

Parallel Multi-swarm Cooperative Particle Swarm Optimization for protein-ligand docking and virtual screening

Chao Li¹, Jinxing Li¹, Jun Sun*¹, Li Mao¹, Vasile Palade², Bilal Ahmad¹

¹ Department of Computer Science and Technology, Jiangnan University, No.1800, Lihu Avenue, Wuxi, Jiangsu, 214122, People's Republic of China

² Center for Computational Science and Mathematical Modeling, Coventry University, Priory Street, Coventry, CV15FB, UK

More Details for Figure 1

The original optimization population in PSO of PSOVina, shown in the left black dotted box, consists of multiple subswarms of N particles. The quantity of subswarms is equal to Exhaustiveness value, and different subswarms are expressed as differently colored columns. The right part of figure displays our optimization population, which is composed of slave subswarms of N particles and a master subswarm with m particles. The master subswarm is the $(\text{Exhaustiveness}+1)$ -th subswarm that is newly added and shown as red color.

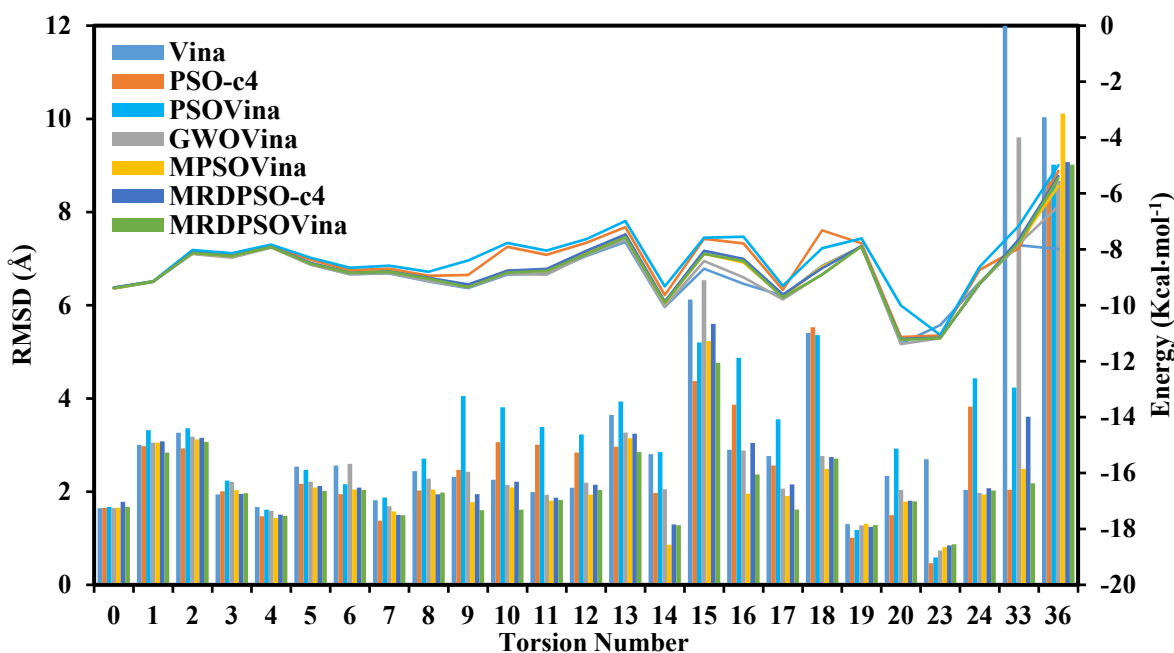


Figure S1. The average RMSD and energy comparison of molecules with different torsions.

Table S1. The scored-energy of 285 test cases obtained by all compared docking programs

		Scored-Energy (Kcal·mol ⁻¹)						
PDB	ntor	Vina	PSO-c4	PSOVina	GWOVi	MPSOVi	MRDPS	MRDPS
					na	na	O-c4	OVina
3jya	0	-8.29	-8.26952	-8.23285	-8.25906	-8.26704	-8.27321	-8.25564
3udh	0	-7.6	-7.60711	-7.60686	-7.60628	-7.60601	-7.5183	-7.60686
4kzu	0	-12.3	-12.2985	-12.3011	-12.2987	-12.3	-12.2989	-12.3003
Average		-9.39667	-9.39171	-9.38027	-9.38801	-9.39103	-9.36347	-9.38758

1bcu	1	-7.5	-7.46477	-7.46625	-7.4637	-7.4639	-7.46458	-7.46436
1gpn	1	-10.88	-10.8516	-10.8513	-10.8513	-10.8495	-10.8518	-10.8516
2xys	1	-11.2	-11.1769	-11.1794	-11.173	-11.1765	-11.1767	-11.1711
3arv	1	-11	-10.9313	-10.9515	-10.964	-10.9491	-10.9564	-10.9569
3rsx	1	-7.8	-7.83536	-7.74313	-7.83371	-7.81408	-7.83302	-7.83496
4ddk	1	-6.61	-6.63366	-6.63074	-6.63062	-6.63414	-6.63377	-6.63648
Average		-9.165	-9.14893	-9.13705	-9.15273	-9.14785	-9.1527	-9.15256
<hr/>								
1c5z	2	-5.8	-5.76589	-5.76628	-5.76831	-5.76748	-5.76579	-5.7665
1o5b	2	-6.6	-6.55485	-6.55505	-6.56257	-6.56305	-6.56358	-6.532
1r5y	2	-7.4	-7.22581	-6.97486	-7.41181	-7.41542	-7.41358	-7.28528
1s38	2	-7.8	-7.8254	-7.42735	-7.81165	-7.80843	-7.62361	-7.80763
2iwx	2	-9	-9.01123	-9.01122	-9.01161	-9.01155	-9.01125	-9.01126
2weg	2	-6.2	-6.13675	-5.83276	-6.18656	-6.13358	-6.0295	-6.10743
2yki	2	-15.56	-16.5619	-16.4941	-16.5621	-16.563	-16.5466	-16.5575
3ary	2	-7.72	-7.49516	-7.36808	-7.70964	-7.62023	-7.59803	-7.64732
3g2z	2	-6.87	-6.19426	-6.22541	-6.85998	-6.59252	-6.66449	-6.56383
3gv9	2	-5.3	-4.90624	-4.8928	-5.34351	-5.2288	-5.13603	-5.29462
3kr8	2	-12	-11.9951	-11.9959	-11.9985	-11.998	-11.9987	-11.9988
3pxf	2	-10.3	-10.2837	-10.1745	-10.2039	-10.175	-10.1976	-10.2746
3twp	2	-5.5	-5.39845	-5.36154	-5.47726	-5.42926	-5.39513	-5.4488
3u5j	2	-8.7	-8.70849	-8.70784	-8.70985	-8.708	-8.57734	-8.70706
3zt2	2	-9.73	-9.73857	-9.5749	-9.7661	-9.75194	-9.75348	-9.73996
4f09	2	-8.1	-8.13877	-8.13727	-8.13669	-8.13856	-8.13868	-8.13981
4gfm	2	-7.81	-7.83044	-7.82084	-7.83062	-7.83549	-7.83215	-7.83453
4jsz	2	-5.28	-5.17107	-5.15606	-5.25978	-5.12507	-5.19935	-5.14348
4k77	2	-8.14	-8.13781	-8.05314	-8.21151	-8.16446	-8.14816	-8.1801
4kzq	2	-11.11	-11.1449	-11.1445	-11.1409	-11.1432	-11.1319	-11.1411
4mme	2	-10.3	-10.2632	-10.2651	-10.2629	-10.2674	-10.2644	-10.2654
4owm	2	-5.4	-5.3701	-5.34065	-5.38479	-5.38417	-5.37965	-5.36773
4u4s	2	-6.3	-6.22296	-6.21874	-6.28802	-6.28241	-6.28347	-6.24
Average		-8.12696	-8.09048	-8.02169	-8.1695	-8.13509	-8.11532	-8.13282
<hr/>								
1e66	3	-12.1	-12.121	-12.1181	-12.1179	-12.1185	-12.1176	-12.1187
1gpk	3	-9.9	-9.92557	-9.92391	-9.924	-9.92458	-9.92432	-9.924
1qkt	3	-10.4	-10.353	-10.353	-10.3533	-10.3525	-10.3519	-10.353
1uto	3	-4.6	-4.54623	-4.49948	-4.57161	-4.56247	-4.56223	-4.5736
1ydr	3	-8.19	-8.15067	-8.11365	-8.15346	-8.1543	-8.15287	-8.1519
2pog	3	-10.3	-10.2654	-10.2662	-10.2655	-10.2658	-10.265	-10.2651
2wer	3	-8.8	-8.7669	-8.7669	-8.7692	-8.7669	-8.76702	-8.76695
3acw	3	-10.95	-10.9425	-10.9472	-10.9491	-10.9403	-10.9446	-10.9504
3ao4	3	-7.45	-7.30944	-7.13426	-7.44897	-7.43175	-7.43742	-7.36924
3bgz	3	-10.9	-10.9225	-10.9203	-10.9218	-10.9206	-10.9234	-10.9228
3g31	3	-5	-4.71843	-4.73352	-4.96841	-4.9662	-4.86076	-4.91351
3gy4	3	-6.13	-6.05207	-6.05336	-6.28246	-6.07903	-6.05776	-6.0551
3kgp	3	-5.7	-5.74779	-5.73657	-5.75245	-5.74974	-5.73044	-5.72357
3pyy	3	-9.1	-9.12769	-9.00722	-9.13391	-9.01559	-9.12447	-9.1197
3wtj	3	-7	-6.95947	-6.94649	-7.00029	-6.98699	-6.85266	-6.974
4cr9	3	-6.7	-6.70902	-6.67282	-6.69373	-6.71108	-6.66646	-6.70688
4de1	3	-8.38	-7.68563	-7.26008	-8.39775	-7.89639	-8.01829	-7.98866
4de3	3	-8.51	-8.58176	-8.1759	-8.48106	-8.61127	-8.41018	-8.43118
4e6q	3	-9.8	-9.76467	-9.75671	-9.80233	-9.79333	-9.78109	-9.78558
4ih5	3	-6.8	-6.43544	-6.47873	-6.74163	-6.55033	-6.53598	-6.60411

4j21	3	-11.6	-11.5588	-11.5593	-11.5591	-11.5585	-11.5573	-11.5591
4llx	3	-4.99	-5.07883	-5.06882	-5.16545	-5.10303	-5.08622	-5.09951
4m0y	3	-9.3	-9.0704	-8.7842	-9.33128	-9.32491	-9.23531	-9.15163
5c28	3	-6.2	-6.00667	-6.02266	-6.18457	-6.1842	-6.13085	-6.18666
Average		-8.28333	-8.19999	-8.13747	-8.29038	-8.24868	-8.22892	-8.23728
1q8u	4	-8.4	-8.36952	-8.36944	-8.36887	-8.36832	-8.37007	-8.3687
1syi	4	-9.1	-9.12155	-9.12203	-9.12595	-9.12655	-9.12263	-9.1268
2al5	4	-8.88	-8.9164	-8.91663	-8.9145	-8.91715	-8.91995	-8.91633
2cbv	4	-7.13	-7.04962	-7.13332	-7.20412	-7.20493	-7.13252	-7.1341
2hb1	4	-6.39	-6.04744	-5.51219	-6.35967	-6.28005	-6.35918	-6.3261
2j7h	4	-6.2	-6.19865	-6.12374	-6.20177	-6.20203	-6.20106	-6.19856
2v00	4	-7.8	-7.77035	-7.53086	-7.78857	-7.78033	-7.78299	-7.63238
2wnc	4	-8.3	-8.31595	-8.24443	-8.29199	-8.29072	-8.29627	-8.31868
2wtv	4	-11.6	-11.6002	-11.5914	-11.6086	-11.5952	-11.5981	-11.6015
2ymd	4	-7.28	-7.447	-7.44726	-7.44487	-7.44664	-7.44813	-7.43972
3b27	4	-6.9	-6.92359	-6.83008	-6.92074	-6.92377	-6.9218	-6.9212
3dx1	4	-6.8	-6.46587	-6.58486	-6.76469	-6.76519	-6.67473	-6.76539
3f3a	4	-8.09	-8.05785	-7.97932	-8.06144	-8.06771	-8.05858	-8.06021
3f3c	4	-7.9	-7.93822	-7.93821	-7.94406	-7.93732	-7.94015	-7.93776
3g0w	4	-10.9	-10.8591	-10.8609	-10.8606	-10.8601	-10.8627	-10.8622
3gr2	4	-5.9	-5.6737	-5.68184	-5.88767	-5.8108	-5.78098	-5.73078
3lka	4	-6.7	-6.62651	-6.65382	-6.72338	-6.74076	-6.7364	-6.69093
3n7a	4	-7.52	-7.56905	-7.5723	-7.5655	-7.5887	-7.56554	-7.57401
3qqs	4	-8.66	-8.58994	-8.59781	-8.66239	-8.591	-8.6465	-8.57492
3rr4	4	-8.1	-7.9968	-7.64063	-8.07222	-8.09455	-8.10659	-8.10022
3u8k	4	-7.1	-7.06323	-7.05988	-7.06115	-7.06479	-7.06662	-7.06609
3u8n	4	-7.41	-7.41107	-7.44145	-7.43965	-7.44079	-7.44139	-7.43621
4abg	4	-5.79	-5.5877	-5.51668	-5.76142	-5.6679	-5.6694	-5.66892
4ddh	4	-7.3	-7.15163	-7.05609	-7.27309	-7.23213	-7.22529	-7.22062
4dli	4	-10	-10.0343	-10.0347	-10.0355	-10.0372	-10.0376	-10.0332
4hge	4	-8.7	-8.91181	-8.73777	-8.68858	-8.68988	-8.70169	-8.83495
4ivb	4	-9.7	-9.73716	-9.73703	-9.73767	-9.73714	-9.73724	-9.73744
4j28	4	-7.3	-7.29096	-7.2609	-7.28704	-7.29021	-7.21993	-7.29103
Average		-7.92321	-7.88304	-7.8277	-7.93056	-7.91971	-7.91514	-7.91318
1nc3	5	-9.8	-9.78649	-9.78955	-9.78907	-9.78733	-9.78737	-9.78551
1o3f	5	-8.89	-8.64203	-7.94988	-8.89972	-8.88383	-8.77963	-8.86436
1oyt	5	-10.92	-10.9491	-10.9275	-10.9442	-10.9499	-10.9469	-10.9484
1p1n	5	-8.1	-8.10344	-8.09713	-8.10207	-8.09556	-8.08923	-8.09321
1p1q	5	-7.49	-7.43261	-7.3891	-7.49853	-7.48918	-7.47788	-7.47491
1ps3	5	-8.2	-7.99013	-8.19479	-8.19505	-8.19479	-8.19553	-8.19695
1q8t	5	-7.8	-7.77236	-7.71928	-7.81643	-7.77798	-7.78384	-7.79713
2r9w	5	-10.24	-9.35382	-8.7688	-10.2573	-9.82737	-9.6752	-9.64525
2wn9	5	-8.3	-7.42704	-7.44785	-8.33629	-7.7272	-8.03733	-8.03596
2xj7	5	-8.61	-8.64526	-8.64629	-8.64618	-8.64578	-8.64752	-8.64713
3d4z	5	-7.15	-6.28014	-6.5027	-7.14562	-7.16821	-6.85787	-7.14621
3d6q	5	-6.6	-6.57576	-6.1232	-6.53028	-6.58775	-6.45726	-6.63585
3dd0	5	-6.3	-6.2298	-5.92896	-6.28692	-6.28446	-6.27871	-6.27931
3fcq	5	-5.5	-5.54807	-5.47024	-5.63951	-5.62015	-5.61545	-5.60651
3fur	5	-11.31	-11.5196	-11.6039	-11.6574	-11.6649	-11.6597	-11.6597
3gbb	5	-9.43	-9.45707	-9.46941	-9.4494	-9.44801	-9.42094	-9.46752
3jvr	5	-7.69	-7.20982	-6.68433	-7.69953	-7.69929	-7.57968	-7.6832

3qgy	5	-9.51	-9.40725	-9.27442	-9.54179	-9.51511	-9.47585	-9.52262
3rlr	5	-8.9	-8.58633	-8.74304	-8.87756	-8.87481	-8.75266	-8.867
3ryj	5	-7.3	-7.25446	-7.18163	-7.2816	-7.2313	-7.27255	-7.24871
3uuo	5	-7.71	-7.74798	-7.74179	-7.74851	-7.74582	-7.73714	-7.74563
4e5w	5	-10.1	-9.80644	-9.76004	-10.0812	-10.0838	-10.0808	-10.0793
4f9w	5	-10	-9.8464	-9.774	-9.97033	-9.9744	-9.87054	-9.97852
4gkm	5	-8.4	-8.40208	-8.5217	-8.40451	-8.46939	-8.43613	-8.4588
4ih7	5	-7	-6.97604	-6.98075	-6.97559	-6.97373	-6.97704	-6.97334
4ivc	5	-9.7	-9.71705	-9.67261	-9.72137	-9.71971	-9.71649	-9.71777
4k18	5	-10.8	-10.5182	-10.5216	-10.8264	-10.8281	-10.7022	-10.7513
4kz6	5	-5.7	-5.60171	-5.36857	-5.74245	-5.63413	-5.65212	-5.68613
4m0z	5	-10.9	-10.8914	-10.8867	-10.8836	-10.8853	-10.8847	-10.8899
4mgd	5	-8.61	-8.59521	-8.6026	-8.63175	-8.59509	-8.6056	-8.60029
4pcs	5	-7.2	-7.18022	-7.1805	-7.20298	-7.17984	-7.18893	-7.18418
4qac	5	-11.27	-11.257	-11.2583	-11.255	-11.2549	-11.2515	-11.258
5aba	5	-6	-5.50487	-5.63886	-6.05027	-5.90943	-6.05498	-6.03658
Average		-8.52818	-8.37016	-8.29758	-8.54813	-8.50686	-8.48331	-8.5141
1owh	6	-14	-13.9689	-13.9809	-13.9819	-13.9716	-8.20316	-13.9798
1pxn	6	-8.4	-8.28315	-8.15497	-8.39977	-8.35793	-8.84503	-8.29865
1w4o	6	-8.8	-8.82301	-8.79289	-8.84449	-8.83753	-6.68985	-8.84237
2brb	6	-6.7	-6.66241	-6.64869	-6.66858	-6.68248	-8.12552	-6.68962
2c3i	6	-8.19	-8.1316	-8.04439	-8.19753	-8.0966	-8.90511	-8.14736
2j78	6	-9	-8.74204	-8.74661	-9.03127	-8.91014	-6.60524	-8.92039
2p15	6	-6.6	-6.43966	-6.27502	-6.58394	-6.58713	-13.8019	-6.61557
2qe4	6	-13.8	-13.8078	-13.7999	-13.8046	-13.8003	-9.74897	-13.8044
2xnb	6	-9.73	-9.75173	-9.75317	-9.7535	-9.75014	-10.3112	-9.75153
3dx2	6	-10.36	-10.1086	-9.91056	-10.3644	-10.3269	-6.7059	-10.3393
3dxg	6	-6.7	-6.26076	-5.84109	-6.70755	-6.61835	-6.3781	-6.59523
3e93	6	-6.4	-6.20367	-6.11646	-6.41952	-6.34732	-13.9824	-6.36939
3ebp	6	-9.7	-9.67356	-9.53204	-9.67169	-9.68303	-9.68086	-9.67528
3f3d	6	-5.8	-5.72966	-5.75522	-5.77437	-5.77832	-5.77343	-5.77542
3f3e	6	-6.3	-6.28565	-6.27669	-6.30987	-6.28849	-6.31853	-6.29449
3gc5	6	-9.6	-9.20643	-9.34282	-9.56467	-9.51414	-9.39069	-9.56615
3k5v	6	-9.9	-9.59632	-9.45976	-9.92882	-9.72818	-9.74431	-9.74361
3l7b	6	-9	-8.97908	-8.98119	-8.97765	-8.97889	-8.97916	-8.9785
3r88	6	-5.74	-5.53506	-5.47735	-5.69035	-5.63997	-5.65395	-5.62654
3syr	6	-9.9	-9.85903	-9.873	-9.85512	-9.85572	-9.85741	-9.85799
3ui7	6	-8.25	-8.2445	-8.20235	-8.24405	-8.24221	-8.24405	-8.24092
3uo4	6	-10.51	-9.85932	-9.86061	-10.6259	-10.1595	-10.1499	-10.0668
4bkt	6	-6.3	-6.31962	-6.32087	-6.31832	-6.3183	-6.31804	-6.31904
4ivd	6	-9.2	-8.80283	-8.25284	-9.23258	-9.0287	-9.08683	-9.09033
4jxs	6	-7.76	-7.17632	-6.77967	-7.6696	-7.59889	-7.60131	-7.51106
4rfm	6	-11.28	-11.3399	-11.3128	-11.2247	-11.3107	-11.3558	-11.316
4twp	6	-10.22	-10.3481	-10.0938	-10.2065	-10.19	-10.2094	-10.1525
5dwr	6	-10.8	-10.7518	-10.8365	-10.8357	-10.8365	-10.7493	-10.8365
Average		-8.89071	-8.74609	-8.65794	-8.88882	-8.83707	-8.83626	-8.83588
1nc1	7	-11.9	-11.9089	-11.9087	-11.9061	-11.9077	-8.32361	-11.9095
1y6r	7	-8.3	-8.32621	-8.32028	-8.3265	-8.32337	-9.66642	-8.32543
1yc1	7	-9.7	-9.65148	-9.64567	-9.66855	-9.66789	-9.81279	-9.66953
1z9g	7	-9.8	-9.81272	-9.8081	-9.81302	-9.82651	-6.14816	-9.80513
2fvd	7	-6.49	-6.06435	-5.8485	-6.61097	-6.1458	-8.93241	-6.10223

2vvn	7	-9.6	-8.69969	-8.64405	-9.06458	-8.91618	-7.0978	-9.00642
2w66	7	-7.11	-6.99337	-6.86672	-7.10967	-7.10615	-7.82905	-7.10472
2wvt	7	-7.8	-7.6917	-7.83118	-7.83266	-7.83004	-6.25206	-7.82426
2x00	7	-6.3	-6.25409	-6.1475	-6.30989	-6.30046	-11.9487	-6.28582
2xbv	7	-11.94	-11.9485	-11.9518	-11.9509	-11.9483	-11.4615	-11.9492
2xii	7	-11.55	-11.1617	-9.49142	-11.4898	-10.9771	-10.0228	-11.4661
2zb1	7	-10	-8.40651	-8.87047	-10.0237	-9.78651	-10.654	-10.023
3b65	7	-10.69	-10.6446	-10.5276	-10.6534	-10.6595	-10.817	-10.6463
3cj4	7	-10.9	-10.8232	-10.8453	-10.9075	-10.8695	-7.39012	-10.8391
3e92	7	-7.4	-7.37826	-7.07853	-7.39488	-7.38146	-11.9082	-7.39117
3ehy	7	-7.1	-7.02351	-6.95772	-7.0808	-7.03771	-7.05969	-7.08407
3fv2	7	-10	-9.97594	-9.97331	-9.97726	-9.97733	-9.97922	-9.97833
3g2n	7	-9.39	-9.34365	-9.33366	-9.35281	-9.35382	-9.35264	-9.35261
3nq9	7	-4.69	-4.63875	-4.50094	-4.98555	-4.74939	-4.80566	-4.71219
3up2	7	-9.59	-9.36241	-9.31718	-9.5815	-9.57333	-9.27174	-9.62407
4ciw	7	-8.3	-8.27404	-8.27143	-8.26979	-8.27202	-8.27137	-8.27477
4de2	7	-8.01	-7.81825	-7.28965	-7.99573	-7.68162	-7.81952	-7.95532
4dju	7	-9.6	-9.58869	-9.23744	-9.59389	-9.60469	-9.58446	-9.59814
4eor	7	-9.3	-9.15954	-9.13632	-9.28007	-9.23989	-9.26765	-9.24793
4f2w	7	-9.1	-9.07128	-9.07518	-9.07611	-9.07319	-9.06873	-9.06942
4j3l	7	-11.1	-11.0828	-10.8813	-11.1287	-11.1203	-11.111	-11.1181
4jfs	7	-6.7	-6.66885	-6.69355	-6.67019	-6.67331	-6.67491	-6.67124
4jia	7	-8.96	-8.8085	-8.82962	-8.98562	-8.88692	-8.80071	-8.79059
4lzs	7	-5.6	-5.55197	-5.62659	-5.57974	-5.57877	-5.58377	-5.58312
Average		-8.85931	-8.69425	-8.58309	-8.84896	-8.77479	-8.7902	-8.80717
1bzc	8	-9.58	-9.2907	-9.29824	-9.57493	-9.54229	-9.48724	-9.57632
1sqa	8	-9.15	-9.0641	-8.64812	-9.08128	-8.96849	-9.02452	-9.08259
1ydt	8	-9.43	-8.83232	-8.83935	-9.41968	-8.99485	-8.94906	-9.07899
1z95	8	-10.51	-10.5322	-10.5595	-10.5019	-10.5082	-10.515	-10.545
2br1	8	-8.39	-8.34049	-8.21989	-8.35607	-8.32121	-8.30419	-8.32804
2cet	8	-9.3	-8.99499	-8.61572	-9.28684	-9.02257	-8.97075	-9.12994
2qbr	8	-8.43	-7.55862	-7.27058	-8.36568	-7.90792	-7.93207	-7.83601
2v7a	8	-9.79	-9.71359	-9.69033	-9.76812	-9.76112	-9.75336	-9.74856
2w4x	8	-7.3	-6.86745	-6.45385	-7.30803	-7.30817	-7.31154	-7.30589
2xb8	8	-10.8	-10.7797	-10.7737	-10.7783	-10.777	-10.7811	-10.7749
2xdl	8	-6.1	-6.08654	-6.07731	-6.08684	-6.08565	-6.08682	-6.09063
2zcg	8	-9.64	-9.4346	-9.3216	-9.63721	-9.4555	-9.45424	-9.48936
2zy1	8	-9.67	-9.38045	-9.19475	-9.55818	-9.38109	-9.42659	-9.4942
3aru	8	-6.07	-5.85683	-5.7791	-6.09739	-6.01568	-6.0345	-6.02492
3b5r	8	-11.28	-11.3151	-11.2912	-11.2662	-11.2913	-11.2999	-11.2608
3fv1	8	-9.84	-9.84893	-9.84318	-9.85249	-9.8458	-9.84147	-9.84296
3ge7	8	-10.5	-10.3866	-10.2807	-10.5298	-10.5195	-10.1626	-10.4983
3ivg	8	-10.1	-9.95919	-9.6844	-10.0997	-10.0081	-10.0418	-10.057
3jvs	8	-8	-8.02084	-7.88946	-8.01151	-8.0165	-8.00813	-8.01404
3mss	8	-7.2	-6.95259	-6.47069	-7.17694	-6.9617	-6.93524	-6.98138
3n76	8	-11.49	-11.3717	-11.3832	-11.4215	-11.3931	-11.4035	-11.3967
3n86	8	-12	-11.9754	-11.9784	-12.0098	-12.0059	-12.0104	-12.0035
3p5o	8	-8.8	-8.81417	-8.61884	-8.81687	-8.81087	-8.8114	-8.81078
4dld	8	-8.33	-8.10177	-7.99923	-8.37988	-8.41964	-8.46283	-8.40664
4qd6	8	-8.5	-7.60143	-7.32223	-8.38858	-7.93403	-8.00245	-7.91897
4wiv	8	-7.52	-7.49565	-7.40844	-7.55207	-7.54843	-7.54801	-7.53493
Average		-9.14308	-8.94523	-8.80431	-9.12791	-9.03095	-9.02149	-9.04736

1k1i	9	-9.4	-8.85392	-6.81535	-9.42281	-9.33207	-9.25385	-9.21668
1mq6	9	-9.1	-7.97378	-7.56691	-9.10487	-8.79442	-8.27328	-9.18112
1nvq	9	-11	-10.5388	-10.6745	-11.0075	-10.9777	-10.9583	-10.9957
1o0h	9	-7.38	-6.68022	-6.48533	-7.3113	-7.06881	-6.88655	-7.07213
2y5h	9	-8.07	-7.08436	-6.78019	-8.02842	-7.84423	-7.8312	-7.91711
2zda	9	-9.8	-9.71974	-9.02435	-9.79805	-9.7812	-9.78372	-9.8035
3e5a	9	-9.29	-9.2561	-8.79544	-9.30544	-9.29906	-9.33739	-9.33466
3gnw	9	-11.9	-11.5128	-10.834	-11.863	-11.8669	-11.8609	-11.8696
3u9q	9	-5.97	-5.75348	-5.65895	-6.00385	-5.87555	-5.87686	-5.84438
3wz8	9	-9.67	-9.52732	-8.84898	-9.61244	-9.5107	-9.51965	-9.60745
4cra	9	-10.01	-9.78162	-9.35427	-10.0355	-9.93149	-10.0466	-9.95451
4crc	9	-10.28	-10.098	-9.1046	-10.1858	-10.2842	-10.2022	-10.1981
4f3c	9	-9.23	-9.51842	-9.525	-9.53531	-9.56602	-9.55466	-9.54251
4ty7	9	-9.89	-8.74073	-8.65331	-9.87669	-9.72367	-9.79534	-9.91904
4w9i	9	-8.21	-8.03223	-7.28034	-8.28248	-8.23749	-8.26265	-8.26237
4x6p	9	-10.97	-9.61853	-8.98706	-10.4523	-10.7627	-10.6461	-10.944
Average		-9.38563	-8.91813	-8.39929	-9.36412	-9.30351	-9.25558	-9.35393
1z6e	10	-10.6	-9.20324	-7.75206	-10.1546	-10.5722	-10.5749	-10.5601
2qbp	10	-9.24	-7.65925	-7.30091	-9.30579	-8.8589	-8.92089	-9.04894
2qnq	10	-10.3	-10.3253	-10.0307	-10.3252	-10.3267	-10.3241	-10.3244
3arq	10	-10.68	-10.1466	-10.2676	-10.6827	-10.5164	-10.5806	-10.6021
3ejr	10	-8.48	-7.0598	-7.24718	-8.51997	-8.0984	-8.45703	-8.32564
3nx7	10	-6.96	-6.67223	-6.49396	-6.93889	-6.71907	-6.67865	-6.62326
3oe4	10	-10.6	-7.41483	-8.37713	-10.5914	-10.1405	-9.67159	-10.5822
3ozt	10	-10.7	-9.03406	-9.73413	-10.7121	-10.701	-10.6917	-10.6477
3zdg	10	-5.2	-5.15984	-5.17233	-5.16467	-5.16752	-5.16674	-5.16258
3zsx	10	-7.78	-7.37424	-7.01964	-8.04837	-7.97284	-7.98541	-7.95364
4w9c	10	-7.4	-6.9232	-6.08717	-7.22885	-7.33915	-7.33109	-7.32643
Average		-8.90364	-7.9066	-7.77116	-8.87932	-8.76479	-8.76207	-8.83246
1vso	11	-6.83	-6.49424	-6.27043	-6.82853	-6.81649	-6.8015	-6.81779
2qbq	11	-7.71	-5.81964	-6.00045	-7.665	-7.11274	-6.93276	-6.99714
2vw5	11	-8.52	-9.03236	-9.02774	-9.0388	-9.03494	-9.03168	-9.03229
2wca	11	-8.3	-7.94507	-7.72154	-8.30983	-7.97531	-8.01828	-7.99725
2yfe	11	-7.4	-7.40348	-7.36367	-7.41197	-7.40634	-7.41654	-7.42215
2zcr	11	-10.08	-10.042	-10.0137	-10.1162	-10.0687	-10.0388	-10.0696
3b68	11	-11.11	-11.1739	-11.1763	-11.1547	-11.1373	-11.1567	-11.1745
3nw9	11	-11.71	-9.68882	-8.85172	-11.7335	-11.6681	-11.1698	-11.5934
3oe5	11	-10.1	-8.36979	-7.31581	-10.1272	-9.94567	-9.83182	-9.89957
3ozs	11	-10.45	-8.69378	-9.4264	-10.4692	-10.0958	-10.4289	-10.0943
3ueu	11	-6.32	-6.11882	-6.0824	-6.36681	-6.22647	-6.26598	-6.16176
4agn	11	-6	-5.02144	-5.04407	-5.98785	-6.08385	-5.94725	-6.09683
4eky	11	-9.84	-9.84582	-9.80156	-9.85035	-9.82884	-9.84125	-9.83885
5c2h	11	-9.62	-9.06946	-8.52899	-9.63074	-9.49423	-8.92977	-9.52976
Average		-8.85643	-8.19418	-8.04463	-8.90648	-8.77819	-8.70079	-8.76608
2p4y	12	-10.86	-10.9665	-10.9187	-10.9601	-10.9616	-10.9714	-10.9749
2wbg	12	-8.4	-7.6839	-8.10459	-8.31501	-8.25317	-8.11246	-8.2302
3b1m	12	-10.12	-10.0933	-10.1135	-10.1354	-10.0494	-10.0682	-10.0471
4agp	12	-6.45	-5.29371	-5.07565	-6.30767	-6.4237	-6.20686	-6.50062
4agq	12	-6.68	-5.47185	-4.62657	-6.64214	-6.32203	-6.11708	-6.50358

4ea2	12	-8.2	-7.97538	-7.96891	-8.15826	-8.03259	-7.99677	-8.04525
4eo8	12	-6.99	-6.92441	-6.69272	-6.95176	-6.9387	-6.92393	-6.94616
Average		-8.24286	-7.77273	-7.64295	-8.21004	-8.14016	-8.05668	-8.17825
1h22	13	-11.39	-9.79514	-9.635	-10.8456	-10.2096	-10.354	-10.6153
2fxs	13	-6.7	-6.2299	-5.8013	-6.62736	-6.60545	-6.497	-6.59784
2yge	13	-8.41	-8.43032	-7.90143	-8.43361	-8.43749	-8.43458	-8.4343
3coz	13	-10	-9.89936	-9.86962	-10.0044	-10.0001	-10.0186	-10.005
3kwa	13	-4.26	-3.80517	-3.87919	-4.35523	-3.99806	-3.96974	-4.00714
3myg	13	-7.41	-7.03088	-6.63351	-7.38454	-7.30927	-7.27886	-7.3618
3uev	13	-6.6	-6.31487	-6.32101	-6.61006	-6.41329	-6.45805	-6.48362
4cig	13	-7.83	-6.99577	-6.77245	-7.51099	-7.1603	-7.28241	-7.42645
4w9h	13	-8.08	-7.73367	-7.22236	-8.10604	-8.10042	-8.05578	-8.02256
5a7b	13	-6.7	-5.81691	-5.81597	-6.71368	-6.44244	-6.30951	-6.67498
Average		-7.738	-7.2052	-6.98518	-7.65915	-7.46763	-7.46585	-7.56291
1g2k	14	-11.39	-11.5277	-11.5562	-11.4263	-11.4908	-11.6164	-11.5203
1lpg	14	-9.3	-8.21807	-8.16114	-9.11595	-9.10283	-8.67034	-8.88857
1qf1	14	-7.93	-7.71902	-7.09365	-7.95866	-7.94665	-7.92483	-7.93657
3coy	14	-10	-9.90927	-9.73016	-10.0212	-10.0275	-10.0198	-10.0217
4gr0	14	-11.69	-10.7878	-10.071	-11.6767	-11.0313	-11.0962	-11.1789
Average		-10.062	-9.63236	-9.32242	-10.0398	-9.91982	-9.86551	-9.90921
1a30	15	-7.01	-6.54055	-6.39915	-7.04512	-6.84088	-6.77916	-6.80272
1h23	15	-11.48	-9.7268	-9.59263	-10.6875	-10.2248	-10.5517	-10.4025
3arp	15	-9.64	-8.44224	-8.72367	-9.1385	-8.94367	-8.91916	-8.92076
3tsk	15	-10.34	-8.86927	-9.18783	-10.3676	-9.54804	-9.18355	-9.68072
3uew	15	-6.66	-6.26372	-6.04818	-6.69985	-6.37838	-6.40299	-6.39766
3zso	15	-8.23	-7.1262	-6.68517	-7.67393	-8.1374	-7.80252	-8.02277
4ogj	15	-7.5	-6.39964	-6.44449	-7.32713	-7.00069	-6.73759	-6.90363
Average		-8.69429	-7.62406	-7.58302	-8.41995	-8.15341	-8.05381	-8.16153
1u1b	16	-8.88	-7.72403	-7.43284	-8.81483	-8.35572	-8.00758	-8.10977
3bv9	16	-8.45	-8.20062	-8.01275	-8.4	-8.34623	-8.40646	-8.26239
3utu	16	-10.37	-7.44688	-7.20214	-9.7956	-8.70549	-8.62518	-8.87726
Average		-9.23333	-7.79051	-7.54924	-9.00348	-8.46915	-8.3464	-8.41647
1eby	17	-12.3	-12.2848	-12.24	-12.2887	-12.288	-12.2913	-12.2916
3o9i	17	-9.84	-9.82637	-9.73357	-9.85004	-9.85681	-9.85151	-9.84509
3pww	17	-10.85	-10.8149	-10.4808	-10.7887	-10.8524	-10.8248	-10.8466
3uex	17	-7.33	-6.94527	-6.81227	-7.40078	-7.05909	-6.96191	-6.97528
4tmn	17	-7.99	-7.37596	-7.27097	-8.6229	-8.38573	-8.1515	-8.6337
Average		-9.662	-9.44946	-9.30753	-9.79022	-9.6884	-9.61621	-9.71845
5tmn	18	-8.59	-7.32244	-7.96168	-8.89372	-8.61936	-8.67471	-8.90335
4w9l	19	-7.9	-7.78076	-7.61016	-7.8647	-7.91336	-7.89053	-7.89637
2vkm	20	-11.37	-11.1374	-10.0048	-11.3854	-11.1913	-11.1976	-11.2348
4gid	23	-10.71	-11.0796	-11.063	-11.1764	-11.1715	-11.1616	-11.1778
3prs	24	-9.18	-8.73614	-8.62536	-9.24632	-9.20561	-9.23789	-9.22512
3uri	33	-7.85	-7.95376	-7.15295	-7.80549	-7.77117	-7.63163	-7.75399
3ag9	36	-7.99	-5.19405	-4.99338	-6.45306	-5.7326	-5.38231	-5.45766

Note: The pdb codes shown in Figure 4 are 3arv, 1q8t, 3nx7 and 3uew. Their ligands have different flexibilities, i.e., 1, 5, 10 and 15 torsions, respectively, which can make docking tests more representative. The visualization of 3arv pdb code is the Chitinase A as protein complexed with the crystallization and docking results of Sanguinarine ; The visualization of 1q8t pdb code is the cAMP-dependent Protein Kinase complexed with the crystallization and docking results of Rho-kinase Inhibitor Y-27632 ; The visualization of 3nx7 pdb code is the human MMP12 as target complexed with the crystallization and docking results of an acetamide inhibitor; The visualization of 3uew pdb code is the Bovine beta-lactoglobulin as protein complexed with the crystallization and docking results of palmitic acid.

Table S2. The average RMSD of 285 test cases obtained by all compared docking programs

		RMSD (Å)						
PDB	ntor	Vina	PSO-c4	PSOVina	GWOVi	MPSOVi	MRDPS	MRDPS
					na	na	O-c4	OVina
3jya	0	4.5286	4.53175	4.5888	4.5289	4.52926	4.52804	4.60274
3udh	0	0.21232	0.21152	0.21165	0.21206	0.21217	0.6142	0.21176
4kzu	0	0.19342	0.20145	0.21355	0.1999	0.21544	0.19727	0.20983
Average		1.64478	1.64824	1.671333	1.646953	1.65229	1.779837	1.674777
1bcu	1	0.46117	0.46324	0.46162	0.46266	0.4612	0.4616	0.47236
1gpn	1	4.42468	4.42469	4.42467	4.42425	4.4247	4.42469	4.42471
2xys	1	0.44453	0.44803	0.44724	0.44783	0.4455	0.44917	0.44764
3arv	1	7.77882	7.04284	7.51012	7.06648	7.64433	7.66039	6.3522
3rsx	1	0.48803	1.07702	2.71351	1.07779	0.49574	1.07581	0.48978
4ddk	1	4.41807	4.39193	4.36039	4.83473	4.83086	4.39644	4.83018
Average		3.00255	2.974625	3.319592	3.05229	3.050388	3.078017	2.836145
1c5z	2	0.50284	0.37733	0.37781	1.13583	0.37799	0.50298	0.37607
1o5b	2	1.02205	0.91278	0.91278	1.02136	1.02191	1.02201	1.03729
1r5y	2	0.22276	1.65597	2.25378	0.22212	0.22247	0.22038	0.71413
1s38	2	0.13502	0.13807	1.29537	0.13908	0.13802	0.71392	0.13563
2iwx	2	0.5695	0.56945	0.5695	0.56938	0.56945	0.5694	0.56935
2weg	2	1.34197	1.45329	2.4006	1.34797	1.51445	1.902	1.51867
2yki	2	2.19573	0.23015	0.23846	0.25544	0.2423	0.23449	0.23954
3ary	2	5.2844	5.99158	5.69327	5.31545	5.54624	5.73446	6.19112
3g2z	2	4.96368	4.49492	4.52499	4.72888	4.8269	4.68976	4.47988
3gv9	2	4.37868	1.8957	3.65574	4.37988	4.00023	3.57804	4.11055
3kr8	2	0.90477	0.56432	0.55753	0.90524	0.68027	0.78753	0.73082
3pxf	2	9.46707	9.37744	9.28807	9.33637	9.34681	9.31641	9.42736
3twp	2	9.34878	6.53269	9.9334	9.33972	8.7688	8.84763	8.22884
3u5j	2	0.22816	0.2282	0.22822	0.22787	0.22817	0.81259	0.22829
3zt2	2	0.7128	0.48273	0.77787	0.71316	0.71283	0.67403	0.67331
4f09	2	0.24435	0.22987	0.23323	0.23613	0.23526	0.23174	0.22969
4gfm	2	6.4969	6.4643	6.49071	6.49886	6.48109	6.46374	6.521
4jsz	2	11.30485	11.28977	10.40552	11.31385	11.12875	11.18049	10.45838
4k77	2	3.0052	2.91859	3.55542	2.66295	2.94281	2.94238	2.82892
4kzq	2	0.22941	0.22959	0.41594	0.22928	0.23211	0.24092	0.23198
4mme	2	0.40994	0.42001	0.41552	0.41195	0.41404	0.4165	0.41555
4owm	2	2.87813	2.71212	4.85434	2.87065	2.86522	2.78415	2.83777
4u4s	2	9.23703	8.18462	8.18304	9.23386	9.2323	8.6831	8.37942
Average		3.264523	2.928413	3.359179	3.178056	3.118627	3.154289	3.067981

1e66	3	0.3854	0.38638	0.38435	0.3896	0.38648	0.38791	0.38776
1gpk	3	0.22189	0.22189	0.22189	0.22197	0.22189	0.22186	0.22186
1qkt	3	0.90469	0.90481	0.90487	0.90498	0.90532	0.90666	0.90474
1uto	3	2.20172	1.06968	2.39818	1.02769	1.09121	1.04461	1.01903
1ydr	3	0.53186	0.52751	0.85777	0.52873	0.53054	0.53369	0.52901
2pog	3	0.37153	0.37188	0.37217	0.37165	0.37121	0.37162	0.37183
2wer	3	0.5368	0.5368	0.5368	0.53665	0.5368	0.5368	0.5368
3acw	3	1.39846	1.3606	1.43319	1.36117	1.32418	1.32374	1.32552
3ao4	3	1.61486	1.78815	2.76403	1.61282	1.48934	1.49369	1.84524
3bgz	3	1.05709	0.93617	0.88783	1.058	0.9972	1.05783	0.99796
3g31	3	3.59422	3.75698	3.6634	3.5941	3.59902	3.89666	3.82395
3gy4	3	1.58908	1.10394	0.98374	1.90434	1.21493	1.252	1.20792
3kgp	3	1.97869	1.35008	1.3268	1.87578	1.5358	1.52149	1.46911
3pyy	3	0.92037	0.54312	1.08672	0.99559	1.22624	0.47049	0.39756
3wtj	3	1.31817	0.81101	0.82202	1.31849	1.21638	1.67852	1.11129
4cr9	3	4.77142	4.77856	4.3702	4.77217	4.77767	4.35408	4.7698
4de1	3	1.19874	2.72623	6.54208	1.10395	2.77597	1.89046	2.79007
4de3	3	2.78122	0.46676	1.58274	5.94763	0.50057	0.63794	1.68422
4e6q	3	1.10289	0.93307	0.90567	1.11763	1.12518	1.11227	1.10831
4ih5	3	2.01441	2.88695	3.50305	1.89346	3.27269	2.70341	2.42568
4j21	3	0.20251	0.2025	0.2025	0.2025	0.20268	0.20355	0.20249
4llx	3	6.28084	10.63988	9.08407	10.7246	9.95499	9.69309	8.47368
4m0y	3	6.98409	6.88052	6.72732	6.98582	6.98334	6.93998	7.0111
5c28	3	2.51949	2.98614	2.15982	2.52033	2.51795	2.55135	2.51972
Average		1.936685	2.007067	2.238384	2.207069	2.031566	1.949321	1.963944
1q8u	4	0.2952	0.29545	0.29566	0.29619	0.29566	0.29586	0.29619
1syi	4	0.78277	0.59247	0.65646	0.78277	0.78282	0.71889	0.78303
2al5	4	0.2225	0.22644	0.28717	0.2275	0.22592	0.22672	0.22513
2cbv	4	1.18177	1.46641	1.18159	0.33454	0.33432	1.18187	1.18257
2hb1	4	4.22938	1.78403	2.6057	3.8517	1.77653	3.1123	2.46276
2j7h	4	2.17399	2.17204	2.54141	2.16903	2.16978	2.16736	2.17469
2v00	4	1.34352	1.01632	1.94185	1.44886	1.22981	1.17933	1.36803
2wnc	4	2.85702	2.85373	3.05361	2.91216	2.89911	2.87587	2.86908
2wtv	4	1.79661	1.63603	1.61779	1.72602	1.71546	1.79675	1.72591
2ymd	4	1.09888	0.23963	0.23917	0.23103	0.23354	0.23344	0.23372
3b27	4	0.40877	0.40895	1.26776	0.40458	0.41018	0.40749	0.40797
3dx1	4	0.45284	1.18191	0.87272	0.45216	0.45214	0.66234	0.45229
3f3a	4	1.67715	1.56843	1.48704	1.67705	1.68571	1.59996	1.58102
3f3c	4	0.89442	0.36586	0.36461	0.89422	0.56371	0.69613	0.63014
3g0w	4	0.17916	0.17909	0.18109	0.17944	0.17939	0.17878	0.1803
3gr2	4	9.00632	10.25825	8.94994	8.76126	8.39146	9.43999	9.80492
3lka	4	5.23287	5.3476	5.31303	5.25343	5.18374	5.17975	5.3263
3n7a	4	0.3029	0.24456	0.23893	0.2533	0.21784	0.24939	0.24334
3qqs	4	5.02439	2.13272	2.36324	5.03672	3.40121	2.40344	2.54528
3rr4	4	0.4496	0.91093	2.93114	0.427	0.47174	0.46957	0.50894
3u8k	4	0.77728	0.75693	0.75714	0.77851	0.82604	0.8378	0.83383
3u8n	4	0.37261	0.36339	0.37236	0.37299	0.37337	0.3761	0.37836
4abg	4	1.41255	0.94121	0.84195	1.41358	1.77433	0.99222	1.02836
4ddh	4	1.55767	1.45579	1.30448	1.55561	1.50234	1.56081	1.56138
4dli	4	0.52989	0.52656	0.52677	0.52896	0.52513	0.52434	0.52747
4hge	4	1.30311	0.9958	1.65828	1.20805	1.30185	1.38848	0.9164

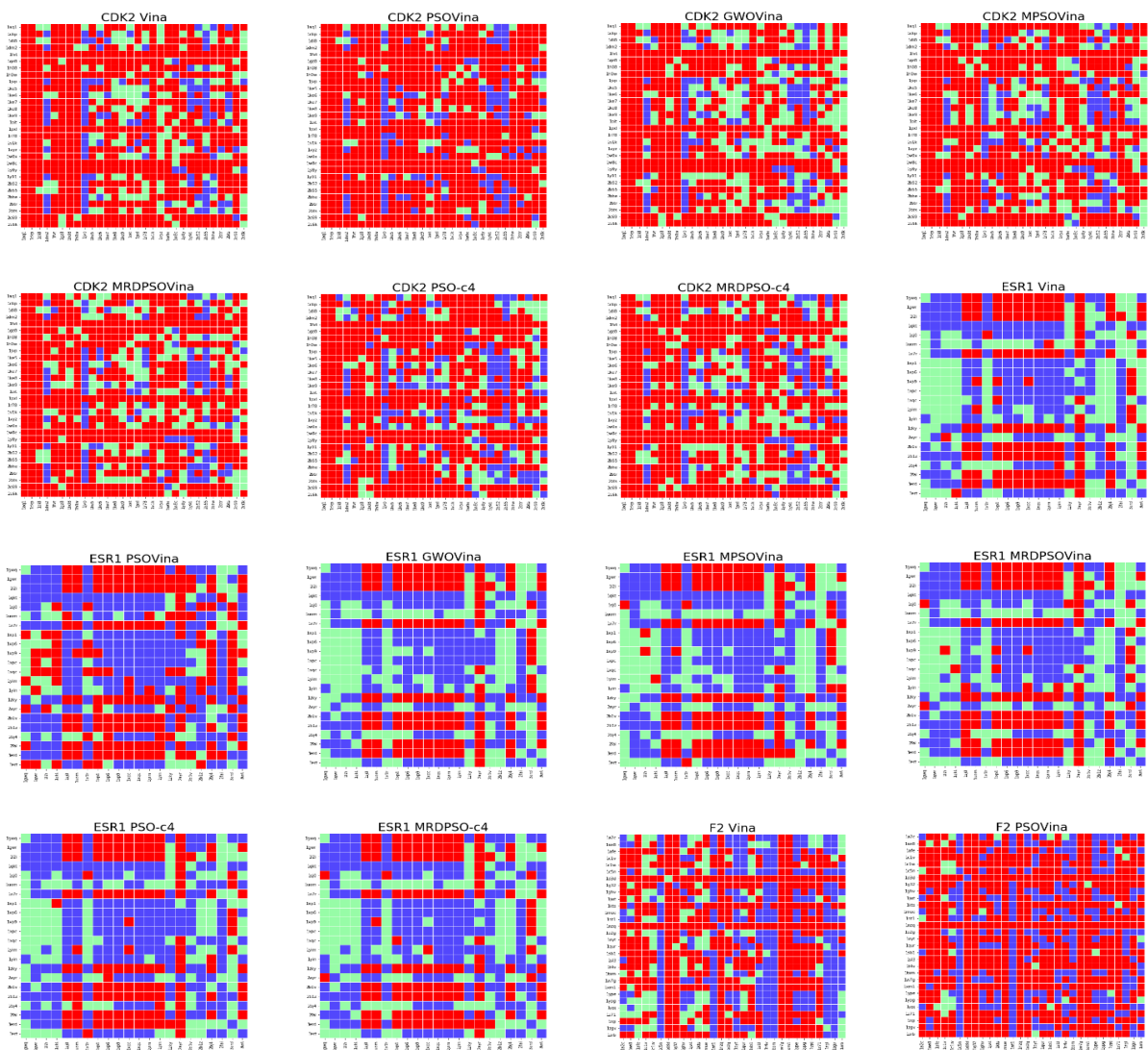
4ivb	4	0.23434	0.23624	0.23638	0.23466	0.23505	0.23731	0.23585
4j28	4	1.00239	1.00061	1.00868	1.00382	1.00259	1.20022	1.00049
Average		1.671425	1.469906	1.61057	1.586255	1.434313	1.506875	1.481563
1nc3	5	0.18233	0.22667	0.25143	0.18221	0.18388	0.24889	0.18432
1o3f	5	1.55459	1.91045	6.25815	1.533	1.53654	2.5194	1.55063
1oyt	5	0.26459	0.26524	0.55058	0.2636	0.26302	0.26489	0.2625
1p1n	5	1.22226	0.88996	0.86073	1.22273	0.98274	0.86126	0.86392
1p1q	5	4.85901	3.63811	4.57653	4.85912	4.86622	5.10061	4.60331
1ps3	5	0.48549	0.70009	0.48452	0.48337	0.4824	0.48482	0.48363
1q8t	5	7.69295	7.74457	7.71577	7.67984	7.74494	7.73735	7.18478
2r9w	5	7.38732	6.57263	6.38475	7.40428	7.28941	7.2686	6.65055
2wn9	5	7.21338	6.73333	6.51904	7.21204	6.79956	7.03743	7.09944
2xj7	5	0.28853	0.28547	0.28899	0.28834	0.28817	0.28827	0.28626
3d4z	5	0.94002	3.53802	2.8398	0.95145	0.93258	1.80944	0.94716
3d6q	5	7.02634	3.06929	5.18596	5.23573	3.88397	4.44927	2.93393
3dd0	5	1.70595	1.83724	3.37157	1.17943	2.22897	1.70469	2.22759
3fcq	5	9.39327	5.56845	3.5869	3.0742	3.05787	2.7894	3.78015
3fur	5	1.60751	0.99882	1.11822	0.88236	0.87369	0.87914	0.88293
3gbb	5	0.77196	0.58307	0.65556	0.80216	0.68571	0.74955	0.79186
3jvr	5	0.69396	3.06163	4.54165	0.69219	0.59886	0.72557	0.62422
3qgy	5	6.19046	1.93551	2.81212	6.19784	6.23152	5.72075	5.68124
3rlr	5	0.28464	0.9516	0.62338	0.28181	0.29868	0.617	0.2924
3ryj	5	1.47718	1.207	1.7363	1.42362	1.27954	0.95811	1.03351
3uuo	5	1.11019	1.03699	1.12141	1.10942	1.11222	1.10942	1.1115
4e5w	5	0.1477	0.45602	0.52016	0.14739	0.14721	0.14714	0.14735
4f9w	5	0.31706	0.72069	1.01147	0.27199	0.26991	0.64429	0.36275
4gkm	5	5.83666	4.41988	5.36238	5.81601	5.61666	5.25892	4.71939
4ih7	5	1.13915	0.90204	0.57743	1.05998	1.13955	0.98076	1.13935
4ivc	5	0.184	0.18176	0.28626	0.18518	0.18255	0.18381	0.18157
4k18	5	0.60979	2.25621	2.2952	0.60984	0.61294	0.70239	1.00807
4kz6	5	5.26356	1.79895	2.40705	5.2587	3.15675	3.55614	4.40819
4m0z	5	0.46942	0.45513	0.45865	0.46806	0.46725	0.46104	0.45849
4mgd	5	0.51393	0.43666	0.48328	0.87352	0.43065	0.51441	0.44303
4pcs	5	0.26784	0.2659	0.34725	0.59773	0.26804	0.35413	0.34763
4qac	5	0.47292	0.47459	0.47069	0.47459	0.47565	0.47385	0.4751
5aba	5	6.15278	6.42645	5.66897	4.35284	4.6023	3.39291	3.40584
Average		2.537174	2.168134	2.465823	2.214381	2.090605	2.12102	2.017351
1owh	6	0.3249	0.32783	0.3293	0.32705	0.32789	2.17488	0.32696
1pxn	6	2.48552	2.82506	2.1801	2.48709	2.44055	0.83728	2.29153
1w4o	6	0.84045	0.75664	0.65299	0.84131	0.80899	1.38599	0.8386
2brb	6	1.48009	1.31747	1.11967	1.4821	1.40112	1.15419	1.38526
2c3i	6	4.28865	1.14818	1.26582	5.10108	1.70462	5.28037	1.27427
2j78	6	4.90807	4.23577	5.25742	4.90865	5.24531	5.84161	5.31339
2p15	6	9.48983	3.80304	4.6053	8.57975	4.4183	0.37085	4.9278
2qe4	6	0.37528	0.36064	0.37001	0.37163	0.3717	0.57722	0.3668
2xnb	6	0.57915	0.57779	0.57781	0.57927	0.58048	1.37097	0.578
3dx2	6	1.2814	1.02089	1.50606	1.3706	1.41343	0.32479	1.36785
3dxg	6	0.32548	1.13423	2.06946	0.32441	0.59627	5.34031	0.46846
3e93	6	5.34743	4.98488	4.81875	5.34603	5.27698	0.32541	5.37676
3ebp	6	0.56778	1.06863	0.90363	0.56225	0.57712	0.57419	0.58326
3f3d	6	1.08224	1.00662	1.12021	1.04269	1.16003	1.08165	1.04113

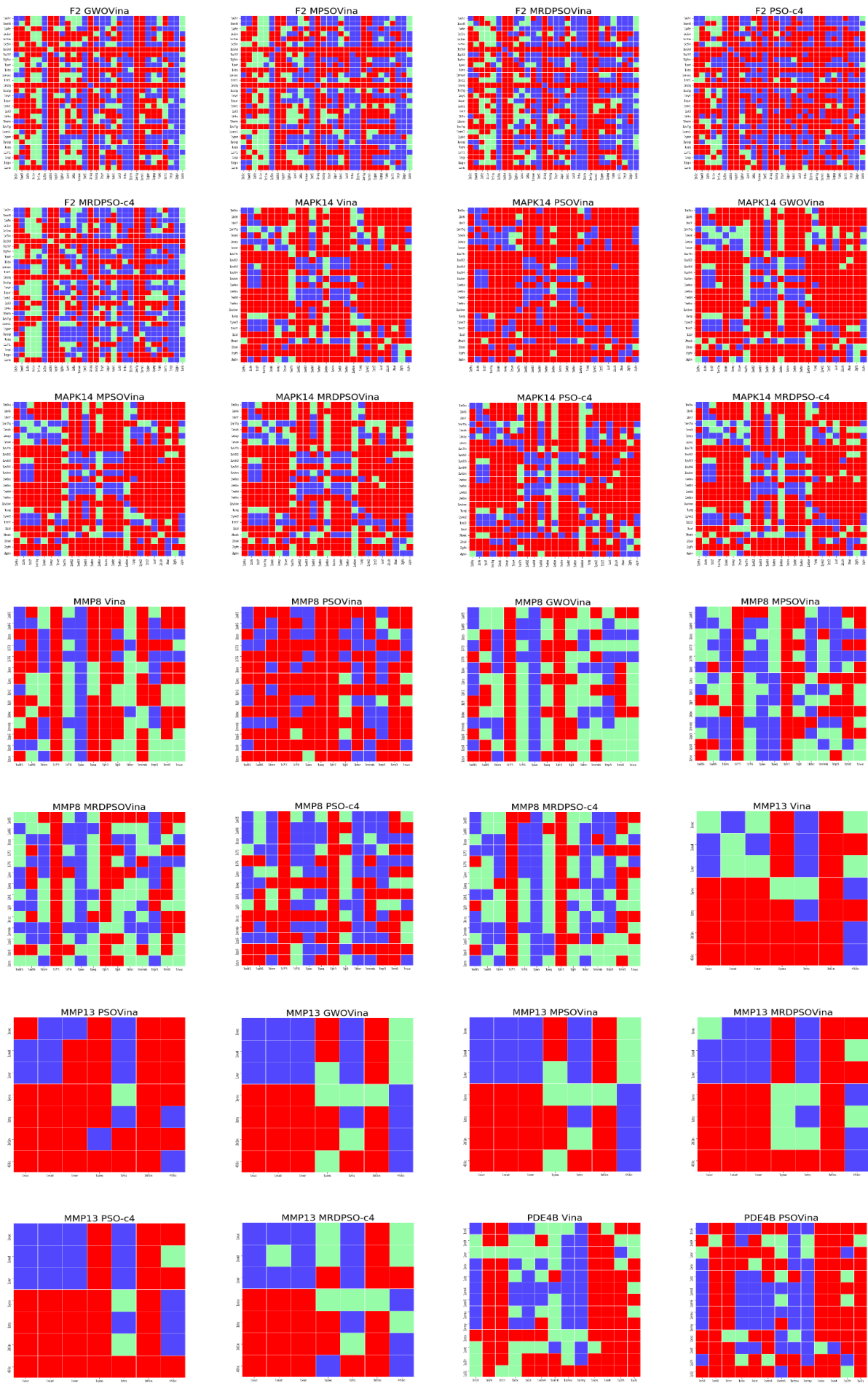
3f3e	6	1.1415	0.94505	0.91161	1.39254	1.15043	1.29182	1.19251
3gc5	6	0.38294	0.76319	0.61311	0.38293	0.40453	0.56541	0.38231
3k5v	6	3.3836	3.27292	3.3041	3.40263	3.52935	3.43132	3.37514
3l7b	6	0.73854	0.73909	0.71408	0.73818	0.73914	0.73851	0.73868
3r88	6	12.77686	10.29806	9.49835	11.99331	11.0295	11.4074	11.16473
3syr	6	0.53472	0.53472	0.50538	0.53464	0.5348	0.53462	0.53473
3ui7	6	0.4941	0.49175	0.82199	0.48942	0.48899	0.49184	0.4909
3uo4	6	7.59781	3.8468	4.92585	8.71276	3.39828	5.43854	5.42998
4bkt	6	0.58224	0.57085	0.57402	0.58818	0.56425	0.57413	0.57731
4ivd	6	0.7292	1.57616	4.00863	0.72725	1.208	0.55829	0.62852
4jxs	6	2.6241	3.26719	4.11975	2.99891	3.24218	2.59335	1.73869
4rfm	6	4.39121	1.53261	1.88207	4.38932	2.57712	1.47343	2.25689
4twp	6	2.45562	1.10092	1.38276	2.61825	1.61578	2.01756	1.98833
5dwr	6	0.42145	0.93723	0.42141	0.42281	0.42143	0.63593	0.42143
Average		2.55822	1.94436	2.159273	2.596966	2.043806	2.085424	2.037865
Inc1	7	0.24066	0.24346	0.24363	0.24829	0.24203	0.41285	0.24747
1y6r	7	0.44136	0.41607	0.4797	0.41476	0.41586	0.55946	0.41631
1yc1	7	0.56123	0.38379	0.38464	0.55903	0.55966	0.67424	0.55931
1z9g	7	0.69094	0.63711	0.89852	0.86677	0.69115	3.09766	0.65379
2fvd	7	5.77053	2.9139	4.71954	5.12309	2.86892	3.58928	3.6917
2vvn	7	9.57708	1.05156	2.19819	4.52459	3.9147	0.26535	5.40565
2w66	7	0.25801	1.97606	3.87185	0.25954	0.25889	0.36234	0.27572
2wvt	7	0.35851	0.83096	0.35915	0.35834	0.36112	0.81171	0.3558
2x00	7	0.65732	0.7375	1.18316	0.6579	0.67021	0.58136	0.69246
2xbv	7	0.5781	0.58661	0.57783	0.57322	0.58683	0.67212	0.57752
2xii	7	0.70027	0.80084	3.89754	0.61683	1.45218	0.55866	0.62423
2zb1	7	0.55438	3.73496	3.43008	0.55852	0.98722	0.34747	0.55842
3b65	7	0.35194	0.40133	0.66284	0.34472	0.34479	0.78482	0.36458
3cj4	7	0.9757	0.85422	0.44698	0.97591	0.67306	2.29943	0.84111
3e92	7	2.31318	2.33906	3.01739	2.31282	2.3124	0.244	2.29754
3ehy	7	3.88354	1.33045	2.70446	2.85535	1.4462	0.88767	1.46771
3fv2	7	0.16258	0.16188	0.33027	0.16235	0.16245	0.1622	0.16257
3g2n	7	1.31933	1.31209	1.3906	1.31971	1.31813	1.31896	1.32209
3nq9	7	5.4585	6.6981	6.42759	7.31686	7.16904	6.80885	5.98151
3up2	7	2.66309	2.32921	3.00595	2.65292	2.44557	3.53549	2.59191
4ciw	7	0.34879	0.34409	0.39973	0.34886	0.34896	0.34391	0.34485
4de2	7	0.54618	1.42138	2.60415	0.56376	2.44103	0.70193	0.55542
4djv	7	0.39782	0.4964	1.70845	0.39443	0.38552	0.40948	0.39661
4eor	7	1.44291	2.30712	2.8152	2.63872	3.67238	3.38206	3.3404
4f2w	7	0.26163	0.25749	0.25783	0.2591	0.26222	0.25754	0.26182
4j3l	7	1.3117	1.29021	1.26819	1.3275	1.31768	1.31734	1.32388
4jfs	7	1.44812	1.37091	1.5096	1.44528	1.43245	1.44433	1.44922
4jia	7	8.77155	1.71753	2.30615	8.69786	6.34986	7.15519	5.94726
4lzs	7	0.57778	0.97093	1.17041	0.57989	0.58351	0.57857	0.57917
Average		1.814577	1.376387	1.871366	1.68817	1.574966	1.502216	1.492622
1bzc	8	1.18168	1.27754	1.77513	1.08486	0.97916	1.04735	0.97047
1sqa	8	1.95677	1.9061	2.62343	1.67183	1.89315	1.8374	1.75725
1ydt	8	4.71815	5.01687	7.19313	4.57889	5.63391	6.44029	6.08275
1z95	8	0.98762	0.70898	0.70965	0.84906	0.61606	0.75692	0.84442
2br1	8	1.93081	1.94698	1.5966	1.93226	1.94846	1.81932	1.95142
2cet	8	7.93321	3.88406	6.11139	7.93673	7.82041	7.26297	7.93634

2qbr	8	6.29572	4.94642	5.63194	6.43807	4.0395	2.4372	2.08543
2v7a	8	1.34039	0.77958	0.92687	1.16813	1.00053	0.83165	0.73698
2w4x	8	0.71503	1.24564	2.64426	0.71454	0.71478	0.71367	0.71516
2xb8	8	0.36444	0.36413	0.32703	0.36836	0.36498	0.36865	0.36591
2xdl	8	0.31951	0.31658	0.51142	0.31754	0.31695	0.31718	0.32131
2zcg	8	5.65792	5.71891	5.57502	5.6306	5.75809	5.73864	5.68189
2zy1	8	5.15022	2.38598	2.88068	2.899	2.94654	2.50345	3.14944
3aru	8	3.31789	1.79968	3.51376	3.30831	1.97934	2.33911	2.27719
3b5r	8	0.66888	0.6544	0.72762	0.67099	0.70947	0.66271	0.6913
3fv1	8	0.70276	0.44466	0.36696	0.49638	0.44521	0.34309	0.34329
3ge7	8	0.92161	1.10715	0.8748	0.92178	0.91832	1.06042	0.88523
3ivg	8	1.68838	1.52451	2.60149	1.679	1.64178	1.62529	1.49646
3jvs	8	3.01946	2.34805	3.23497	2.77201	2.50014	2.34957	2.43147
3mss	8	2.79076	2.59432	4.50898	2.79513	3.26226	2.66983	2.85134
3n76	8	1.46596	0.97354	1.12795	1.28705	1.11721	1.11725	1.13169
3n86	8	0.95558	0.90634	0.89671	0.95914	0.95811	0.95321	0.96233
3p5o	8	1.16947	1.17084	1.29415	1.17574	1.16765	1.17017	1.17175
4dld	8	1.8973	2.04796	2.9603	1.12811	0.66815	0.54735	0.59874
4qd6	8	5.07934	4.65817	5.37919	5.1733	2.59941	2.41781	2.79801
4wiv	8	1.21453	1.93269	4.38154	1.24426	1.15794	1.13468	1.2039
Average		2.44013	2.025388	2.70673	2.276964	2.04452	1.940968	1.978518
1k1i	9	4.75855	3.40564	6.35836	4.73076	4.48193	4.48188	3.65537
1mq6	9	1.3627	4.49616	4.67114	1.35284	1.95052	4.20733	1.03745
1nvq	9	5.34053	3.01967	3.78508	5.34206	5.33895	4.95344	5.34092
1o0h	9	1.39461	3.96663	5.82607	2.26493	2.94649	1.83814	1.23234
2y5h	9	2.21677	4.27262	5.28479	2.10607	1.35176	1.91968	1.96663
2zda	9	0.89595	0.49449	2.23291	0.53363	0.47085	0.49139	0.59684
3e5a	9	1.18398	1.20739	3.24625	1.14686	1.12904	1.05009	1.05769
3gnw	9	0.29316	1.06046	2.29311	0.29469	0.29582	0.29372	0.29317
3u9q	9	1.14655	0.88457	1.13842	1.13383	1.36235	1.11418	1.0313
3wz8	9	2.11855	1.8226	4.92274	2.00509	1.87043	1.82968	1.95058
4cra	9	2.15297	1.40533	4.50436	1.29636	0.43194	0.33065	0.83838
4crc	9	0.67806	1.35073	5.03315	2.56121	0.52286	1.40983	0.73989
4f3c	9	1.34634	0.4678	0.39678	0.59447	0.39836	0.37277	0.46752
4ty7	9	9.80336	6.67716	5.69553	9.79886	2.64055	3.67502	3.07386
4w9i	9	1.45983	1.31287	2.71138	1.43209	1.44113	1.35618	1.35955
4x6p	9	0.88988	3.643	6.67568	2.21373	1.73309	1.79413	0.96288
Average		2.315112	2.467945	4.048484	2.425468	1.772879	1.944882	1.600273
1z6e	10	1.18685	3.13794	7.25234	1.11378	0.36085	0.34293	0.37161
2qbp	10	1.03503	3.89592	5.00297	0.93612	1.05946	1.11179	0.81616
2qnq	10	0.48288	0.48411	2.34965	0.48399	0.48409	0.48495	0.48531
3arq	10	10.19791	3.40043	3.90753	10.19364	9.13494	9.33094	8.37431
3ejr	10	1.78485	5.64191	5.03424	1.33114	3.43925	1.55881	2.42855
3nx7	10	1.47026	1.24115	2.73731	1.34656	1.37326	1.98409	1.37474
3oe4	10	0.63582	6.34745	3.93124	0.63766	1.66254	4.32871	0.53952
3ozt	10	1.05731	4.06038	2.38057	1.04107	0.58601	0.52271	0.47046
3zdg	10	0.51626	0.51634	0.72256	0.5132	0.51399	0.51497	0.51984
3zsx	10	5.4442	3.82755	4.71521	4.31782	3.96547	3.55943	1.84238
4w9c	10	0.97269	1.11428	3.87351	1.65637	0.39846	0.61064	0.50423
Average		2.253096	3.060678	3.809739	2.14285	2.088938	2.213634	1.611555

1vso	11	1.50242	2.56596	3.12116	1.38238	1.39305	1.46593	1.53672
2qbq	11	2.17251	8.38656	8.35867	3.60895	3.3898	2.46415	2.80466
2vw5	11	1.65155	0.2072	0.21144	0.22266	0.21361	0.20934	0.20729
2wca	11	3.91884	3.84726	4.06423	3.92724	3.9666	3.78817	3.70149
2yfe	11	1.47749	1.20453	1.39538	1.48307	1.47193	1.44147	1.44564
2zcr	11	3.20755	1.71029	1.45441	2.73713	2.50355	2.17485	2.72631
3b68	11	1.07552	0.79567	1.01253	1.08871	0.80536	0.77868	0.77564
3nw9	11	0.34428	4.14505	5.89853	0.34807	0.44146	1.34721	0.55198
3oe5	11	0.68607	4.02839	6.02372	0.58666	0.66271	0.77913	0.77156
3ozs	11	0.69827	3.33288	2.06077	0.52031	1.63051	0.54104	1.61739
3ueu	11	4.35596	4.2991	3.82336	4.38155	4.46242	4.31145	5.30922
4agn	11	4.58765	4.86874	4.58869	4.62351	2.56636	2.8968	1.91326
4eky	11	0.65612	0.65611	0.6331	0.65533	0.6575	0.65575	0.65526
5c2h	11	1.52201	2.01719	4.76873	1.45511	1.10996	3.29897	1.46447
Average		1.989731	3.004638	3.386766	1.930049	1.805344	1.868067	1.820064
2p4y	12	1.38927	0.57693	0.5962	0.71767	0.68373	0.65932	0.56945
2wbg	12	2.74531	3.74911	2.61654	2.70283	3.10654	3.24061	3.15412
3b1m	12	0.70251	1.02026	0.71069	1.18929	1.35186	1.51678	1.51798
4agp	12	3.72278	6.04213	7.49918	4.33918	2.54862	2.2602	2.52818
4agq	12	2.81875	4.90779	7.25982	3.30261	2.68283	4.11794	3.46834
4ea2	12	2.4135	2.75877	2.39154	2.34184	2.25033	2.28684	2.26917
4eo8	12	0.78287	0.80168	1.50751	0.74124	0.91554	0.95914	0.74366
Average		2.082141	2.836667	3.225926	2.190666	1.934207	2.14869	2.035843
1h22	13	9.64256	3.31598	4.67747	7.32938	6.93513	6.44473	7.26746
2fxs	13	6.01932	4.91184	4.91078	5.89046	5.60782	6.07173	5.99627
2yge	13	0.5578	0.55486	1.93813	0.55618	0.55907	0.56117	0.55801
3coz	13	0.65931	1.23855	1.27833	0.67858	0.6144	0.62591	0.60005
3kwa	13	3.79003	3.93038	4.67608	3.65918	3.9876	4.18097	4.10297
3myg	13	3.02405	1.92773	6.02241	1.41102	2.2426	1.54247	0.95833
3uev	13	1.75649	2.10079	2.77857	1.76574	1.83453	2.67864	2.75985
4cig	13	6.34777	6.10362	6.11168	6.2843	5.2896	5.79614	2.46914
4w9h	13	1.5825	1.79827	3.09346	1.54667	1.56581	1.47617	1.44984
5a7b	13	3.0614	3.7829	3.85084	3.54125	2.8477	3.05287	2.30456
Average		3.644123	2.966492	3.933775	3.266276	3.148426	3.24308	2.846648
1g2k	14	0.99409	0.90261	0.89198	1.11665	1.00176	0.97449	0.95391
1lpg	14	9.54336	4.50576	4.79628	5.80945	1.12713	3.26108	3.19973
1qfl	14	0.78445	1.3336	3.43038	0.71747	0.65151	0.67852	0.76824
3coy	14	0.32919	1.09458	1.57415	0.4067	0.29055	0.28806	0.33177
4gr0	14	2.36354	2.02892	3.54389	2.21469	1.22383	1.2816	1.13808
Average		2.802926	1.973094	2.847336	2.052992	0.858956	1.29675	1.278346
1a30	15	7.37267	5.86502	5.21152	8.29383	6.18523	5.81915	6.88113
1h23	15	9.76612	6.25236	6.4895	7.4932	5.55406	6.79313	4.60313
3arp	15	10.12363	4.81637	6.90944	9.48277	10.01933	8.40873	7.87461
3tsk	15	3.83177	2.46799	3.21978	3.84614	2.27556	2.917	2.4618
3uew	15	3.85362	3.25654	4.07584	3.31679	4.26717	5.48226	2.8406
3zso	15	0.94985	4.6343	5.42365	5.91373	1.1606	3.73352	1.69536
4ogj	15	6.95353	3.32914	5.08547	7.42102	7.17069	6.04413	6.99399
Average		6.121599	4.374531	5.202171	6.538211	5.233234	5.599703	4.764374

1u1b	16	2.45255	4.07582	6.25476	4.47402	1.89108	4.85934	3.17784
3bv9	16	0.88078	1.68325	2.37323	0.88355	0.77469	0.83775	0.77129
3utu	16	5.36746	5.83622	5.98811	3.29256	3.20212	3.43651	3.15768
Average		2.900263	3.865097	4.872033	2.883377	1.955963	3.044533	2.368937
1eby	17	0.36822	0.36807	1.41598	0.36648	0.36751	0.36556	0.3694
3o9i	17	0.41138	0.41586	1.25927	0.35341	0.36372	0.36372	0.35507
3pww	17	1.97791	1.06775	3.00877	1.37583	0.8008	0.91613	0.94559
3uex	17	4.22664	3.80814	3.90297	4.36656	4.17119	4.1552	3.79085
4tmn	17	6.83212	7.14642	8.16875	3.86872	3.82819	4.97444	2.61689
Average		2.763254	2.561248	3.551148	2.0662	1.906282	2.15501	1.61556
5tmn	18	5.40224	5.52766	5.35895	2.76089	2.48901	2.74153	2.70734
4w9l	19	1.3026	1.01213	1.1766	1.27555	1.30811	1.24374	1.2822
2vkm	20	2.33779	1.49402	2.92473	2.03441	1.78716	1.80564	1.78867
4gid	23	2.69205	0.4652	0.58878	0.73502	0.80647	0.84427	0.87129
3prs	24	2.0391	3.82227	4.43011	1.9732	1.93766	2.07144	2.02506
3uri	33	11.99391	2.04019	4.2325	9.59937	2.48888	3.60815	2.17813
3ag9	36	10.03285	8.67705	9.01488	8.67273	10.11324	9.07064	9.01759





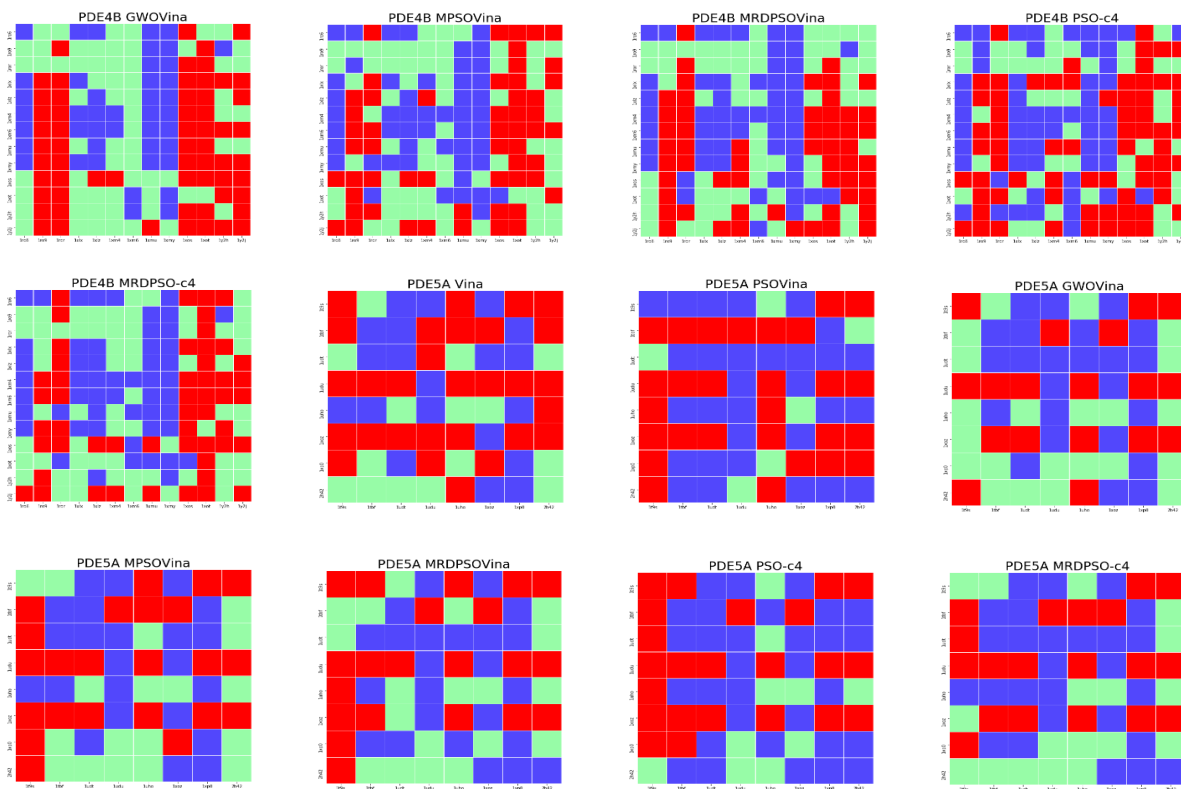


Figure S2. The cross-docking comparison of Vina and Vina-based programs. The cross-docking results were divided into failed sampling (red), failed scoring (green) and successful docking (blue).