

SUPPLEMENTARY MATERIALS

TABLES

Table S1. Cross-docking results on the HIV protease set for (a) rigid docking using LigDockCSA, (b) GalaxyDock with 2 flexible residues (ARG8 of the two chains), and (c) GalaxyDock with 4 flexible residues (ARG8 and ILE50 of the two chains). Ligand RMSD of the predicted binding pose (starting from ligand A + protein structure B) from that of the crystal structure (ligand A + protein structure A) is presented for each cross docking of ligand A (row) to protein structure B (column).

(a)

		Ligands																			
Proteins		1HBV	1HEF	1HEG	1HIH	1HIV	1HPS	1HTE	1HTF	1HTG	1HVI	1HVJ	1HVK	1HVL	1HVS	1SBG	4HVP	4PHV	5HVP	8HVP	9HVP
	1HBV	1.023	0.558	1.416	1.024	1.441	0.629	7.524	6.745	2.380	1.752	1.276	1.785	1.631	12.025	0.942	2.010	0.608	1.131	1.533	12.585
	1HEF	1.708	1.508	1.436	0.674	0.929	1.145	9.938	3.269	0.910	1.594	12.102	14.770	1.669	12.075	0.739	1.111	10.754	1.087	1.538	0.588
	1HEG	1.547	0.837	1.290	1.107	1.205	0.848	6.449	3.172	0.981	2.339	2.078	14.385	1.779	2.771	0.689	1.856	0.870	1.090	1.455	12.610
	1HIH	10.954	1.386	1.393	0.698	1.551	0.826	6.594	2.797	1.129	2.213	2.032	12.095	2.299	12.907	9.758	2.371	0.767	1.647	1.435	1.147
	1HIV	10.987	2.047	1.464	0.910	0.653	0.667	6.866	1.337	1.206	1.107	1.362	0.720	1.429	0.768	0.391	1.350	0.459	1.235	1.698	1.479
	1HPS	1.739	1.209	1.349	0.890	0.954	0.556	10.010	1.004	1.267	2.133	1.935	14.877	2.082	11.187	1.450	1.474	0.627	1.135	1.356	1.062
	1HTE	2.177	1.092	1.494	0.491	0.860	1.085	0.878	2.264	2.769	0.951	1.351	1.090	1.206	0.484	0.657	1.374	0.590	1.213	1.758	1.265
	1HTF	11.026	1.026	1.388	1.046	1.270	0.467	6.133	1.096	0.415	11.232	11.294	1.739	2.118	1.823	0.731	2.341	0.555	1.222	1.416	1.070
	1HTG	1.744	1.008	1.121	0.764	0.881	0.716	0.717	1.286	0.847	12.031	1.313	0.930	0.985	11.991	0.667	1.258	10.748	1.207	1.517	0.969
	1HVI	10.985	1.575	11.409	1.365	1.496	1.381	6.771	1.580	2.822	1.063	1.016	1.320	1.135	0.830	1.209	1.861	0.673	1.111	1.447	1.499
	1HVJ	1.665	1.632	1.298	1.226	1.508	1.452	7.042	1.522	2.415	1.018	0.959	1.205	0.899	0.762	1.488	1.185	0.635	1.214	1.970	1.601
	1HVK	1.787	1.640	1.318	0.880	1.390	1.364	6.920	1.498	2.489	1.037	1.074	1.172	1.248	0.539	1.217	1.208	0.610	1.305	1.644	1.553
	1HVL	1.812	1.578	1.380	1.294	1.753	1.486	6.914	1.562	2.451	1.024	1.074	1.138	0.922	1.065	1.283	1.293	10.757	1.307	1.504	1.554
	1HVS	2.086	1.588	1.599	0.932	1.181	1.441	10.035	1.491	2.733	0.773	1.090	1.197	1.086	0.744	0.971	2.011	0.834	1.250	1.483	1.259
	1SBG	11.095	1.311	1.120	0.951	1.103	0.484	8.296	3.177	0.995	1.722	1.602	14.908	1.450	2.246	0.827	2.352	0.643	0.976	1.406	12.605
	4HVP	1.896	1.441	1.081	0.944	0.566	0.998	6.600	1.594	0.945	0.881	1.803	1.124	1.056	12.005	0.425	1.151	0.496	1.316	2.052	1.143
4PHV	10.983	11.685	1.270	0.789	1.206	1.378	6.363	2.663	0.987	2.429	1.808	14.102	11.866	1.384	1.062	2.291	0.875	0.854	1.265	0.804	
5HVP	2.036	1.562	1.113	9.595	1.095	0.857	6.757	9.415	1.311	0.983	1.426	1.174	1.407	0.828	9.677	1.390	10.770	1.058	1.485	1.154	
8HVP	10.895	2.009	1.958	1.227	1.018	0.774	1.262	1.784	2.541	1.245	1.160	12.086	1.376	0.833	9.747	1.383	0.532	0.821	1.563	1.186	
9HVP	1.380	1.596	1.153	1.292	1.350	0.452	6.334	1.368	0.436	11.996	1.696	6.899	1.570	11.993	0.993	1.104	0.624	1.482	1.222	0.650	

0Å~	2Å~	4Å~	6Å~	8Å~	10Å~
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(b)

		Ligands																			
Proteins		1HBV	1HEF	1HEG	1HIH	1HIV	1HPS	1HTE	1HTF	1HTG	1HVI	1HVJ	1HVK	1HVL	1HVS	1SBG	4HVP	4PHV	5HVP	8HVP	9HVP
	1HBV	0.862	0.853	1.016	0.958	1.498	0.657	1.054	0.847	1.630	0.626	0.691	0.566	0.727	0.556	0.907	1.636	0.708	1.056	1.239	0.808
	1HEF	1.406	1.115	1.156	0.649	1.788	0.846	0.829	0.630	0.763	1.126	0.669	0.570	0.570	1.262	1.780	1.566	0.592	0.949	1.261	0.525
	1HEG	1.397	0.776	1.233	0.903	0.983	0.702	0.988	0.686	1.544	1.155	0.992	0.564	0.507	0.683	0.595	0.919	1.915	0.770	1.232	0.646
	1HIH	1.347	1.269	1.169	4.581	1.047	0.506	0.874	0.874	1.589	0.629	0.621	0.674	0.789	0.277	1.103	1.112	0.600	1.021	1.134	0.971
	1HIV	1.699	1.487	0.924	0.662	0.479	0.491	1.207	0.928	0.929	1.566	0.581	0.971	0.836	0.809	0.378	1.248	0.457	1.039	1.424	1.592
	1HPS	1.257	1.676	1.111	0.791	0.784	0.526	0.967	0.675	1.694	0.671	0.875	0.638	0.652	0.763	1.194	1.349	0.568	0.868	1.152	0.718
	1HTE	1.633	0.990	1.439	4.833	0.699	0.807	0.603	0.913	0.442	0.657	0.716	0.602	0.712	0.702	0.692	1.780	1.968	0.913	1.200	0.981
	1HTF	1.575	0.697	1.077	0.903	0.989	0.736	0.543	0.783	1.596	0.716	0.845	0.645	0.764	0.800	1.466	1.345	0.626	1.003	1.175	0.863
	1HTG	1.463	0.806	0.887	0.719	1.132	0.696	0.896	0.772	0.359	1.113	0.883	0.697	1.259	0.879	0.506	1.686	0.724	1.013	1.301	0.773
	1HVI	1.414	1.083	1.132	0.822	1.477	1.083	1.319	1.279	1.759	0.862	0.666	0.686	0.643	0.507	1.884	1.624	0.566	0.966	1.139	1.156
	1HVJ	1.330	1.096	1.015	0.843	1.186	1.001	1.272	1.203	1.809	0.669	0.597	0.710	0.720	0.474	0.982	0.996	0.591	1.028	1.355	1.185
	1HVK	1.323	1.737	1.111	0.784	1.274	0.854	1.097	1.254	1.859	1.729	0.613	0.644	0.769	0.372	0.794	1.056	0.550	1.086	1.328	1.526
	1HVL	1.399	1.040	1.135	0.874	1.315	0.901	1.317	1.067	1.772	0.588	0.535	0.735	0.708	0.526	1.009	1.051	0.583	1.012	1.157	1.596
	1HVS	1.565	5.002	1.303	0.971	1.025	0.877	1.133	1.082	1.764	0.517	0.585	0.687	0.675	0.366	1.726	1.661	0.643	1.080	1.240	0.994
	1SBG	1.316	1.105	0.974	0.417	0.982	0.390	0.790	0.768	1.556	0.863	1.049	0.608	0.611	0.674	0.665	1.619	0.688	0.791	1.229	1.460
	4HVP	1.553	1.184	1.038	0.707	0.445	0.727	1.311	1.122	0.560	0.862	0.891	0.617	1.126	0.687	0.406	1.078	0.464	1.106	1.182	0.781
	4PHV	1.586	1.590	1.108	0.784	0.921	0.397	0.719	0.986	1.544	0.898	0.914	0.708	0.904	0.958	0.811	0.941	0.494	0.792	1.098	1.522
	5HVP	1.633	1.102	0.935	0.915	4.894	0.478	1.413	1.174	0.790	0.924	0.855	0.865	0.816	0.919	0.285	1.331	0.397	0.855	1.150	0.831
	8HVP	1.626	1.584	0.897	0.914	0.903	0.818	1.085	1.256	1.531	0.608	0.779	0.647	0.874	0.578	4.494	0.925	0.436	0.864	1.273	1.448
	9HVP	0.926	1.329	1.085	0.842	1.239	0.414	0.769	0.774	0.436	1.616	0.878	0.670	0.801	0.623	1.922	1.672	0.570	0.736	1.136	0.485

0Å~	2Å~	4Å~	6Å~	8Å~	10Å~
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(c)

		Ligands																	
Proteins		1HBV	1HEF	1HEG	1HHH	1HIV	1HPS	1HTE	1HTF	1HTG	1HVI	1HVJ	1HVK	1HVL	1HVS	1SBG	4HVP	4PHV	5HVP
		1HBV	1HEF	1HEG	1HHH	1HIV	1HPS	1HTE	1HTF	1HTG	1HVI	1HVJ	1HVK	1HVL	1HVS	1SBG	4HVP	4PHV	5HVP
	1HBV	0.954	0.726	0.963	0.751	3.212	0.985	0.975	0.717	1.736	0.541	0.721	0.646	0.824	0.421	0.910	0.893	0.729	1.032
	1HEF	1.393	1.734	1.002	4.910	0.608	0.511	0.851	0.795	1.680	1.494	1.694	0.568	1.042	1.025	0.631	1.658	0.652	1.048
	1HEG	1.329	0.813	1.023	0.703	1.022	0.732	0.661	0.830	0.426	0.952	0.840	0.641	0.867	0.717	0.625	0.873	1.954	0.766
	1HHH	1.380	1.262	1.147	2.834	1.205	0.646	0.702	0.739	0.928	0.684	0.614	0.663	0.721	0.417	1.829	1.737	0.595	0.974
	1HIV	1.695	1.449	0.953	0.741	0.487	0.524	0.788	1.102	0.901	0.657	1.169	0.639	0.829	0.777	0.492	1.362	0.464	1.085
	1HPS	1.323	0.751	1.098	0.741	0.819	0.494	1.001	0.718	0.638	0.670	1.622	0.620	0.797	0.984	1.238	0.922	0.543	0.848
	1HTE	1.887	0.843	1.218	4.938	0.688	0.754	0.885	0.930	1.737	1.429	0.748	0.587	0.681	0.704	0.626	1.173	0.813	0.848
	1HTF	1.438	0.800	1.110	0.649	0.904	0.475	0.256	0.762	1.622	1.069	0.888	0.795	0.756	0.797	0.441	1.031	0.674	0.983
	1HTG	1.632	0.654	1.054	0.511	0.718	0.639	0.585	0.696	0.498	1.290	0.878	0.699	0.962	0.892	0.607	1.790	0.571	1.014
	1HVI	1.292	1.238	1.161	0.935	1.491	0.614	1.113	1.153	1.803	0.881	0.674	0.795	0.800	0.745	0.678	1.616	0.568	1.034
	1HVJ	1.442	1.236	1.010	0.642	1.194	0.890	1.241	1.135	1.773	0.642	0.734	1.369	1.418	0.496	0.902	0.984	0.556	1.018
	1HVK	1.389	1.591	1.122	0.591	1.423	0.842	4.604	1.144	1.727	0.755	0.593	0.664	0.720	0.507	0.855	1.071	0.538	1.114
	1HVL	1.419	1.079	1.092	0.788	1.217	0.877	1.413	1.227	1.774	0.700	0.727	0.726	0.795	0.554	1.860	1.719	0.548	1.076
	1HVS	1.657	1.264	1.408	0.666	1.152	0.632	1.090	1.127	1.712	0.667	0.957	0.631	0.660	0.435	0.700	1.522	0.601	1.081
	1SBG	1.308	1.166	0.989	0.635	0.966	0.461	0.484	0.815	1.553	0.837	0.841	0.536	0.658	0.610	0.500	1.631	0.633	0.784
	4HVP	1.542	1.506	0.692	0.694	0.458	0.709	4.563	1.092	0.604	0.950	1.039	1.071	0.676	1.056	0.452	1.245	0.402	1.079
	4PHV	1.280	0.831	1.091	0.651	1.021	0.338	0.864	0.847	1.583	1.011	0.829	0.686	1.639	1.014	0.798	0.959	0.644	0.779
	5HVP	1.586	0.962	0.889	0.804	0.973	0.416	1.353	1.200	0.826	1.564	0.847	1.080	0.801	0.917	1.649	1.240	0.512	0.744
	8HVP	1.411	1.603	1.103	1.374	0.877	0.693	1.162	1.240	1.547	0.899	0.851	0.936	0.835	0.546	4.716	0.933	0.424	0.827
	9HVP	1.157	1.590	1.003	0.339	1.095	2.942	0.638	0.650	0.471	0.735	0.811	0.671	0.690	0.642	0.964	0.563	0.566	0.724

0Å~	2Å~	4Å~	6Å~	8Å~	10Å~
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Table S2. Accuracy of χ_1 angles on the HIV protease set for flexible docking with GalaxyDock for (a) 2 flexible residues (2 ARG8's) and (b) 4 flexible residues (2 ARG8's and 2 ILE50's). The χ_1 angle prediction is considered accurate if its value is within 30° from the experimental value.

		Ligands																			
Proteins		1HBV	1HEF	1HEG	1HH	1HIV	1HPS	1HTE	1HTF	1HTG	1HVI	1HVJ	1HVK	1HVL	1HVS	1SBG	4HVP	4PHV	5HVP	8HVP	9HVP
	1HBV	1.000	0.500	0.500	1.000	1.000	1.000	0.500	1.000	1.000	1.000	0.500	0.500	0.000	0.500	1.000	0.500	1.000	1.000	1.000	0.000
	1HEF	1.000	1.000	1.000	1.000	1.000	1.000	0.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.500
	1HEG	1.000	0.500	0.000	0.000	0.000	0.500	1.000	0.000	0.000	1.000	1.000	0.000	1.000	0.500	0.500	1.000	0.000	0.500	0.000	1.000
	1HH	1.000	1.000	1.000	1.000	1.000	1.000	0.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.500	1.000	0.000
	1HIV	1.000	1.000	1.000	1.000	1.000	1.000	0.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.000
	1HPS	0.500	1.000	0.500	1.000	1.000	1.000	0.500	0.500	0.500	0.500	1.000	0.500	0.500	0.500	1.000	1.000	1.000	0.500	1.000	0.500
	1HTE	0.500	0.500	0.500	0.500	0.500	0.500	1.000	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500
	1HTF	1.000	1.000	1.000	1.000	1.000	1.000	0.500	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.500	1.000	1.000	1.000	0.500
	1HTG	1.000	1.000	1.000	1.000	1.000	0.500	0.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.500	1.000	1.000	1.000	1.000	0.500
	1HVI	1.000	1.000	1.000	1.000	1.000	1.000	0.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.000
	1HVJ	1.000	1.000	1.000	1.000	1.000	1.000	0.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.000
	1HVK	1.000	1.000	1.000	1.000	1.000	1.000	0.500	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.000
	1HVL	1.000	1.000	1.000	1.000	1.000	1.000	0.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.000
	1HVS	1.000	1.000	1.000	1.000	1.000	1.000	0.500	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.500
	1SBG	1.000	1.000	1.000	0.500	1.000	1.000	0.500	0.500	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.500
	4HVP	1.000	1.000	1.000	1.000	1.000	1.000	0.500	0.500	1.000	1.000	1.000	1.000	0.500	1.000	1.000	1.000	1.000	1.000	1.000	0.500
	4PHV	1.000	1.000	1.000	1.000	1.000	0.500	1.000	0.500	1.000	1.000	1.000	0.500	0.000	0.500	0.500	1.000	1.000	1.000	1.000	0.000
	5HVP	1.000	1.000	1.000	1.000	1.000	1.000	0.500	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.500
	8HVP	1.000	1.000	1.000	1.000	1.000	1.000	0.500	0.500	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	0.000
	9HVP	0.500	1.000	0.500	1.000	1.000	0.500	0.500	0.500	1.000	1.000	0.500	1.000	1.000	0.500	1.000	1.000	0.500	1.000	1.000	0.500

100%	50%	0%
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(b)

Ligands																					
	1HBV	1HEF	1HEG	1HHI	1HIV	1HPS	1HTE	1HTF	1HTG	1HVI	1HVJ	1HVK	1HVL	1HVS	1SBG	4HVP	4PHV	5HVP	8HVP	9HVP	
1HBV	1.000	1.000	1.000	0.500	0.750	0.750	0.250	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.750	0.750	0.500	0.500	0.500	0.500	
1HEF	0.500	0.750	0.500	0.750	0.500	0.500	0.250	0.500	0.500	0.750	0.750	0.500	0.750	0.500	0.500	0.500	0.500	0.500	0.500	0.250	
1HEG	0.500	0.750	1.000	0.250	0.250	0.750	0.250	0.000	0.500	0.250	0.250	0.250	0.500	0.250	0.500	0.750	0.250	0.250	0.500	0.750	
1HHI	0.500	0.500	0.500	1.000	0.750	0.500	0.500	0.750	1.000	1.000	0.750	1.000	0.750	1.000	0.500	0.750	0.750	0.750	0.500	0.000	
1HIV	0.500	0.500	0.500	0.750	0.750	0.500	0.500	0.500	0.750	0.500	0.750	0.750	0.750	0.500	0.500	0.750	0.750	0.500	0.750	0.000	
1HPS	0.750	0.750	0.750	0.500	0.750	0.750	0.250	0.500	0.500	0.250	0.500	0.500	0.500	0.250	0.500	0.750	0.250	0.500	1.000	0.500	
1HTE	0.000	0.250	0.000	0.250	0.500	0.500	1.000	0.750	0.500	0.500	0.500	0.500	0.500	0.750	0.250	0.250	0.500	0.750	0.000	0.250	
1HTF	0.500	0.500	0.500	1.000	0.750	0.500	0.500	1.000	0.750	1.000	1.000	0.750	0.750	1.000	0.500	0.750	0.750	0.500	0.500	0.000	
1HTG	0.500	0.500	0.500	1.000	0.750	0.500	0.750	1.000	1.000	1.000	0.750	0.750	0.500	0.750	0.500	0.500	1.000	1.000	0.500	0.250	
1HVI	0.500	0.500	0.500	1.000	0.500	0.500	0.500	1.000	1.000	1.000	0.750	0.750	0.750	1.000	0.500	0.500	1.000	1.000	0.750	0.000	
1HVJ	0.500	0.500	0.500	0.750	0.750	0.750	0.250	0.750	0.750	0.750	1.000	0.750	1.000	0.750	0.750	0.750	0.750	0.750	0.750	0.000	
1HVK	0.500	0.500	0.500	1.000	0.750	0.750	0.250	0.750	1.000	1.000	1.000	0.750	1.000	0.750	0.750	0.750	0.750	0.750	0.750	0.250	
1HVL	0.500	0.500	0.500	0.750	0.750	0.500	0.250	0.750	0.750	0.750	1.000	1.000	1.000	0.750	0.750	0.750	0.750	0.750	0.750	0.000	
1HVS	0.500	0.500	0.500	1.000	0.750	0.500	0.250	0.750	1.000	1.000	0.750	0.750	0.750	1.000	0.750	0.750	0.750	1.000	0.750	0.250	
1SBG	0.750	0.750	0.750	0.500	1.000	1.000	0.250	0.500	0.500	0.250	0.750	0.750	0.750	0.500	1.000	1.000	0.500	0.500	1.000	0.500	
4HVP	0.500	0.500	0.500	0.750	0.750	0.500	0.250	0.500	0.500	0.250	0.750	0.750	0.500	0.500	0.500	0.750	0.750	0.750	0.750	0.000	
4PHV	0.500	0.500	0.500	0.750	0.500	0.500	0.500	1.000	0.750	0.750	1.000	1.000	1.000	1.000	0.750	0.500	0.750	1.000	0.500	0.000	
5HVP	0.500	0.500	0.500	1.000	0.500	0.500	0.750	1.000	1.000	1.000	0.500	0.750	0.750	0.750	0.500	0.500	0.750	1.000	0.500	0.250	
8HVP	0.500	0.500	0.500	0.500	0.750	0.750	0.500	0.500	0.500	0.500	0.750	0.750	1.000	0.500	0.750	0.750	0.500	0.500	0.750	0.000	
9HVP	0.500	1.000	1.000	0.500	0.750	0.750	0.500	0.500	0.500	0.250	0.500	0.500	0.750	0.250	0.750	0.750	0.500	0.500	0.750	0.500	

100%	75%	50%	25%	0%
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Table S3. Comparison of the LXR β cross-docking experiment with RosettaLigand²⁸ and AutoDock4.

Receptor	Ligand	Galaxy-Dock	Rosetta-Ligand 1 ^a	Rosetta-Ligand 2 ^b	AutoDock4 ^c	LigDock-CSA
1P8D	1P8D	1.33 Å	1.49 Å	1.39 Å	2.11 Å	2.01 Å
	1PQ6	2.41 Å	2.06 Å	2.24 Å	4.82 Å	3.73 Å
	1PQC	1.97 Å	1.78 Å	2.29 Å	4.42 Å	4.58 Å
1PQ6	1P8D	1.75 Å	1.20 Å	1.27 Å	2.91 Å	2.08 Å
	1PQ6	0.89 Å	2.05 Å	2.08 Å	1.45 Å	1.64 Å
	1PQC	1.84 Å	3.46 Å	3.61 Å	3.65 Å	2.41 Å
1PQC	1P8D	1.60 Å	0.98 Å	0.98 Å	4.57 Å	9.27 Å
	1PQ6	1.90 Å	3.70 Å	2.20 Å	2.73 Å	4.31 Å
	1PQC	1.00 Å	0.49 Å	0.53 Å	1.62 Å	1.81 Å
Average		1.63 Å	1.91 Å	1.84 Å	3.14 Å	3.64 Å
Success Rate		88.9%	55.6%	44.4%	22.2%	22.2%

- a. Flexible side-chain with rigid backbone.
b. Backbone flexibility allowed during minimization after side-chain and ligand placing.
c. Rigid docking. The values were taken from the RosettaLigand paper²⁸

Table S4. Cross-docking results of GalaxyDock for the cAPK set. RMSD (in Å) and χ_1 angle accuracy (in %, in parenthesis) are shown.

Receptor \ Ligand	1BKX	1BX6	1STC	1YDT
1BKX	1.11 (100)	2.94 (100)	2.93 (100)	1.37 (100)
1BX6	0.99 (50)	2.96 (100)	4.15 (50)	0.96 (50)
1STC	1.04 (0)	3.75 (50)	0.56 (50)	5.92 (50)
1YDT	1.06 (100)	1.19 (100)	0.97 (100)	1.21 (100)

Table S5. Cross-docking results of GalaxyDock for the diverse set. RMSD (in Å) is shown.

Protein	Receptor	Ligand	Flexible residues	Known pocket		Predicted pocket	
				Galaxy Dock	LigDock CSA	Galaxy Dock	LigDock CSA
Aldose Reductase	2ACR	2FZB	F122, L300	3.651	4.882	3.430	3.653
Anti-Steroid Fab	1DBA	1DBB	W100	4.318	6.568	3.825	6.822
CDK2	1AQ1	1DM2	H84	1.742	6.628	1.206	1.764
	1DM2	1AQ1	I10, H84, Q131, L148	0.512	0.788	1.314	1.124
COX-2	1CX2	3PGH	R120	0.986	1.042	1.010	0.952
	3PGH	1CX2	F518	1.055	1.007	0.829	1.088
Estrogen Receptor	1ERR	3ERT	E419, M421, L525	1.646	1.239	1.894	2.435
	3ERT	1ERR	M421, L525, L539	1.297	2.518	1.563	1.203
Factor Xa	1KSN	1XKA	Y99	1.687	1.585	1.686	2.941
	1XKA	1KSN	Q192	0.797	2.485	4.184	4.892
GSK-3 β	1Q4L	1UV5	R141	0.825	1.219	0.956	1.219
	1UV5	1Q4L	S66, R141, Q185	1.945	2.637	1.974	2.637
Hiv1 RT	1C1C	1RTH	K102, W229, P236	5.273	3.310	3.534	2.908
	1RTH	1C1C	K102, W229, P236	1.482	1.320	1.450	1.368
JNK3	1PMN	1PMV	I124, M146	1.087	1.116	0.919	5.071
	1PMV	1PMN	I124, M146	0.911	5.549	0.920	5.058
LXR β	1P8D	1PQ6	L330, F340, I353	1.955	2.113	1.888	3.274
	1PQ6	1P8D	R319, I353	1.637	1.798	1.749	1.734
Neuroaminidase	1A4Q	1NSC	E274	0.911	1.107	1.135	1.181
	1NSC	1A4Q	E274	1.009	4.476	1.387	2.288
P38 Kinase	1BMK	1DI9	M109	1.758	5.980	3.635	4.006
	1DI9	1BMK	I84, M109	1.197	1.025	1.048	4.023
PKA	1STC	1YDS	T183, F327	1.601	1.283	1.568	1.310

	1YDS	1STC	F54, F327	1.737	3.914	1.728	2.096
PPAR γ	1FM9	2PRG	F282, F363	1.296	5.255	5.655	3.135
	2PRG	1FM9	E259, F282, Q286, F363, L453	4.459	3.830	6.394	7.891
TK	1KI4	1KIM	Y101, Y132, Y172	1.419	1.398	1.462	0.870
	1KIM	1KI4	Y101, Y132	0.894	4.120	0.907	1.367
Trypsin	1PPC	1PPH	Q192	1.069	8.458	0.680	2.904
	1PPH	1PPC	Q192, Y228	1.691	1.655	1.700	1.655

FIGURES

Figure S1. An example of LXR β cross-docking experiments. When the ligand of 1PQC was docked to 1P8D (predicted: red and cyan, native: yellow and green, ligand RMSD: 1.97 Å, and χ_1 accuracy: 66.7%), some π - π interaction was preserved although the predicted pose has some error.

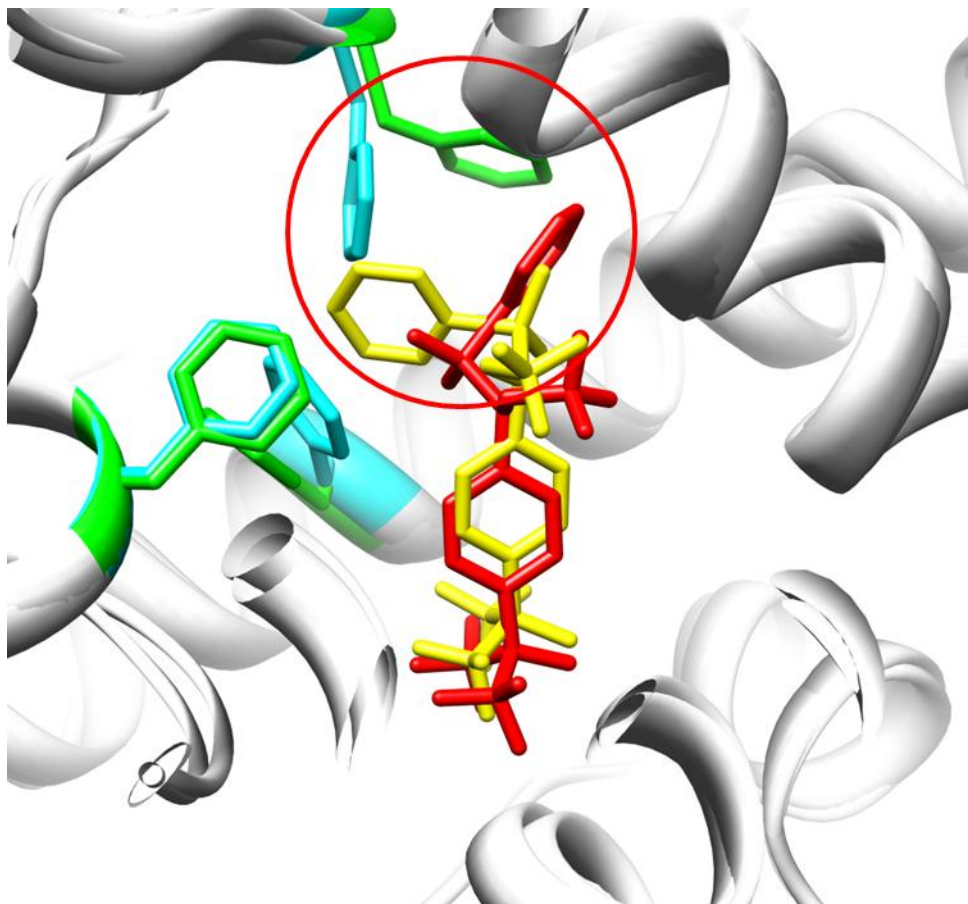


Figure S2. Correlation plot of the diverse set using experimental pocket between degrees of freedom and time. The green line is a trend line except two outliers.

