231
N...1.....	0.17308	0.51616	0.25322	NOSP11100000	0.25536	0.50542	0.42514	PT4-O...5...	-0.7774	0.40466	0.45625	c...n...2...	0.38215	0.43564	-0.8165
N...1...C...	-2.29436	-5.1167	-2.73363	S...(.....	0.08992	0.34873	0.58056	PT4-O...6...	0.00257	0.69735	-0.94362	c...n...c...	0.15493	6.28061	6.96756
N...2...(...	0.18823	2.02126	-0.13518	S...(...=...	1.3745	0.33608	-0.48343	Nmax.3.....	-1.86652	-0.54421	-3.19986	n.....	0.08171	-0.05604	0.66769
N...2.....	0.22795	0.35763	0.31143	S.....	0.77772	-0.6587	0.70181	Nmax.4.....	1.58594	0.1059	0.3467	n...1.....	-0.28004	0.46033	0.32107
N...2...C...	0.35162	0.19733	0.31038	S...N.....	-0.03954	-0.59169	0.06431	Nmax.5.....	1.21875	1.98948	2.74845	n...1...c...	0.3328	-1.00692	-0.27801
N...3.....	0.11617	0.06477	-0.61864	S2E0C...0-..	0.44771	0.07249	0.30197	Nmax.6.....	0.27603	0.32609	0.47205	n...2.....	0.34896	0.00608	0.42966
N...3...C...	-0.48873	0.30211	2.22132	S2E0C...1-..	0.13317	0.10635	0.2638	Nmax.7.....	0.02347	0.04176	2.30045	n...2...c...	0.40952	0.33272	0.10139
N...=...(...	-0.85647	-0.24181	0.01573	S2E0C...10-.	0.368	0.10243	0.31378	Omax.0.....	0.35726	0.42531	0.02329	n...c...(...	0.08604	-0.04637	0.06217

N...=.....	3.03005	6.17479	-0.64472	S2E0C...2-..	0.08118	0.30835	0.02718	Omax.1.....	-1.13545	-0.53371	2.09431	n...c.....	0.71129	0.28342	0.18897
N...=...C...	0.41696	0.48447	-0.28322	S2E0C...3-..	0.33097	0.00924	0.4594	Omax.2.....	0.10007	0.16523	0.12462	n...c...2...	0.17219	-0.59589	0.39194
N...C...#...	0.08093	2.00605	-2.37117	S2E0C...4-..	-0.73548	-1.17562	0.18469	Omax.3.....	0.2999	0.02127	0.07819	n...c...3...	-0.25666	0.47514	0.42112
N...C...(...	0.1207	0.282	0.22092	S2E0C...5-..	2.03379	0.34411	0.42773	Omax.4.....	0.18116	0.00052	-0.83168	n...c...n...	4.35072	6.97674	6.40472

Table S4. Score values (kcal/mol) for all computer-aided designed compounds

	Cofactor (VdW)	E-Inter (cofactor - ligand)	E-Inter (protein - ligand)	E-Inter total	Energy	HBond	NoHBond90	Steric	VdW	MolDock Score	Rerank Score
A	-1.63023	-8.65188	-160.006	-168.658	-165.027	-1.2981	-4.69246	-158.708	-25.6903	-166.348	-119.961
HA1	-0.554653	-1.10049	-169.64	-170.74	-177.189	-2.37791	-3.90548	-167.346	-9.03714	-174.868	-113.426
HA2	-0.459641	-0.99038	-166.725	-167.715	-174.735	-3.97457	-6.09645	-162.75	-42.7887	-174.472	-129.537
HA3	-2.53515	-9.74414	-173.311	-183.055	-188.183	-2.7931	-7.80976	-170.518	-38.9693	-190.578	-138.405
HD1	-2.42472	-8.10204	-171.24	-179.342	-181.596	-9.08808	-2.5	-171.24	-42.4677	-179.718	-136.979
Hy1	-2.3936	-7.40262	-158.247	-165.649	-167.376	-2.5	-5.17528	-155.747	-16.5851	-166.866	-113.824
Hy2	-1.43223	-5.17812	-162.46	-167.639	-168.229	-1.30022	-1.30022	-161.16	-50.7057	-166.67	-133.162
Hy3	-0.71222	-8.98228	-169.17	-178.152	-178.487	-2.5	-5	-166.67	-40.5211	-177.445	-134.945
Hy4	-2.33439	-8.06146	-175.756	-183.818	-184.916	-1.70001	-2.30071	-175.756	-45.774	-184.374	-141.41
S1	-1.84519	-8.15288	-168.008	-176.16	-172.086	-2.46252	-4.93173	-165.545	-44.395	-170.422	-133.922
S2	-2.39735	-8.38029	-168.567	-176.947	-177.72	0	-2.5	-168.567	-42.4076	-177.747	-134.971
S3	-2.40127	-8.03289	-170.661	-178.694	-180.813	0	-2.5	-170.661	-33.9678	-179.852	-131.712
S4	-2.50553	-8.22988	-173.437	-181.667	-183.942	0	-2.5	-173.437	-42.0336	-183.623	-138.355
S5	-1.17601	-4.95744	-161.186	-166.143	-177.776	0	-5.61107	-159.486	-20.8689	-179.771	-119.46
S6	-2.44434	-8.14543	-172.615	-180.761	-182.41	0	-2.5	-172.615	-46.6343	-182.114	-139.897
S7	-1.99364	-2.66602	-176.381	-179.047	-186.972	0	-11.4276	-167.293	-40.5561	-186.674	-135.995

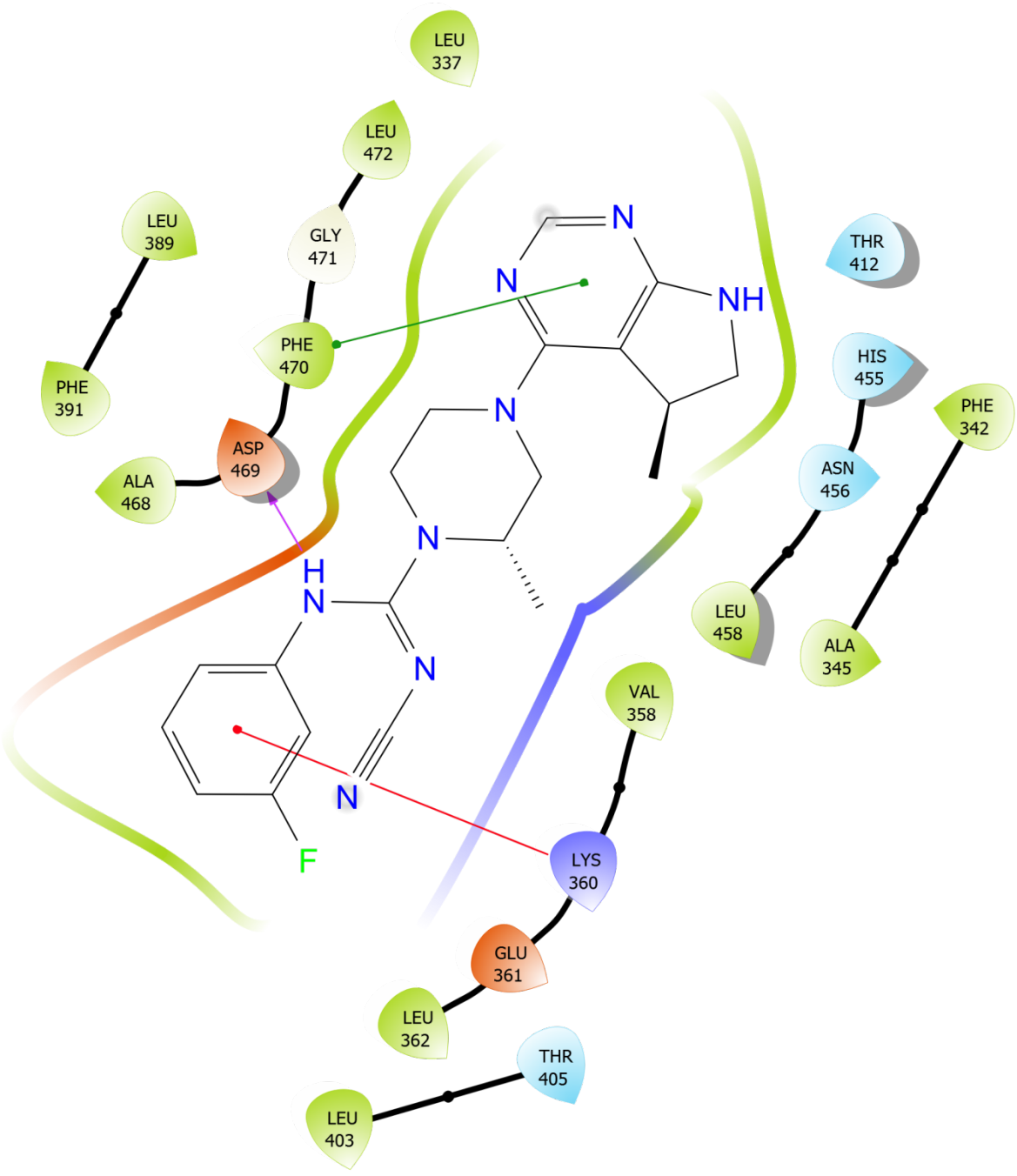


Figure S1. Two-dimensional representation of the interaction between molecule A and amino acids inside LIMK2 binding pocket.

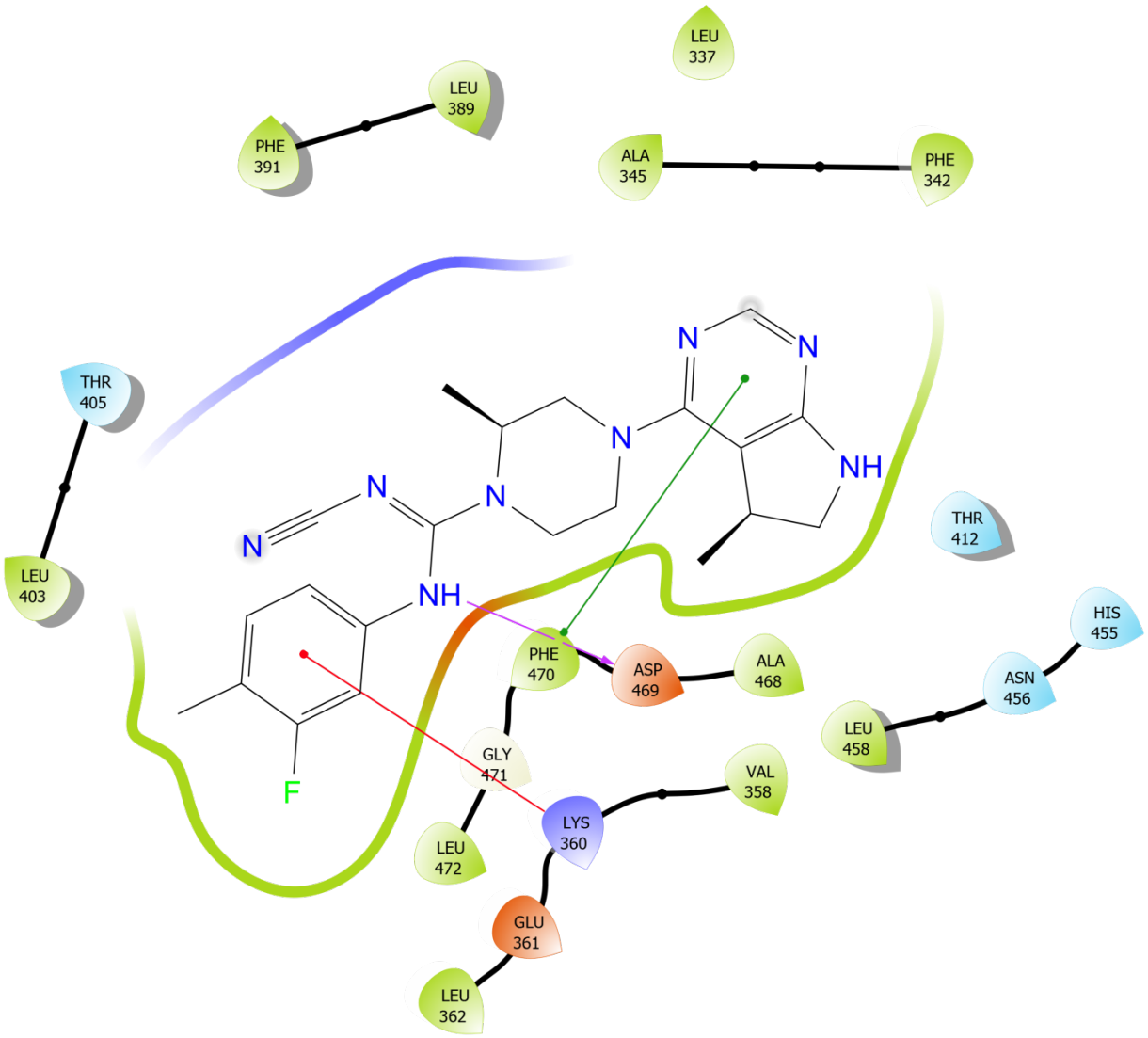


Figure S2. Two-dimensional representation of the interaction between molecule S1 and amino acids inside LIMK2 binding pocket.

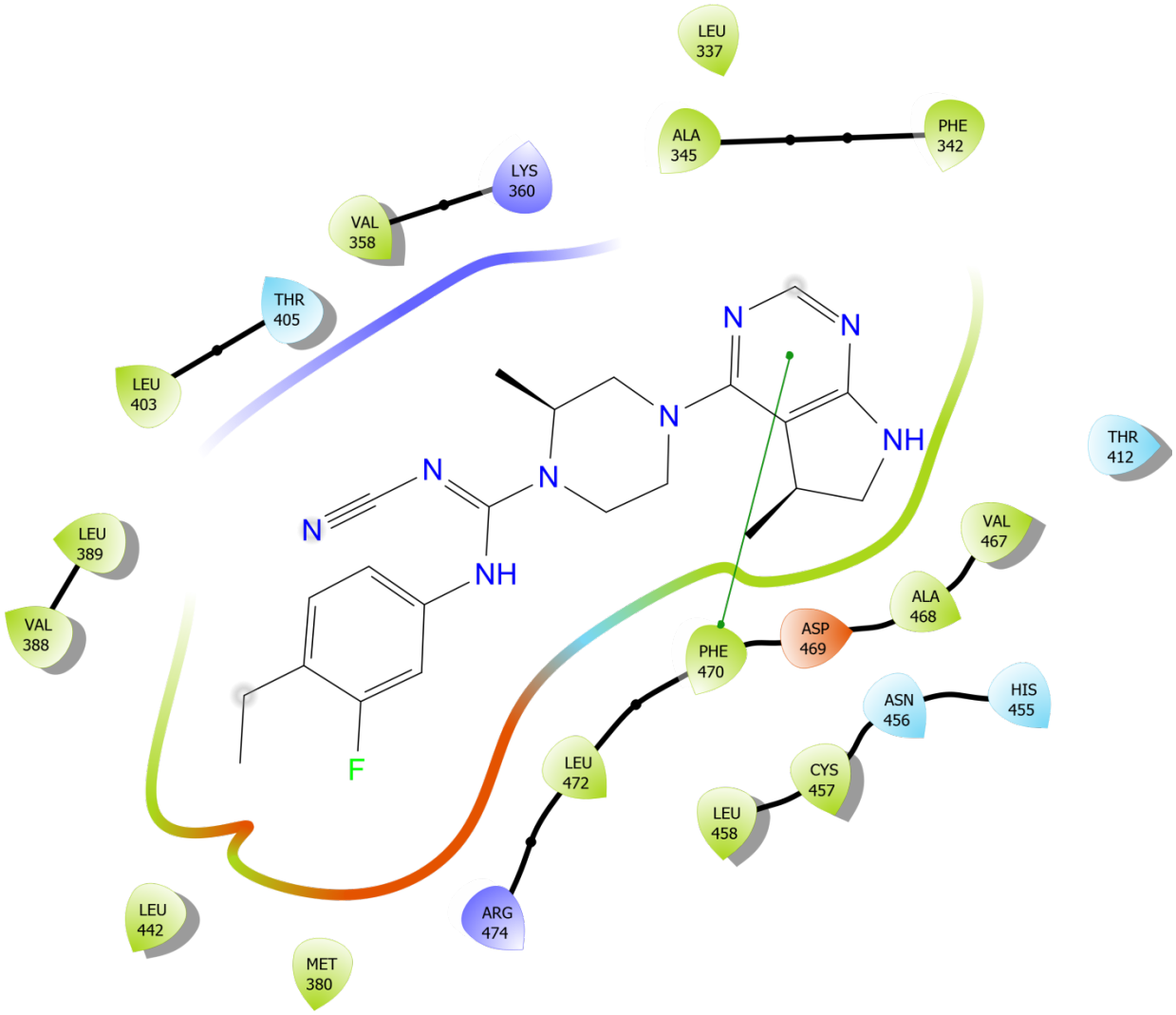


Figure S3. Two-dimensional representation of the interaction between molecule S2 and amino acids inside LIMK2 binding pocket.

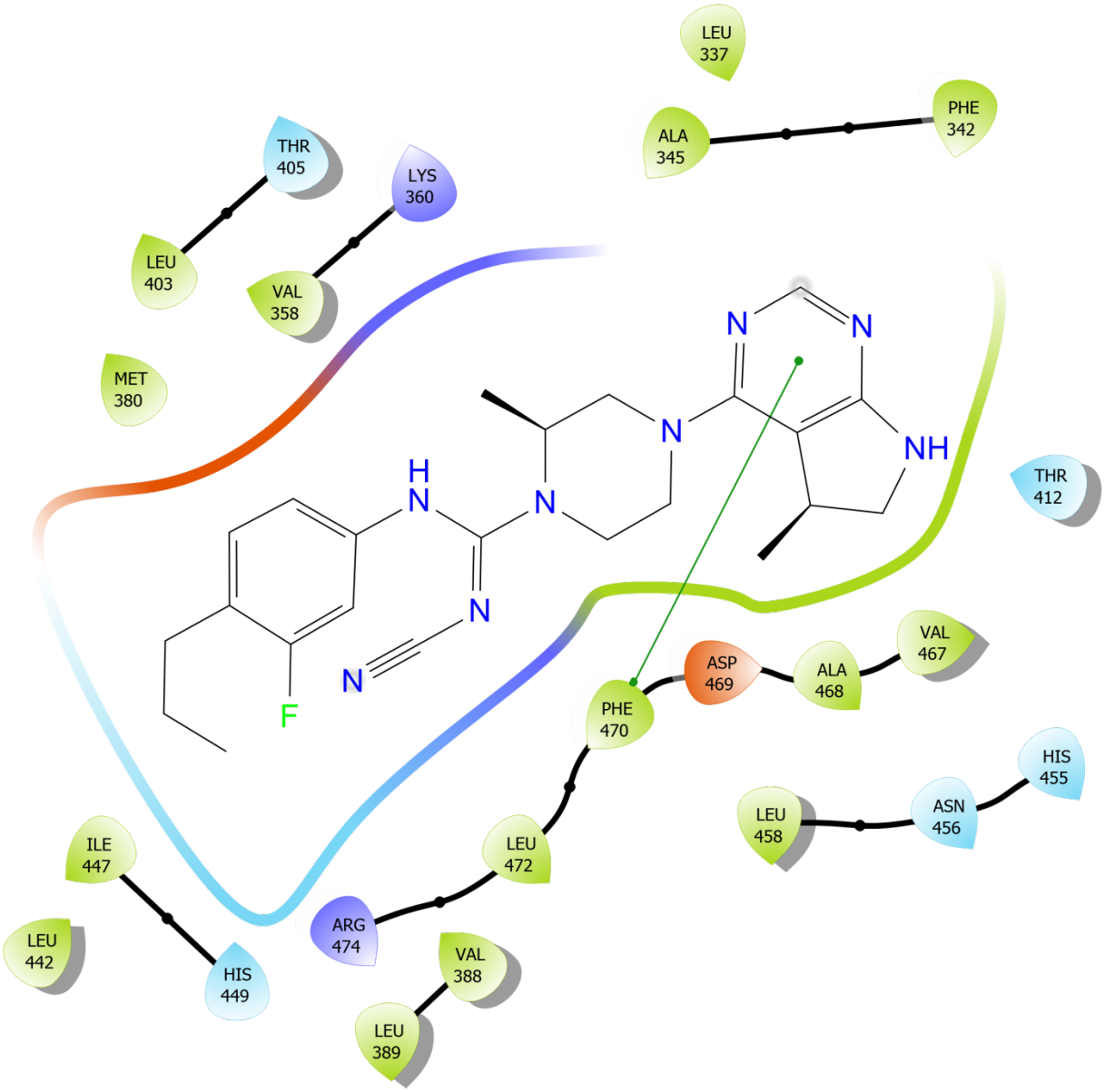


Figure S4. Two-dimensional representation of the interaction between molecule S3 and amino acids inside LIMK2 binding pocket.

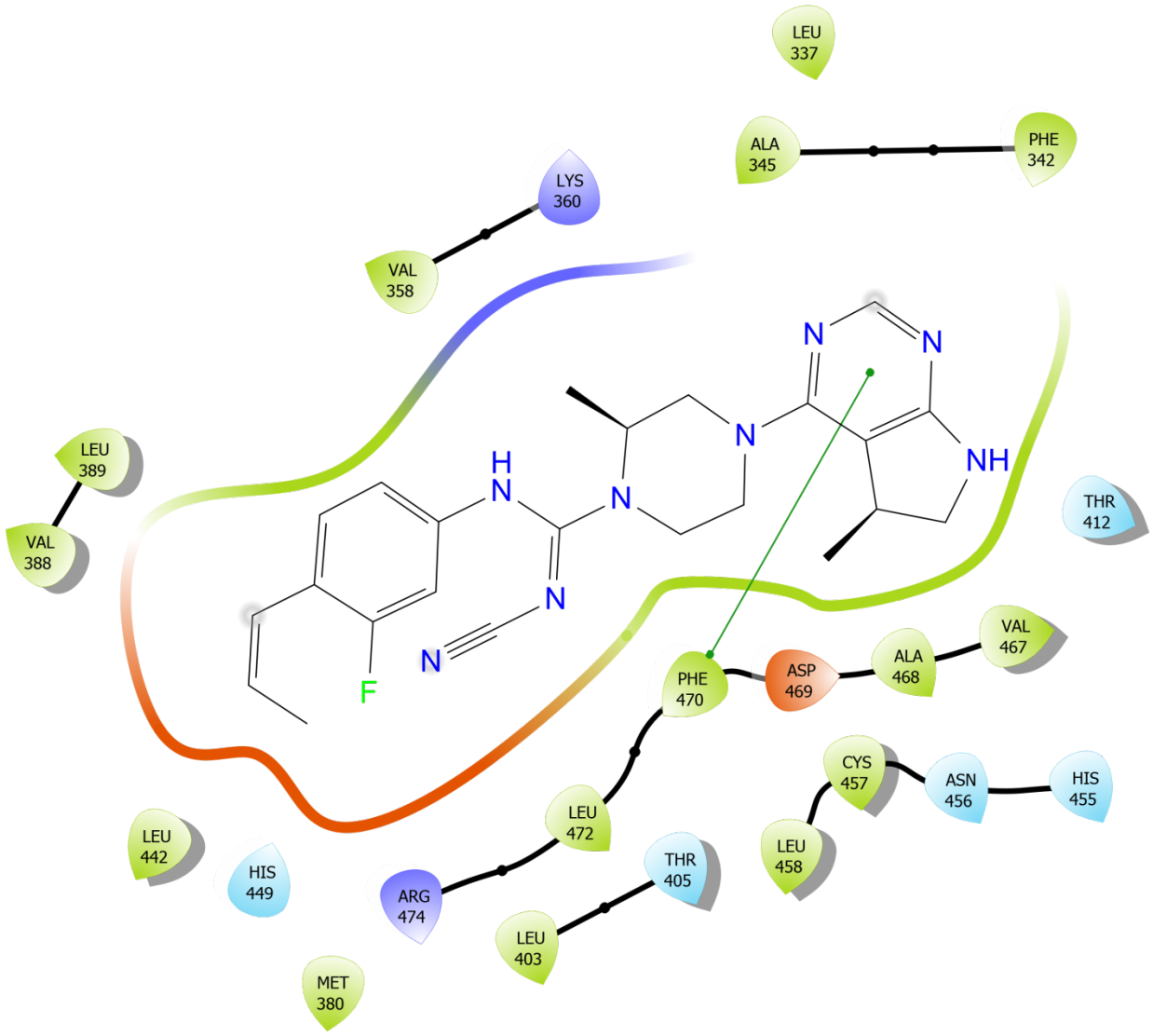


Figure S5. Two-dimensional representation of the interaction between molecule S4 and amino acids inside LIMK2 binding pocket.

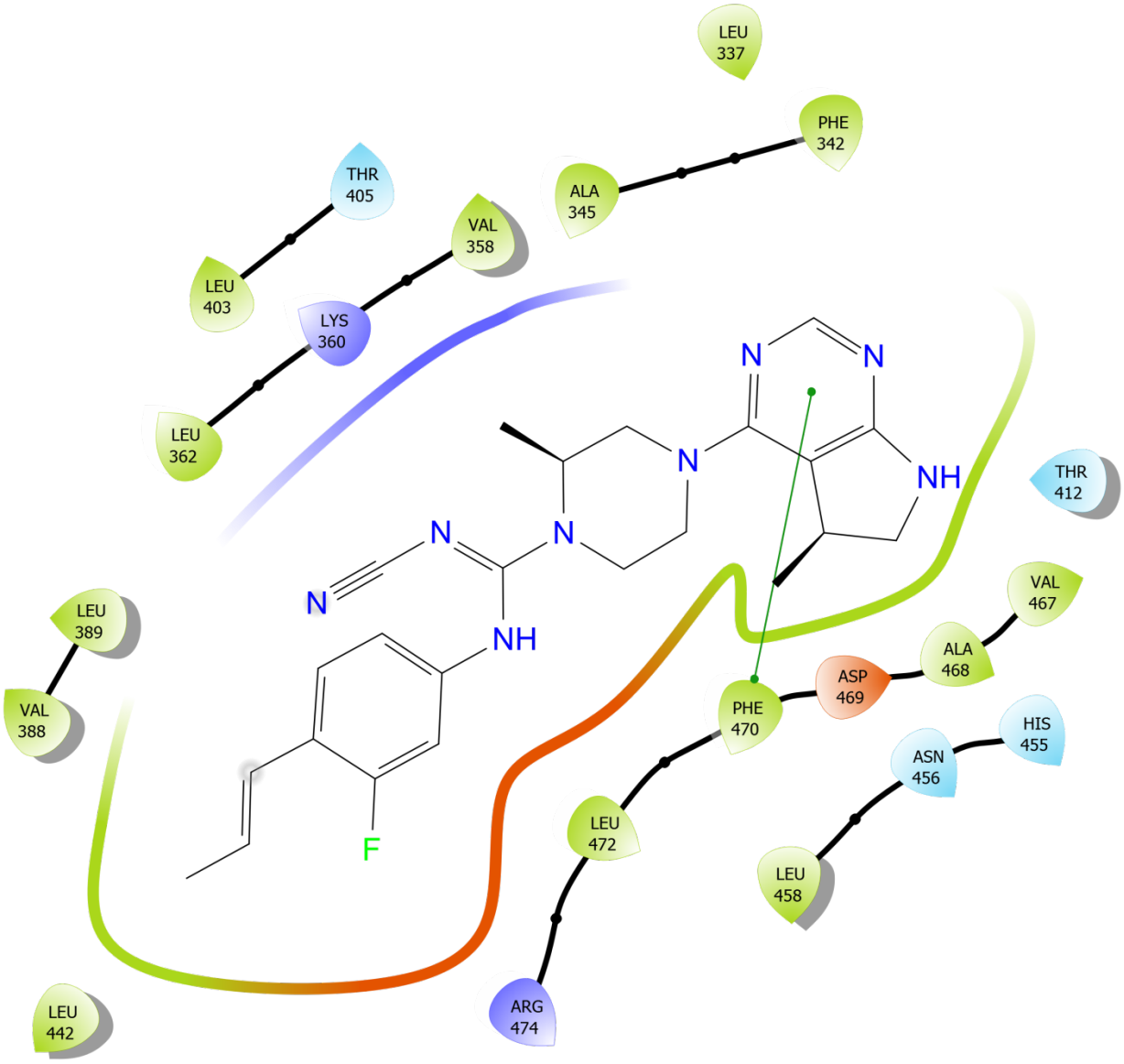


Figure S6. Two-dimensional representation of the interaction between molecule S5 and amino acids inside LIMK2 binding pocket.

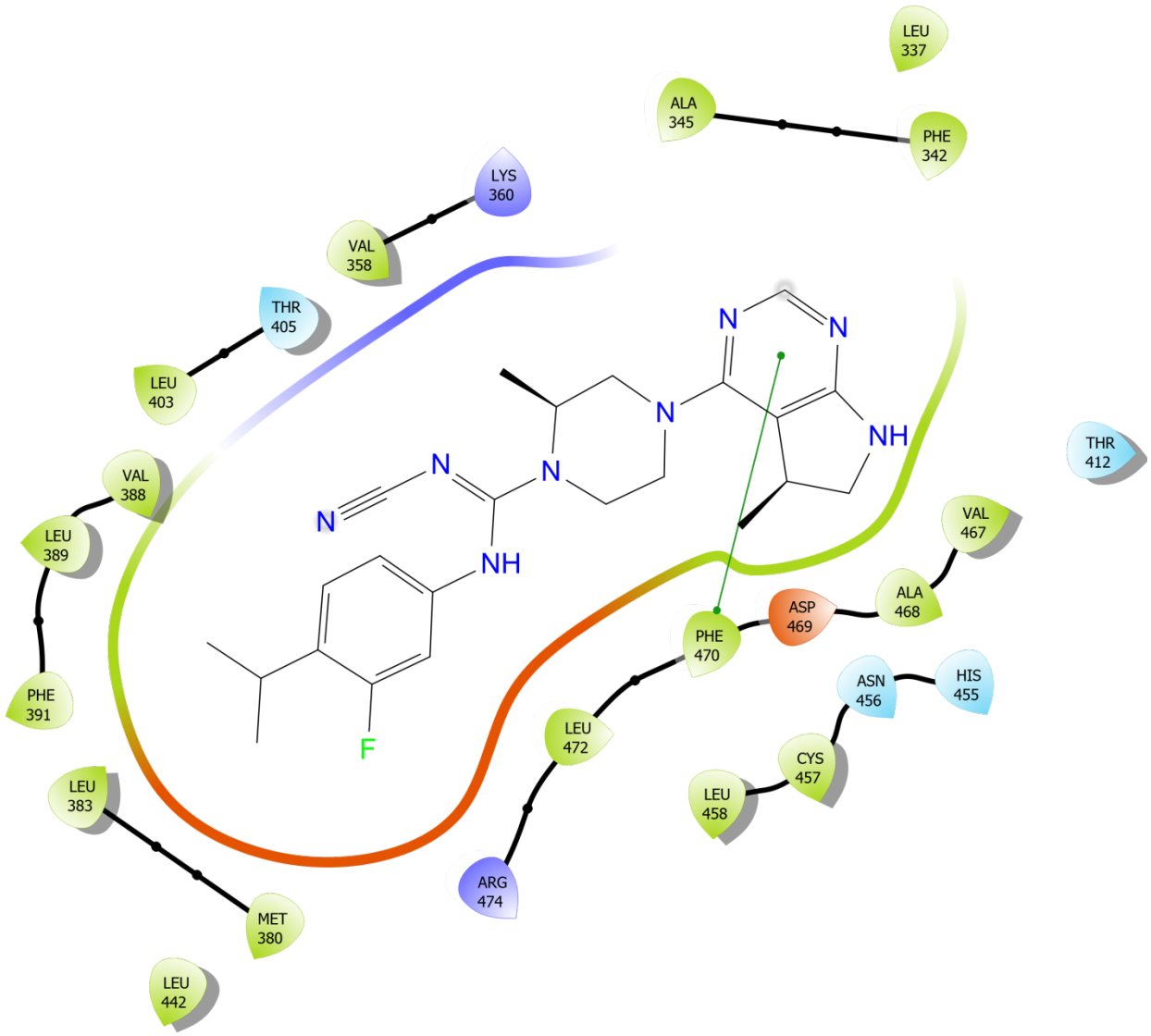


Figure S7. Two-dimensional representation of the interaction between molecule S6 and amino acids inside LIMK2 binding pocket.

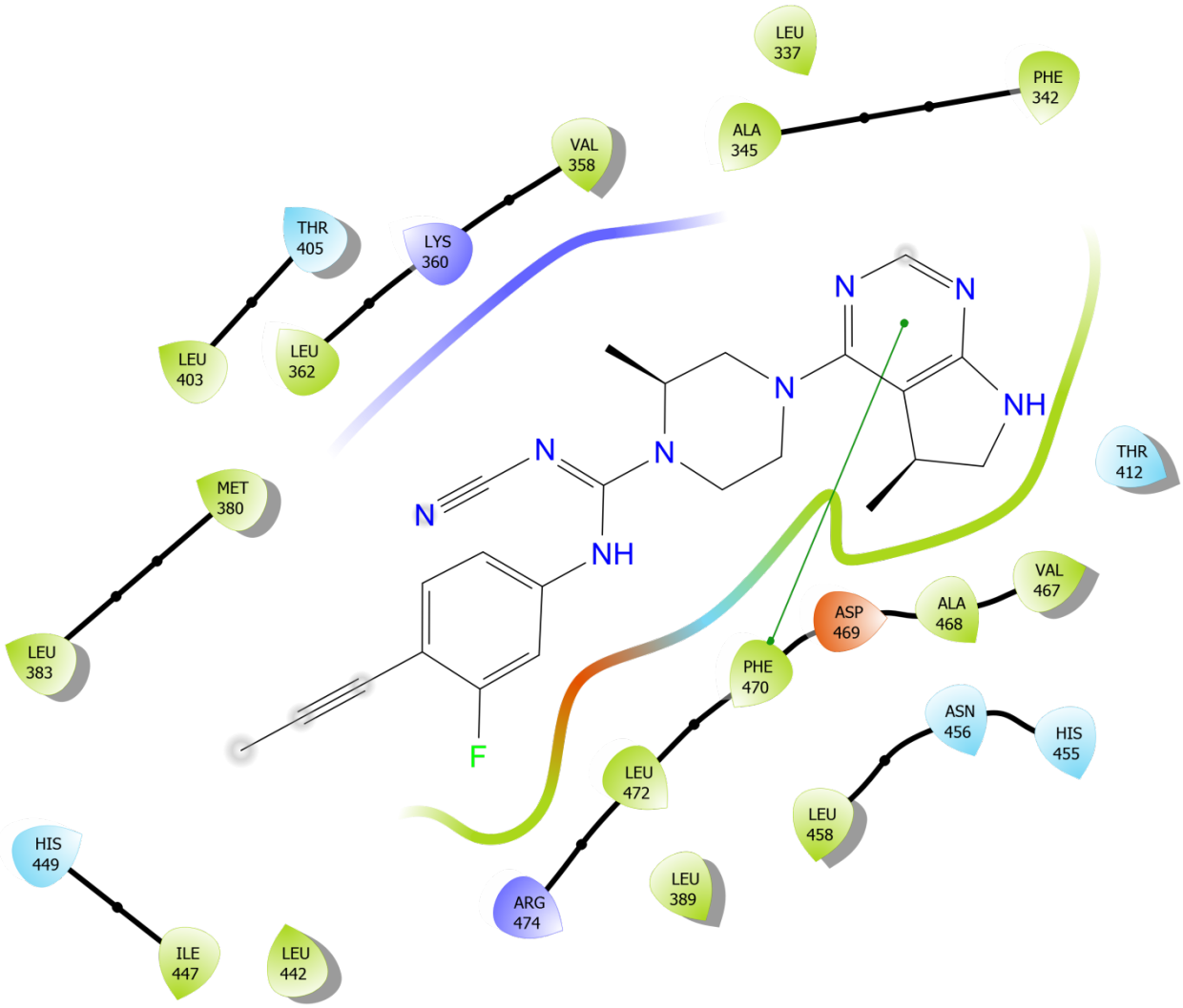


Figure S8. Two-dimensional representation of the interaction between molecule S7 and amino acids inside LIMK2 binding pocket.

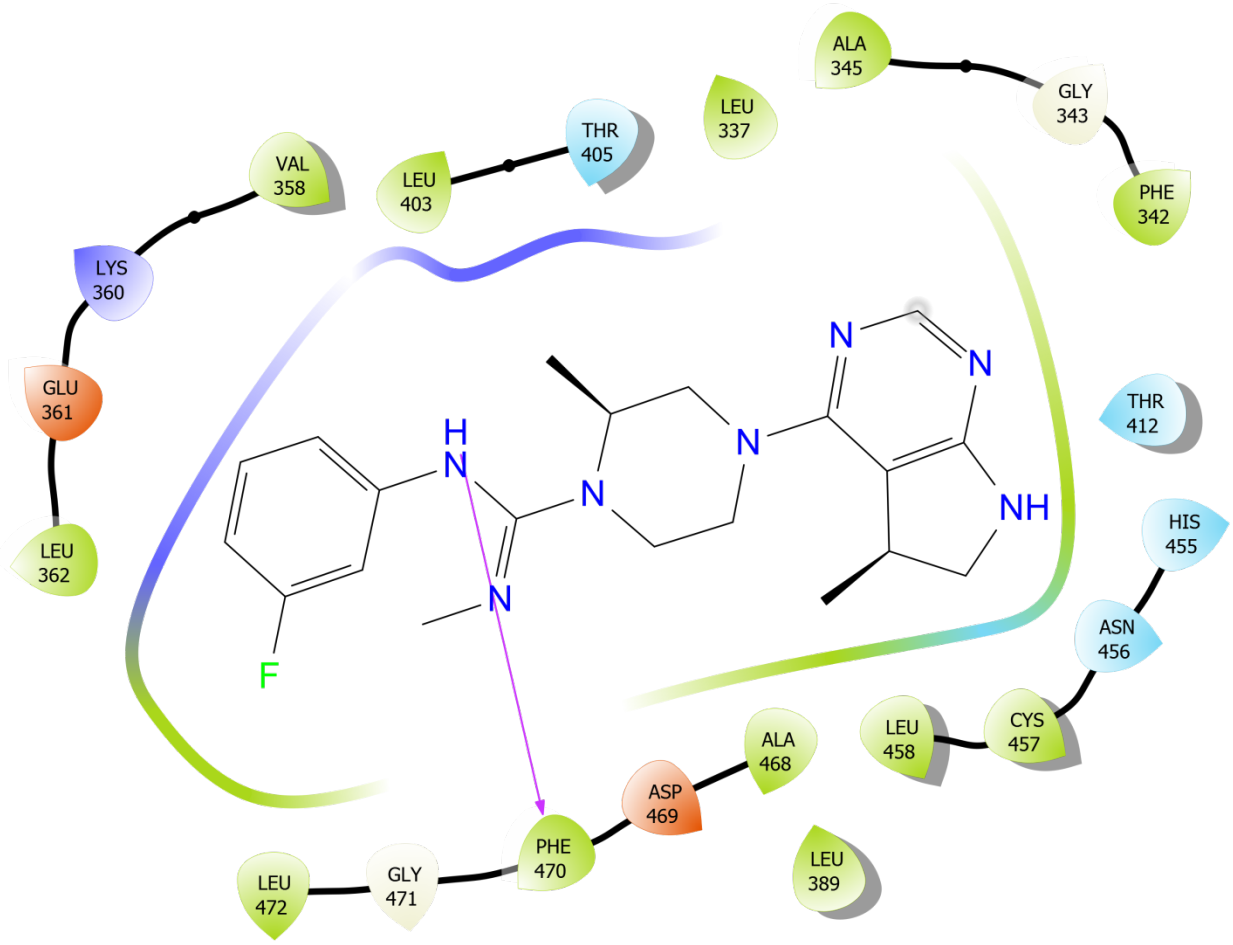


Figure S9. Two-dimensional representation of the interaction between molecule Hy1 and amino acids inside LIMK2 binding pocket.

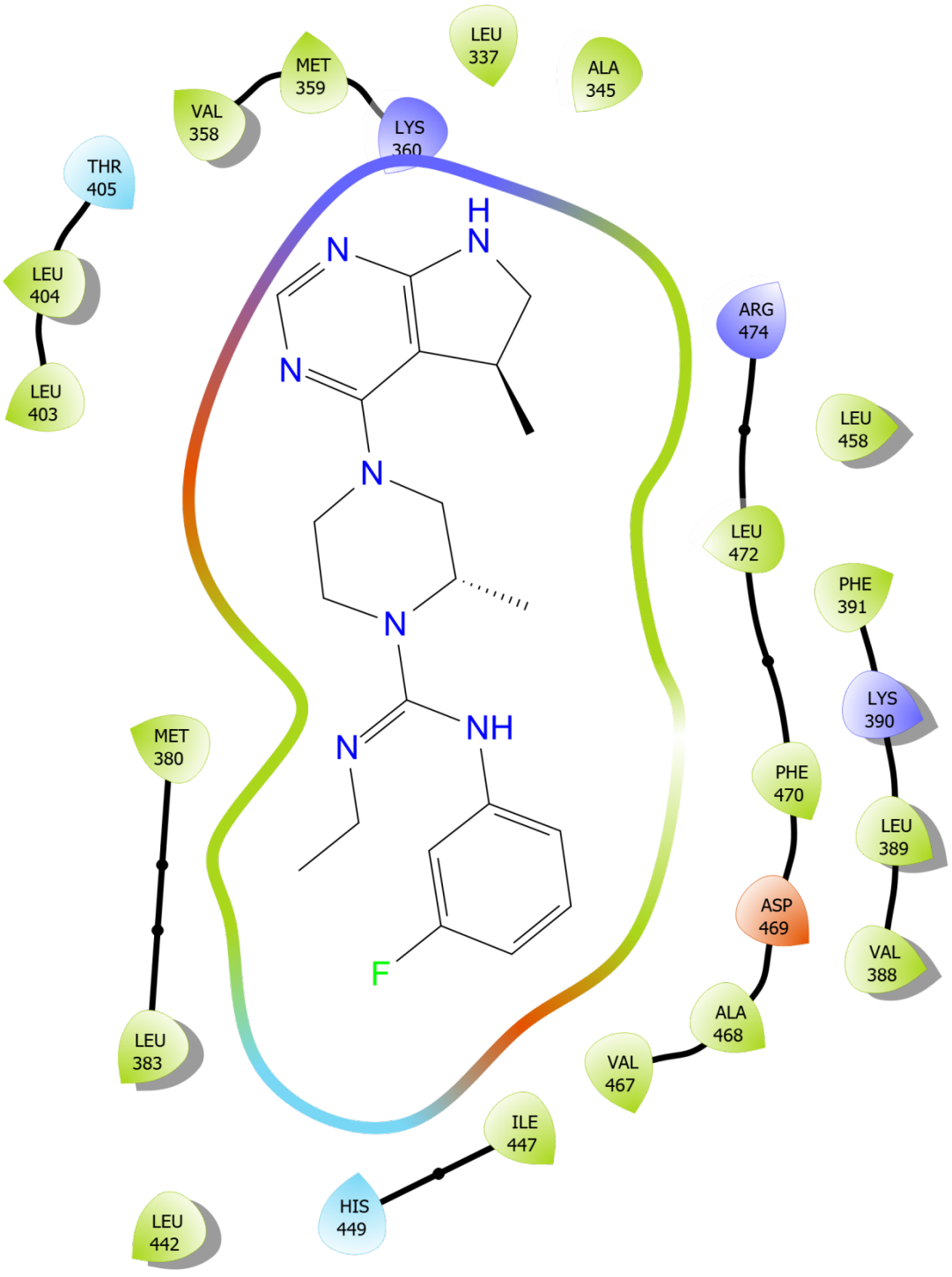


Figure S10. Two-dimensional representation of the interaction between molecule Hy2 and amino acids inside LIMK2 binding pocket.

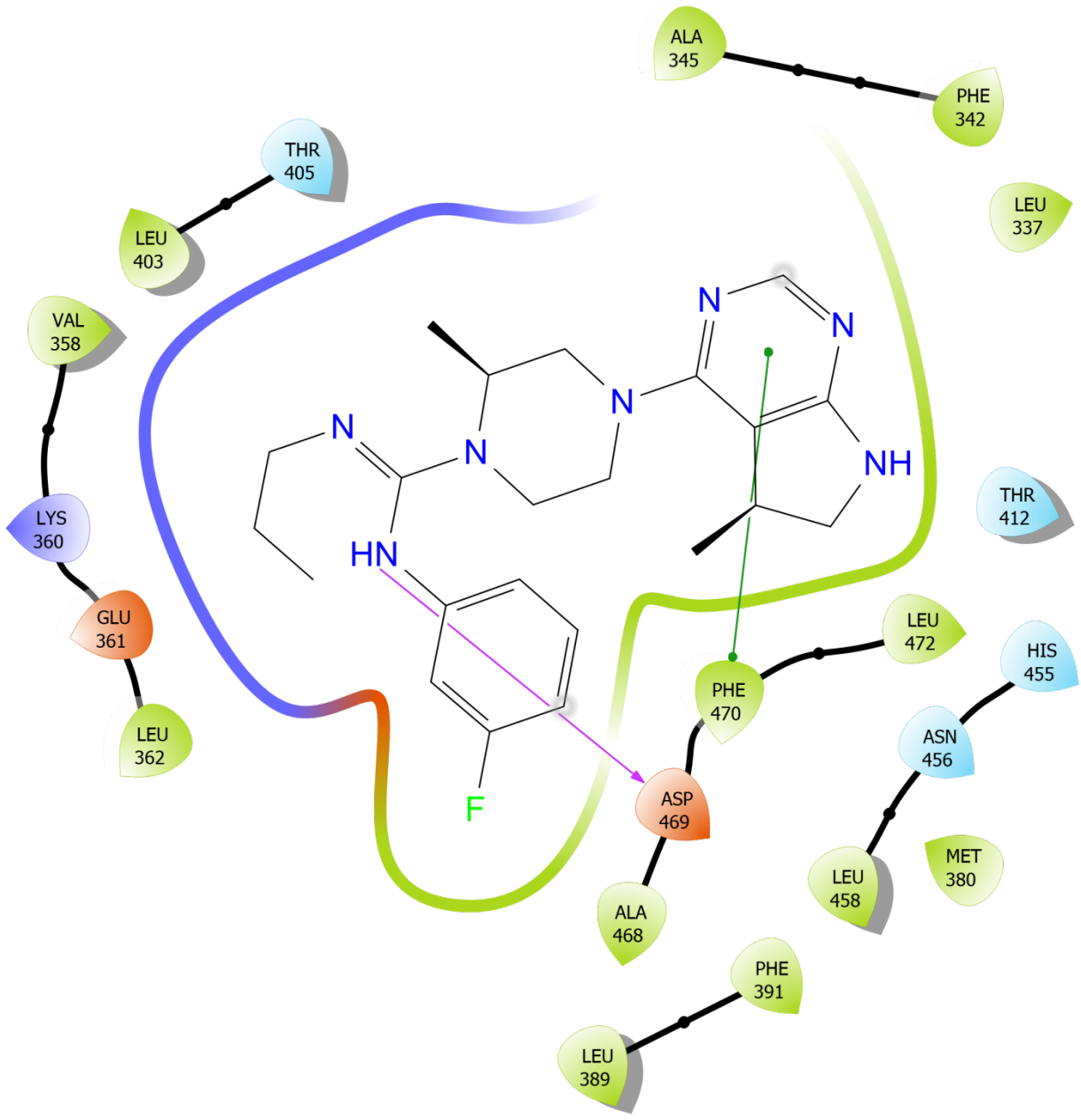


Figure S11. Two-dimensional representation of the interaction between molecule Hy3 and amino acids inside LIMK2 binding pocket.

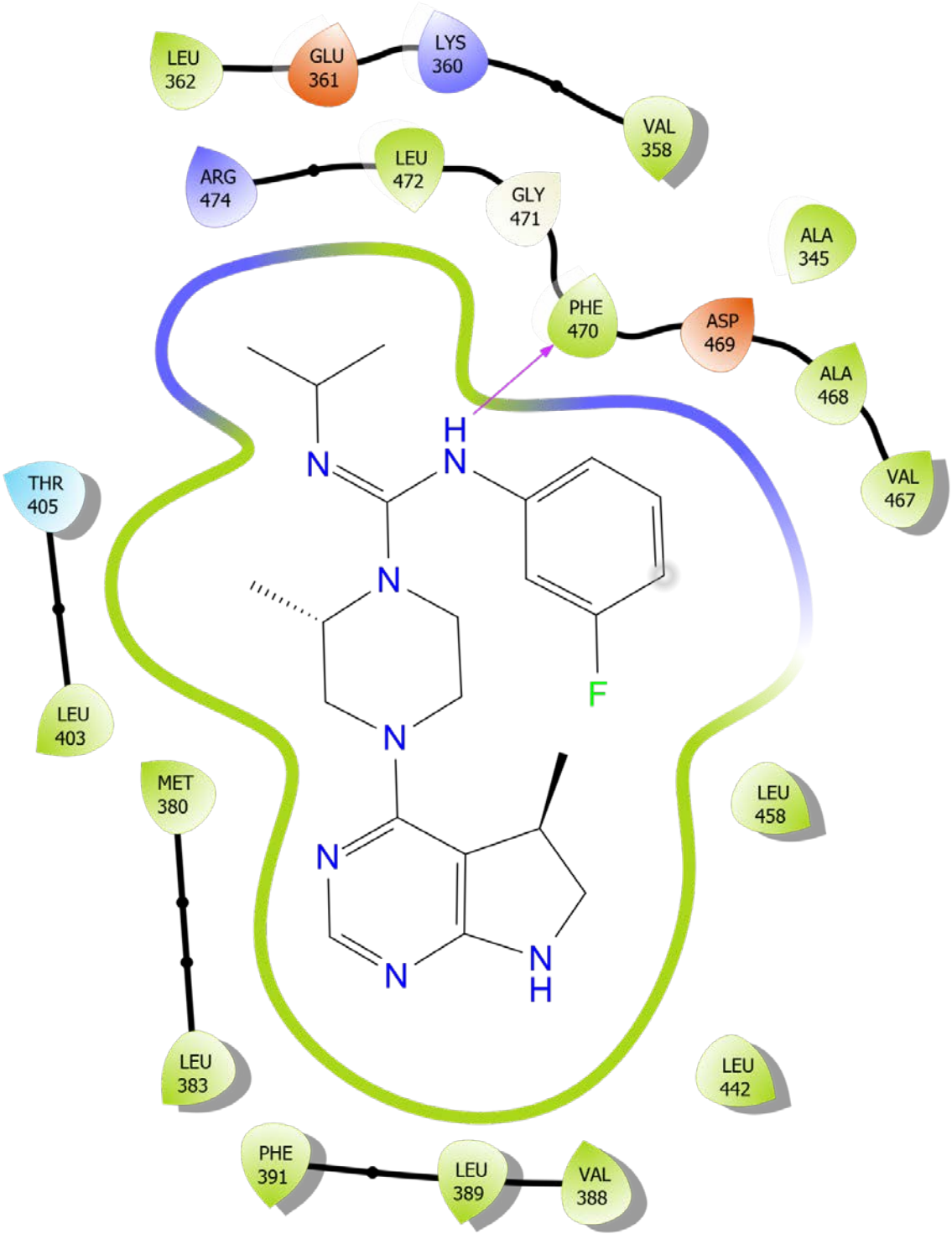


Figure S12. Two-dimensional representation of the interaction between molecule Hy4 and amino acids inside LIMK2 binding pocket.

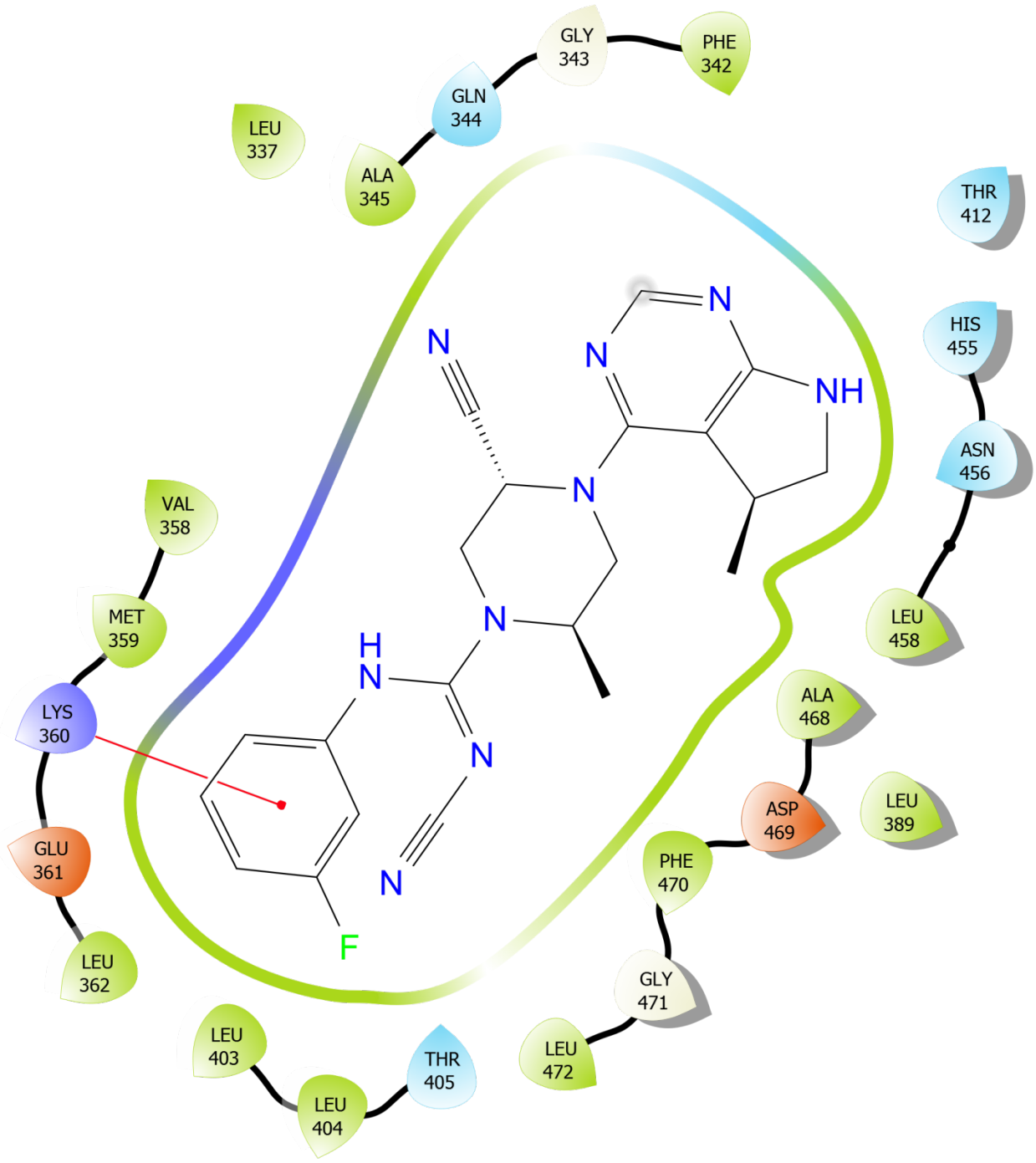


Figure S13. Two-dimensional representation of the interaction between molecule HA1 and amino acids inside LIMK2 binding pocket.

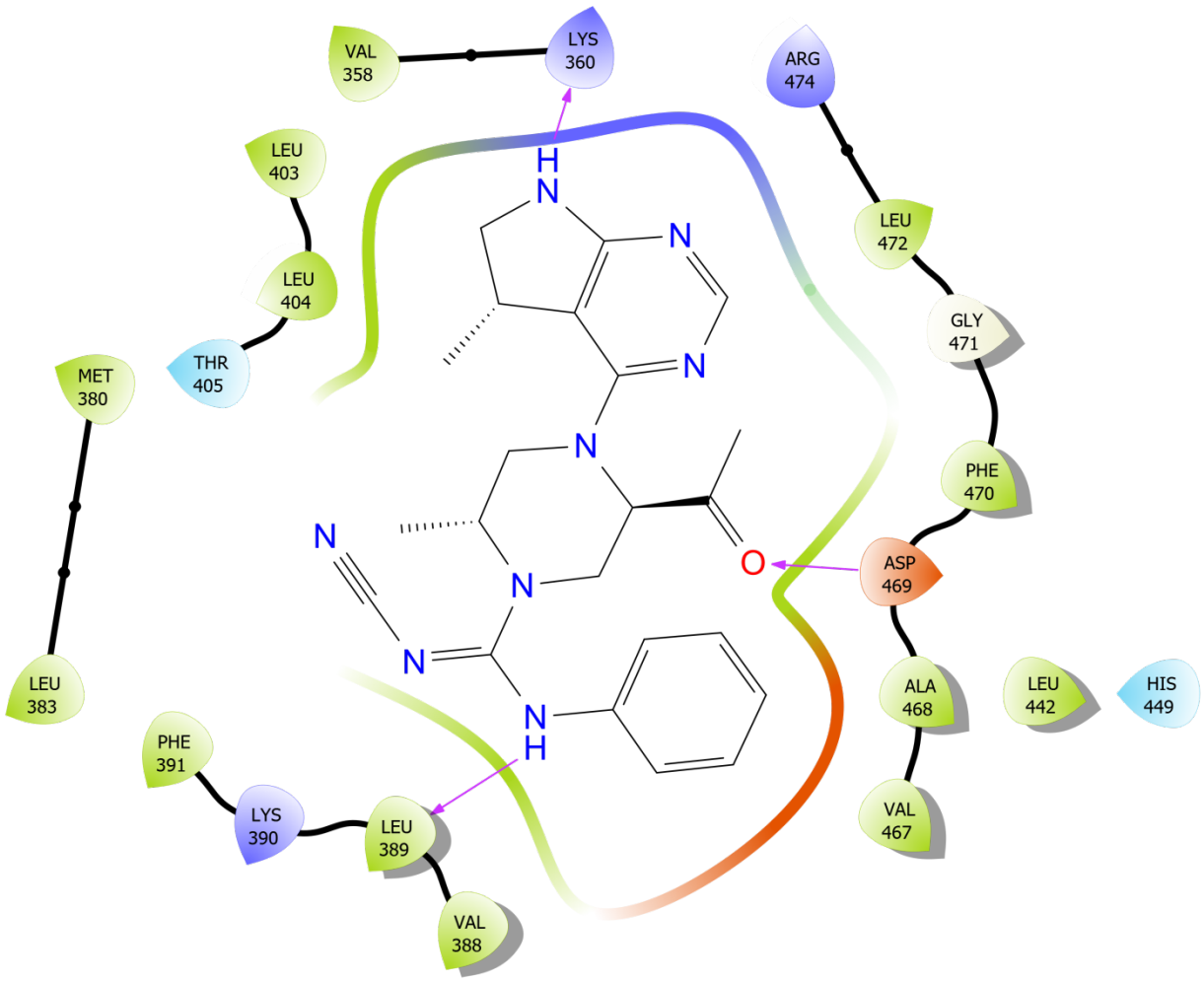


Figure S14. Two-dimensional representation of the interaction between molecule HA2 and amino acids inside LIMK2 binding pocket.

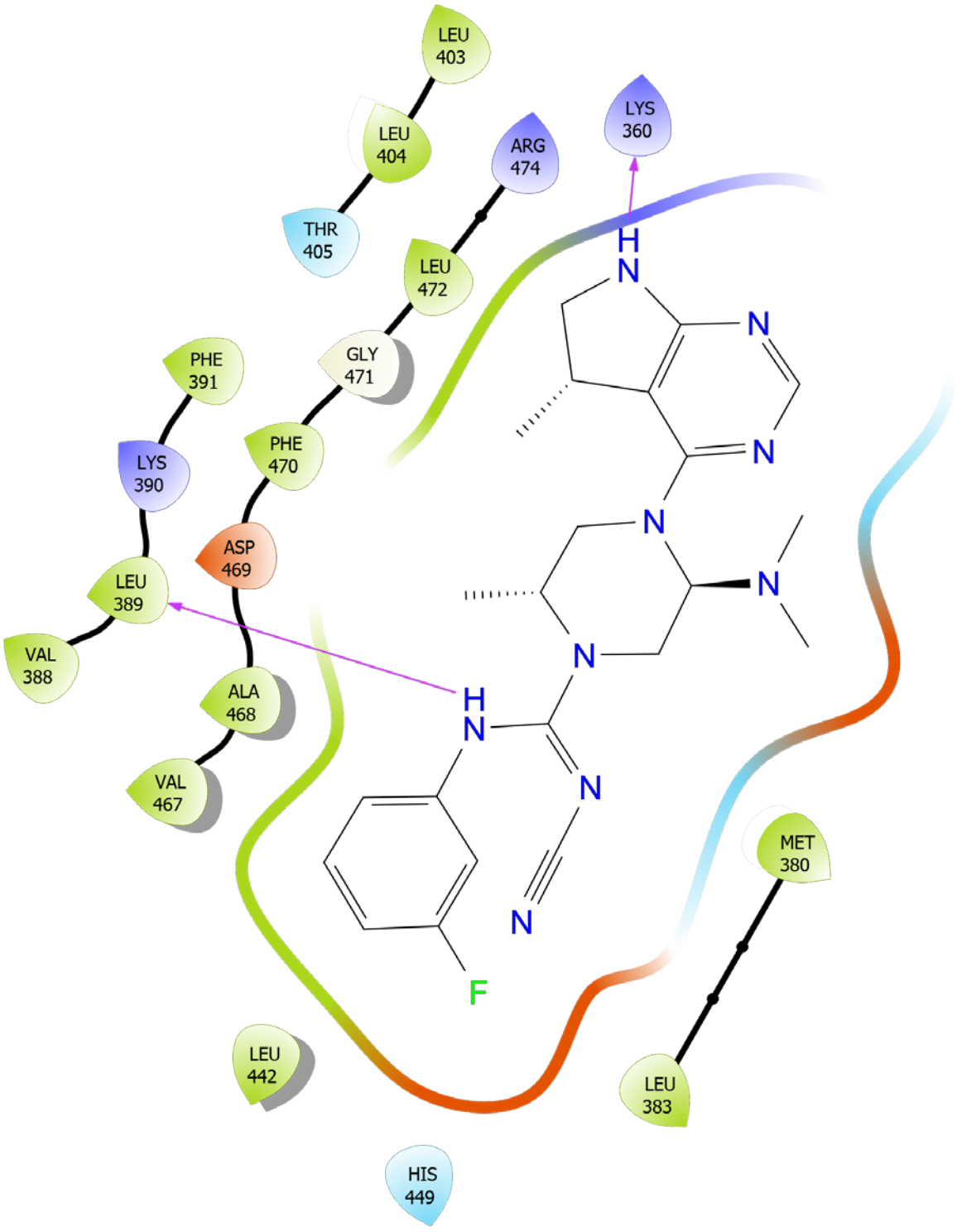


Figure S15. Two-dimensional representation of the interaction between molecule HA3 and amino acids inside LIMK2 binding pocket.

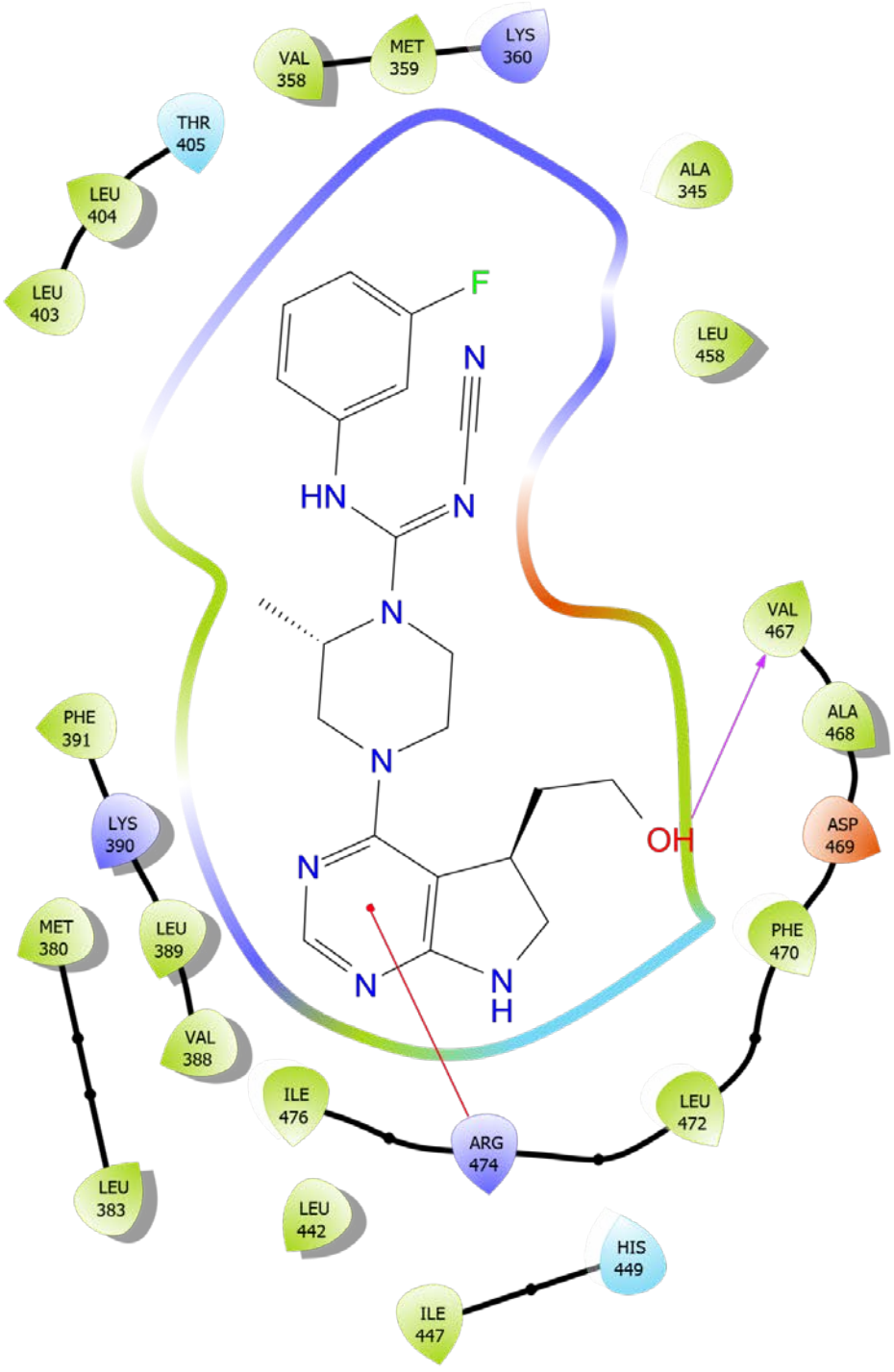


Figure S16. Two-dimensional representation of the interaction between molecule HD1 and amino acids inside LIMK2 binding pocket.