

Supporting Information

A hybrid docking and machine learning approach to enhance the performance of virtual screening carried out on protein-protein interfaces

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a

1	Selection of PPI sites and protein-ligand complexes	2	Datasets curation PAINS filter ligand preparation	3	Docking with Surflex, rescoring with GOLD fns.
	10 PPIs, 2 structures per target (BAZ2B, Bcl-2, Bcl-xL, BRD4-1, CREBBP, HIV IN, XIAP, Mcl-1, Mdm2, Menin)		ChEMBL, PubChem K_i , K_d , IC_{50} , EC_{50} , % Inhibition Activity cut-off < 10 μ M		10 x 2 dockings, N = 3 poses/cpd, retain best-pose VS performance estimation
4	Calculation of SASA descriptors (bound/unbound)	5	VS performance estimation of SASA descriptors	6	Construction of ML models using SASA descriptors
	32 Protein SASA descriptors 32 Ligand SASA descriptors 16 Prot-Lig SASA descriptors		Area under the curve (AUC), BEDROC, Enrichment factors (EF1/5%)		Estimation of Sensitivity, Specificity, Precision, Accuracy, AUC, J, MCC, k, F_1

b

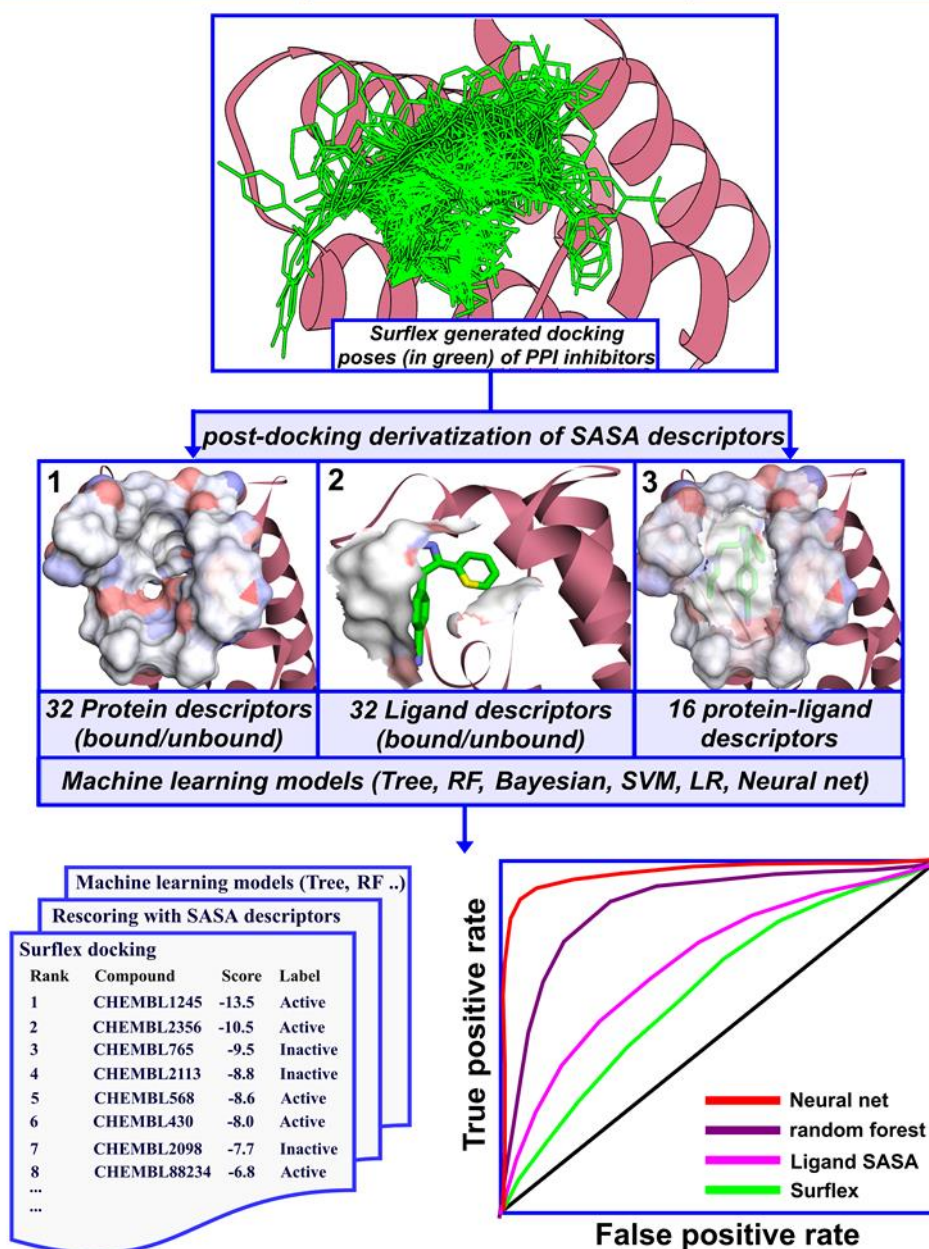
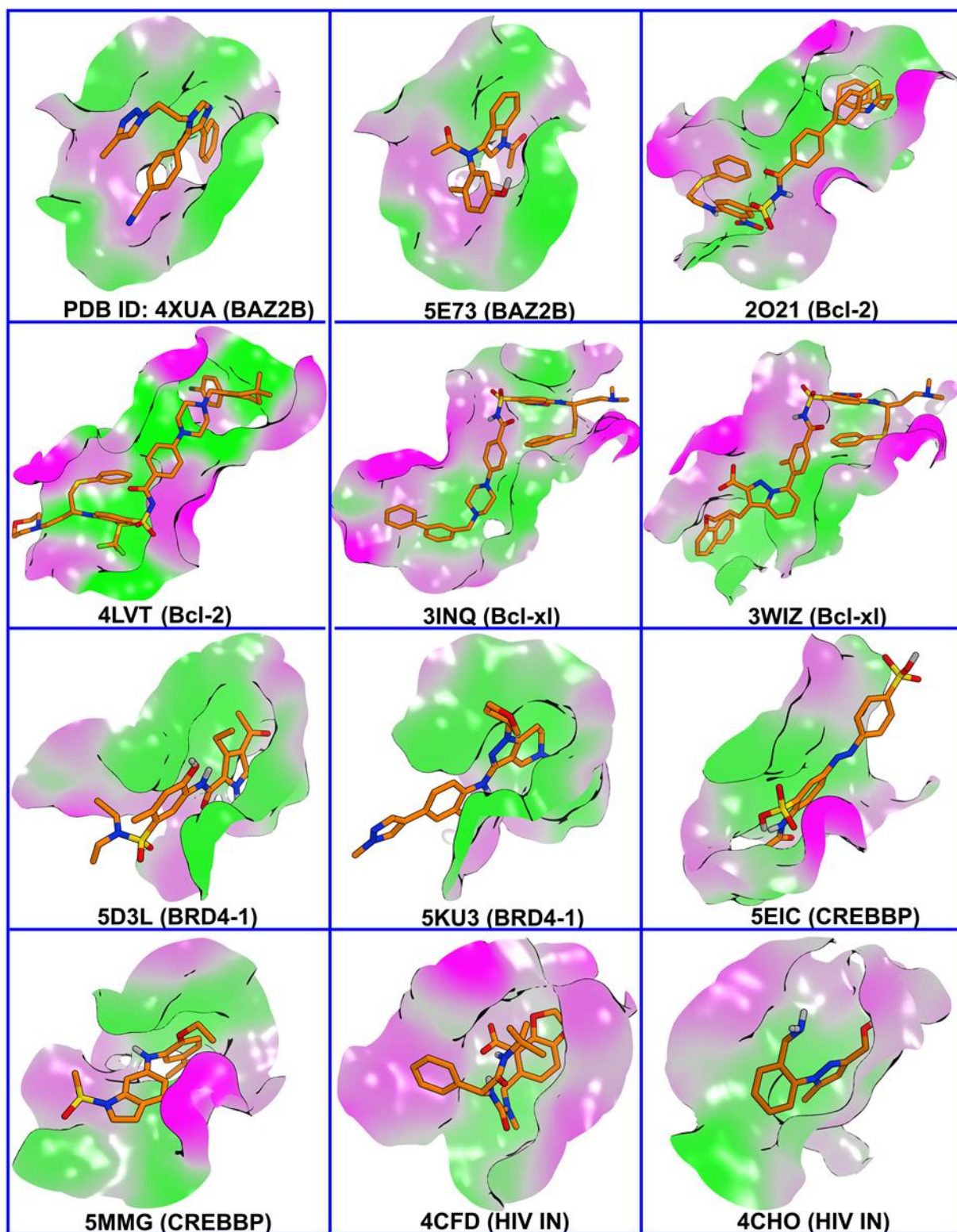


Figure S1. (a) Workflow diagram describing a hybrid computational approach developed in this study that combines structure-based virtual screening, rescoring, and machine learning algorithms: (1) selection of the PPI targets and their protein-ligand structures from the PDB; (2) collecting compounds from ChEMBL and PubChem followed by their categorization into actives or inactives, and then curation and ligand preparation; (3) flexible molecular docking (from the ligand side as two protein structures were used) with the fast ligand docking-scoring protocol of Surflex “pscreen” with several docking poses (e.g., $N = 3$) generated for each compound. These steps were followed by rescoring of all poses with GOLD scoring functions (GoldScore, ChemScore, ASP, ChemPLP, ChemScore RDS) and through consensus scoring utilizing all scoring functions; (4) post-docking derivatization of SASA descriptors of the protein and the ligand in the bound and unbound states for the top-ranked pose of the compounds obtained from Surflex docking. A set of protein-ligand SASA descriptors were calculated by combining protein and ligand SASA values; (5) VS performance estimation of SASA descriptors; (6) construction of machine learning models (Single tree, Bagged forest, Random forest, Bayesian, SVM, Logistic regression, Neural network, and Neural network with bagging) using SASA descriptors.

(b) Schematic representation of the post-processing technique applied to the docking poses and building of the machine learning models. Eighty SASA descriptors were calculated from the top-ranked docking pose of the compounds: (1) 32 protein descriptors; (2) 32 ligand descriptors; and (3) 16 protein-ligand descriptors. These descriptors were used to construct diverse machine learning models. The VS performance of the rescoring methods was assessed by estimating the ROC-based measures such as AUC, log EF1%, EF5%, and BEDROC ($\alpha = 20$). The performance of the machine learning models was estimated by calculating ROC AUC, sensitivity, specificity, precision, concordance (overall accuracy), J, MCC, F_1 , and k.



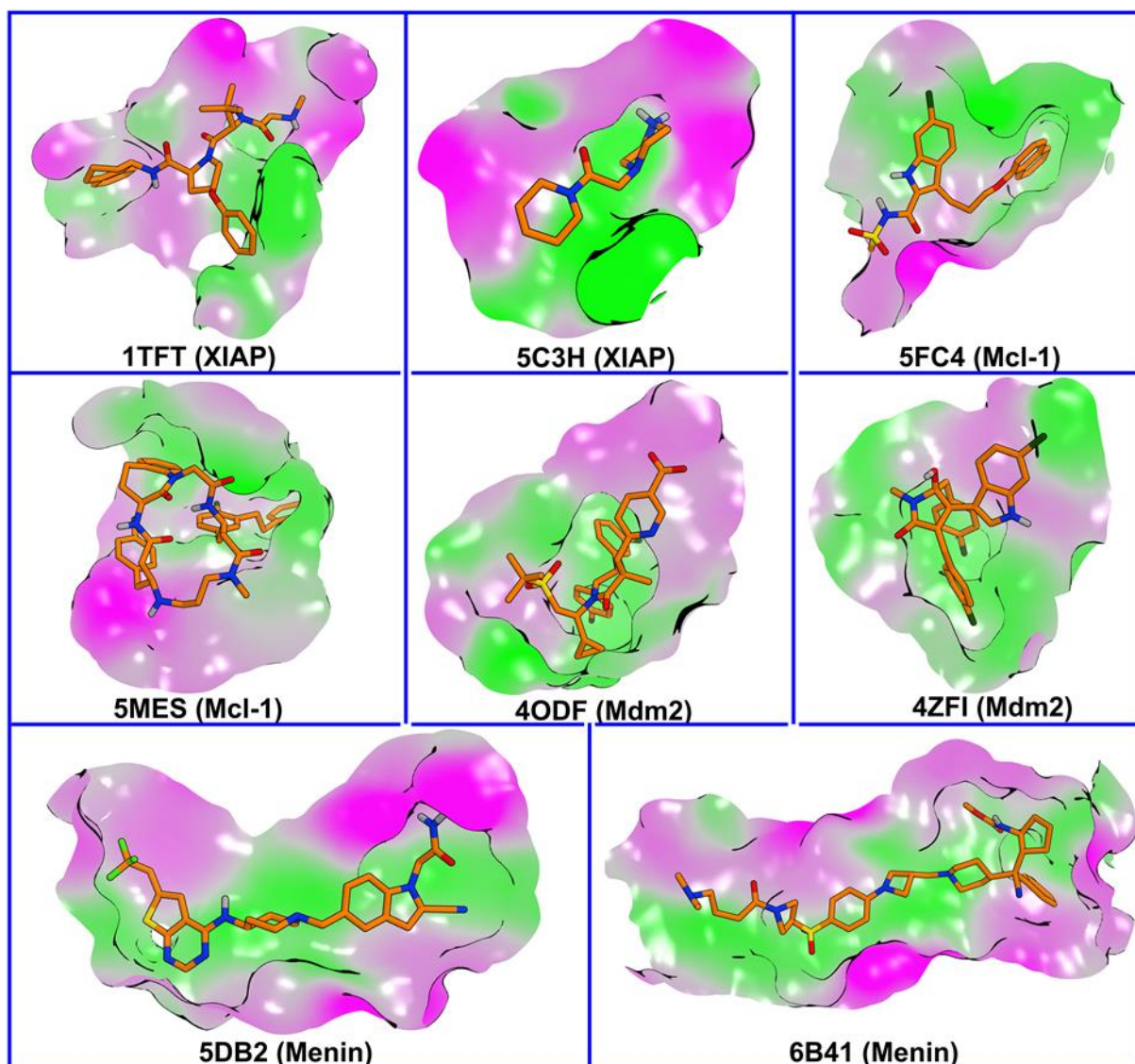


Figure S2. The ligand-binding cavities for the cluster protein representatives of the investigated PPI targets: BAZ2B (PDB ID: 4XUA, 5E73), Bcl-2 (2O21, 4LVT), Bcl-xL (3INQ, 3WIZ), BRD4-1 (5D3L, 5KU3), CREBBP (5EIC, 5MMG), HIV IN (4CFD, 4CHO), XIAP (1TFT, 5C3H), Mcl-1 (5FC4, 5MES), Mdm2 (4ODF, 4ZFI), and Menin (5DB2, 6B41). The binding site surface is colored according to the type of residue surrounding the ligand (magenta: hydrophilic residues, green: hydrophobic residues, and grey: neutral areas). The inhibitor bound to the target proteins is shown in stick (orange) representation. The figure was generated using MOE.

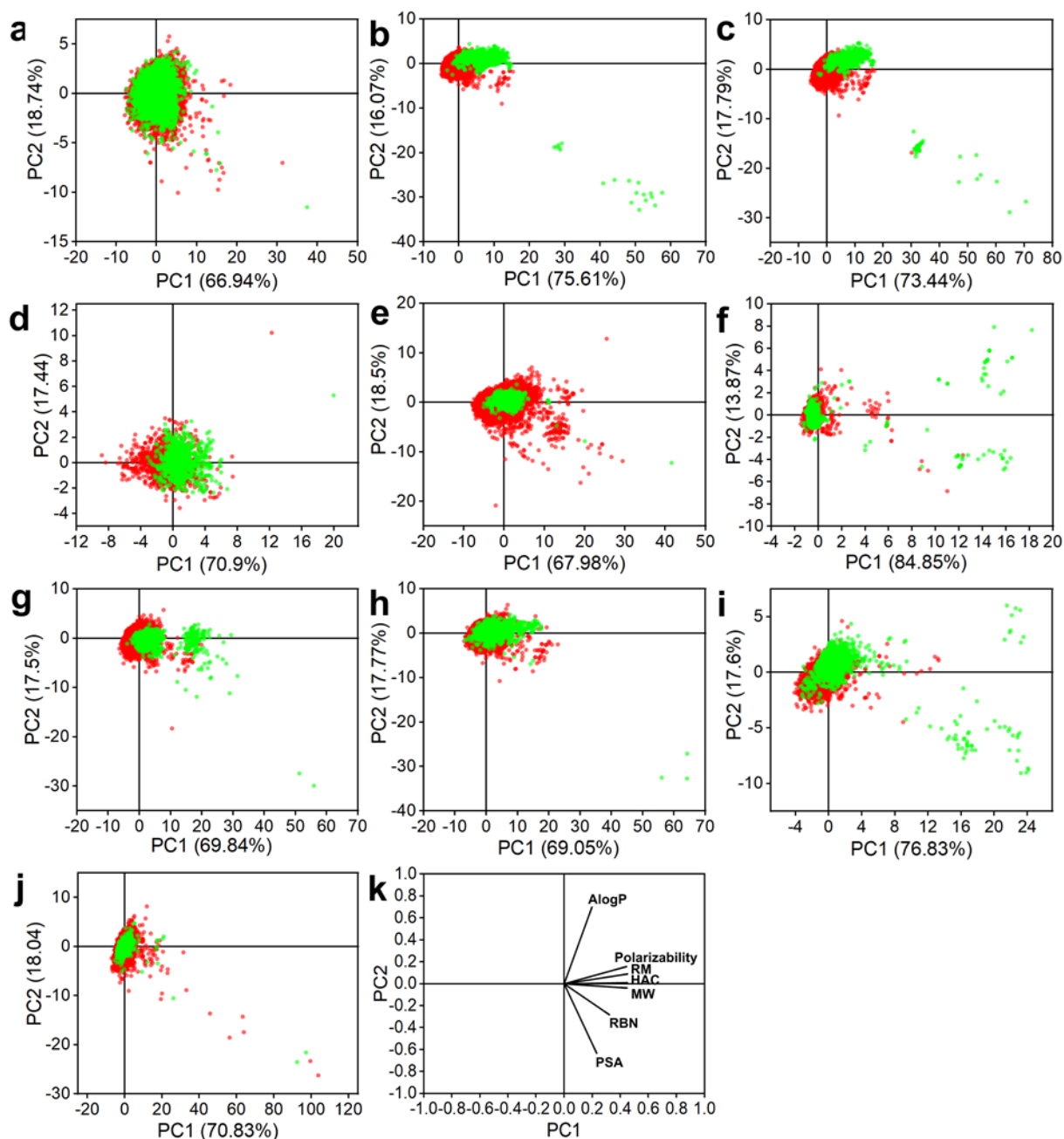


Figure S3. PCA score plots of the PPI datasets. Compounds included in the score plots are (a) BAZ2B, (b) Bcl-2, (c) Bcl-xL, (d) BRD4-1, (e) CREBBP, (f) HIV IN, (g) XIAP, (h) Mcl-1, (i) Mdm2, and (j) Menin. Figure (k) shows the loading plot of descriptors used for PCA analysis. The compounds were described by seven simple descriptors: Number of heavy atoms (HAC), Molecular weight (MW), Number of rotatable bonds (RBN), AlogP, Polar surface area (PSA), Molar refractivity (RM), and Polarizability. Active and inactive compounds are shown in green and red circles, respectively. The first principal component describes in part the size (HAC and MW), and the second gives insights about polarity (PSA) and lipophilicity (AlogP).

Figure S4. Comparison of AUC values (y-axis) attained for ten PPI targets (twenty protein structures) using Surflex and different docking-pose derived SASA descriptors (x-axis). Each boxplot shows twenty AUC values for a given scoring method. A marked increase in mean and scoring performance (measured as AUC) can be seen for several SASA scoring metrics compared to Surflex.

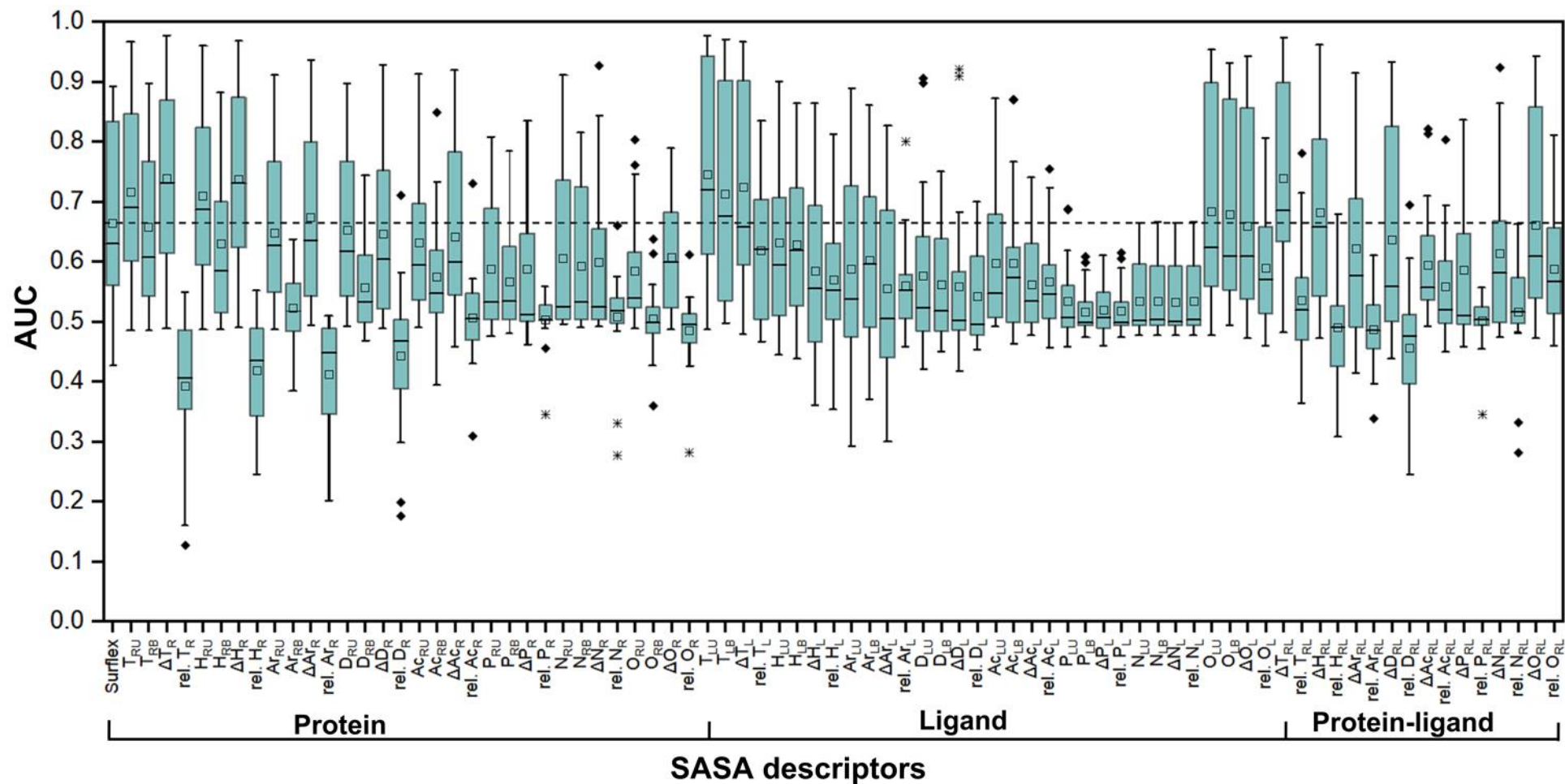


Figure S5. Comparison of EF 1% (a) and EF 5% (b) (y-axis) results attained for ten PPI targets (twenty protein structures) using Surflex and different SASA scoring methods (x-axis). Each boxplot shows twenty EF values for a given scoring method. A marked increase in mean and scoring performance (measured as EF1% and EF5%) can be seen in scoring methods SASA receptor total unbound (T_{RU}), SASA receptor total delta (ΔT_R), SASA receptor hydrophobic delta (ΔH_R), SASA ligand total unbound (T_{LU}), SASA ligand total bound (T_{LB}), SASA ligand total delta (ΔT_L), SASA ligand other unbound (O_{LU}), SASA receptor-ligand total delta (ΔT_{RL}) as compared to the Surflex scoring function.

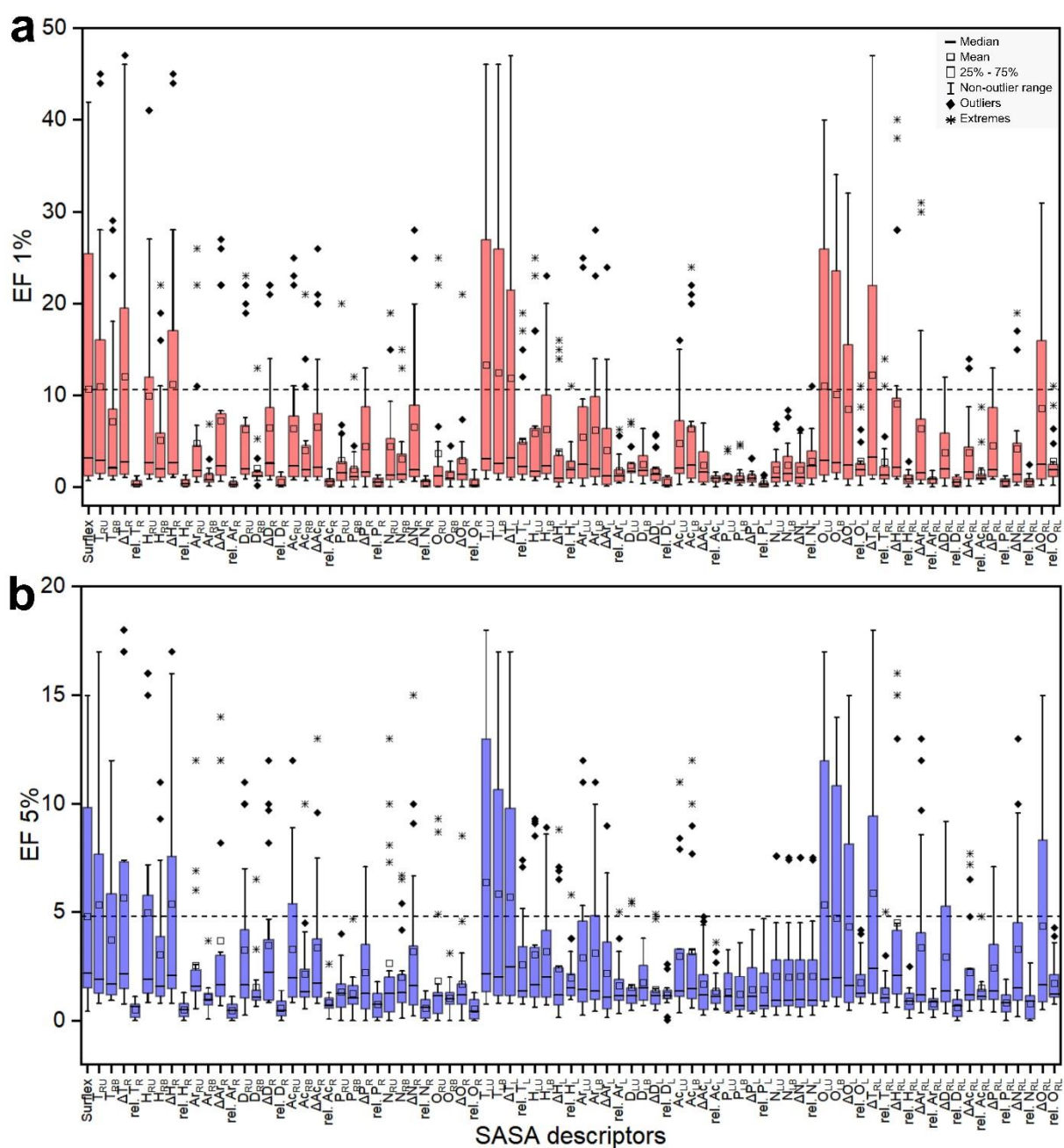
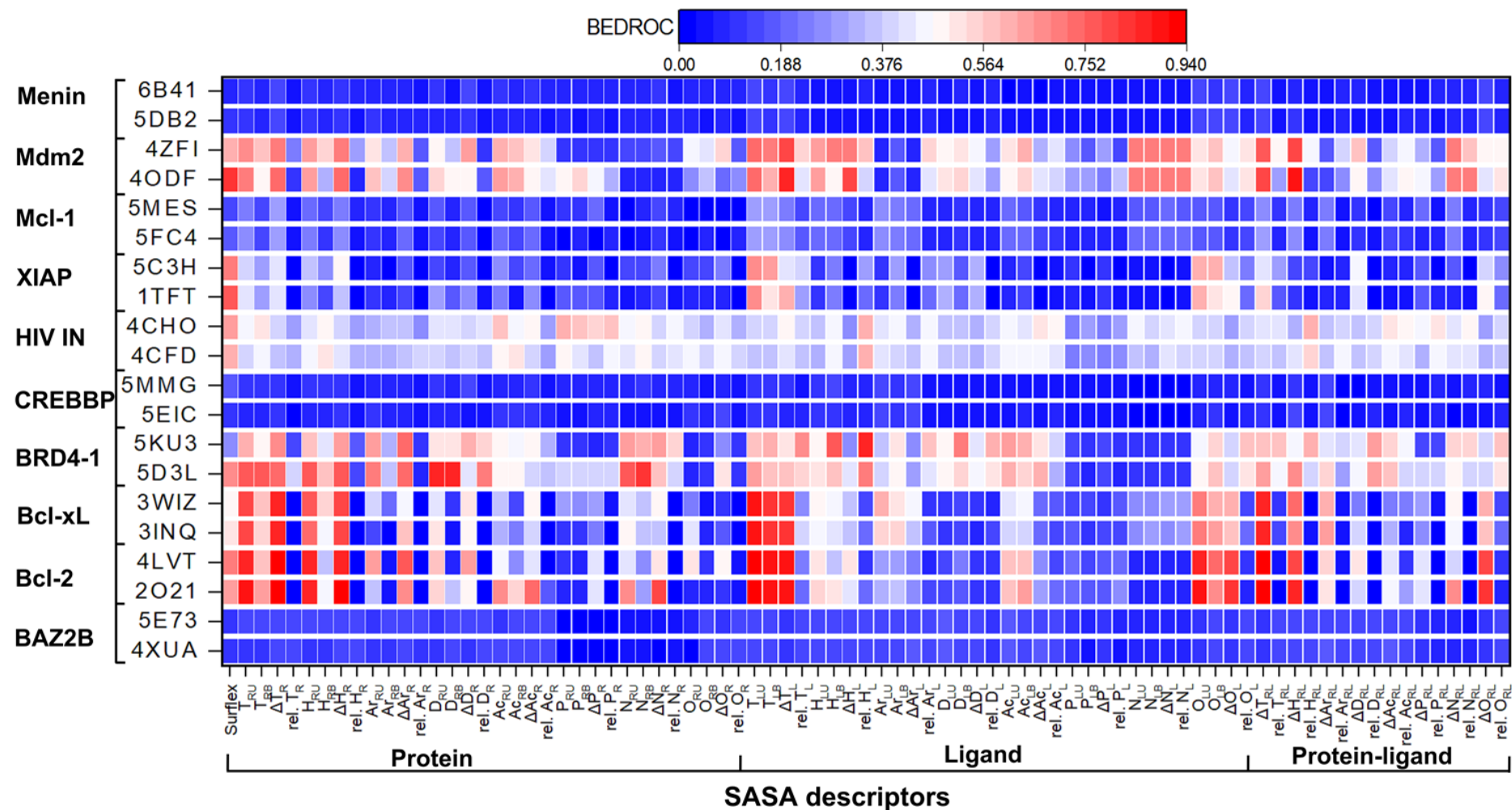


Figure S6. Heat map plot showing the BEDROC values for the ten PPI targets and their protein structures (y-axis) obtained using 32 protein SASA descriptors, 32 ligand SASA descriptors, and 16 protein-ligand SASA descriptors. The calculations were performed for each target-specific set of actives and inactives.



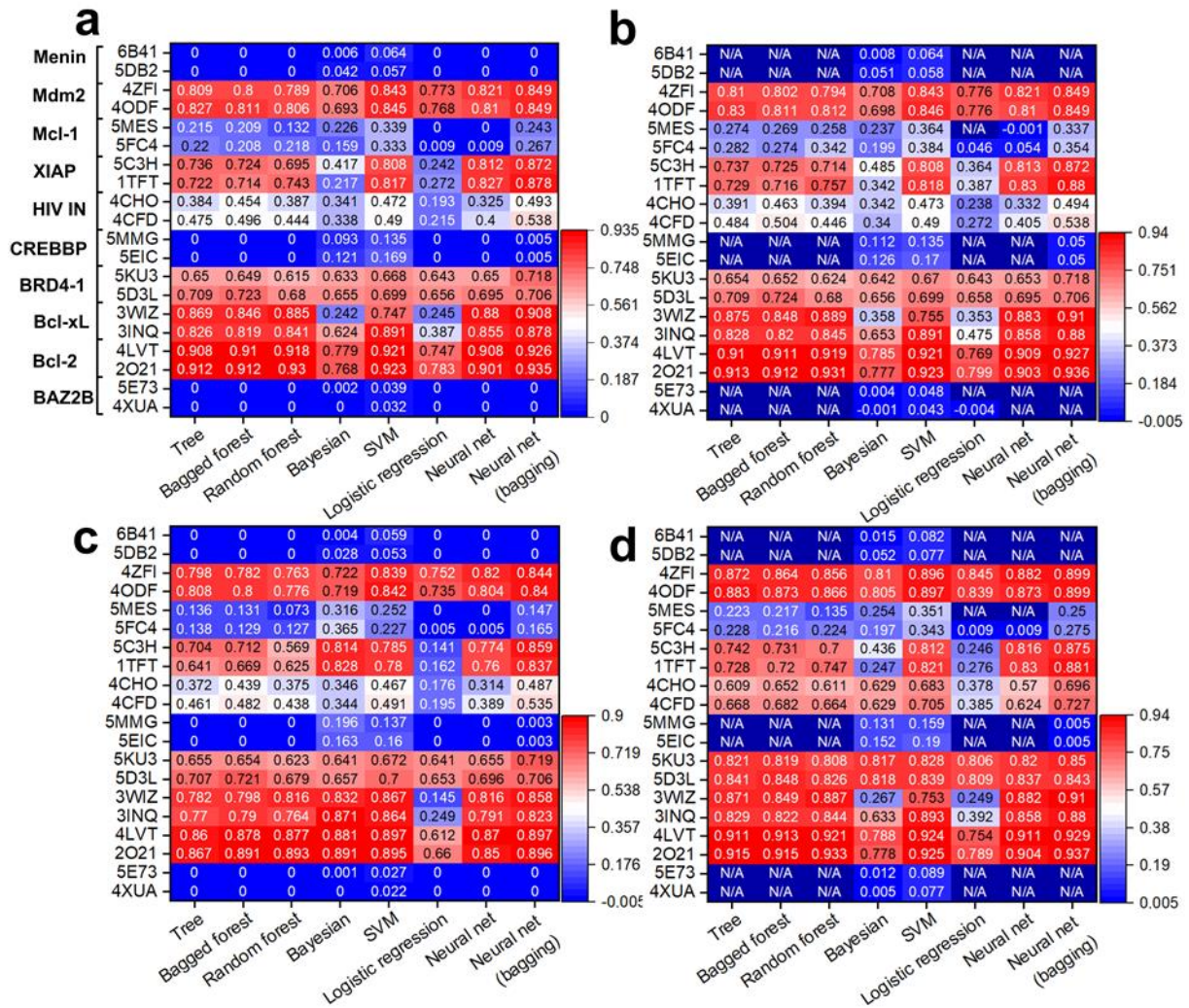


Figure S7. The heat maps show the additional external statistics for the machine learning models: (a) κ (b) MCC (c) J (d) F1.

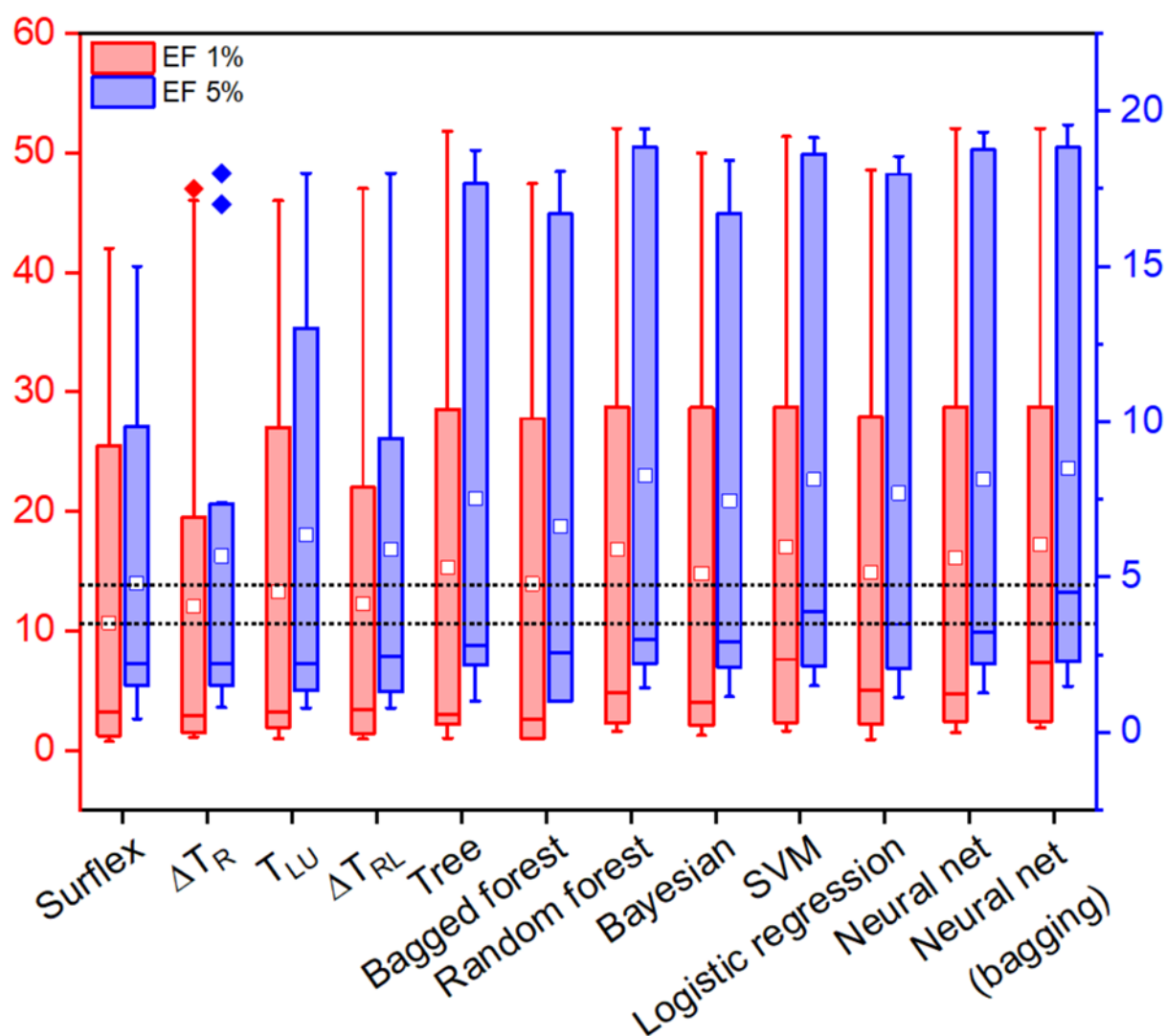


Figure S8. Comparison of EF1% and EF5% (y-axis) results attained for ten PPI targets (twenty protein structures) using Surflex; the best performing receptor SASA descriptor ΔT_R ; the best performing ligand SASA descriptor T_{LU} ; the best performing receptor-ligand SASA descriptor ΔT_{RL} ; and different machine learning methods (x-axis): Each boxplot shows twenty EF values for a given method. The horizontal black dotted lines in the plot indicate a marked increase in mean and scoring performance (measured as EF 1% and EF 5%) of the 3D descriptors and ML models compared to Surflex. Among the different ML methods, neural net (bagging) produced the best results on this PPI dataset.

Figure S9. Relative molecular descriptor importance inferred from the Neural network (bagging) models. Each box plot underlines the relative importance of the descriptors inferred from the 20 Neural networks (bagging) classifier models trained to discriminate between active and inactive PPI molecules. The importance of the descriptors is sorted from highest (SASA receptor hydrophobic delta) to lowest (relative SASA receptor other). The x-axis reports the SASA descriptors, and the y-axis the relative importance of the descriptors.

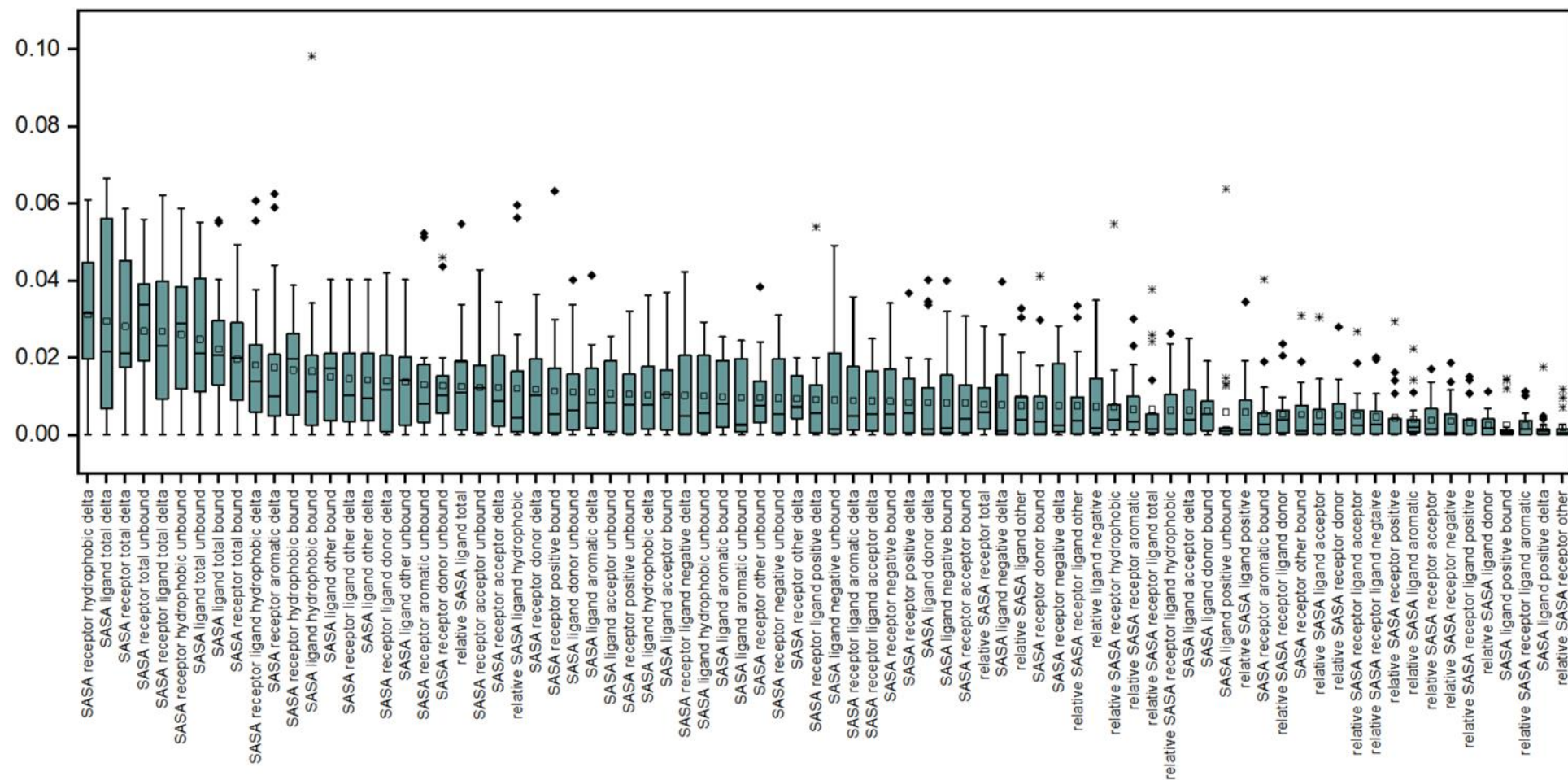


Table S1. The Enrichment Factors (EF 1% and EF 5%) for the protein structures of ten PPI targets obtained after Surflex docking, re-scoring with GOLD scoring functions, and the consensus scoring method. The best enrichment values corresponding to each target protein (across rows) for EF 1% and EF 5% are shown in bold.

Target	PDB ID	Enrichment factors	Surflex	GoldScore	ChemScore	ASP	ChemPLP	ChemScore RDS	Consensus scoring
BAZ2B	4XUA	EF 1%	0.77	0.77	1.2	1.4	0.92	1	1
		EF 5%	0.88	0.94	1.1	1	0.95	0.98	1
	5E73	EF 1%	0.86	0.7	1.3	1	1	1.1	0.93
		EF 5%	0.89	0.84	1	0.98	0.93	1	0.96
Bcl-2	2O21	EF 1%	25	26	23	22	28	6.6	21
		EF 5%	11	11	10	11	13	3.4	9.8
	4LVT	EF 1%	28	27	28	28	28	16	28
		EF 5%	12	12	12	12	13	6.2	13
Bcl-xL	3INQ	EF 1%	26	25	19	20	27	7.3	21
		EF 5%	10	8.8	8	7.8	9.9	3.6	8.6
	3WIZ	EF 1%	27	30	27	21	33	6.5	30
		EF 5%	9.7	9.9	10	9.1	12	3.3	11
BRD4-1	5D3L	EF 1%	0.96	1.4	1.9	1.9	1.9	2.2	1.9
		EF 5%	1.4	1.7	1.9	1.7	1.9	1.9	1.8
	5KU3	EF 1%	0.72	1.3	0.6	1.8	0.84	0.48	1.3
		EF 5%	0.43	1.4	1.2	1.3	1.1	1.1	1.4
CREBBP	5EIC	EF 1%	1.8	1.6	2.8	1.8	2.8	1.4	2.9
		EF 5%	1.6	1.9	2.1	2.7	2.2	1.3	2.6
	5MMG	EF 1%	5.1	2.3	2.7	2.5	2.4	1.1	2.9
		EF 5%	2.7	2.1	1.9	2.4	1.9	1.3	2
HIV IN	4CFD	EF 1%	1.4	0.35	0.7	1.2	0.7	0.35	1.4
		EF 5%	1.6	0.8	0.94	1.4	1.1	0.82	1.3
	4CHO	EF 1%	1.5	0.46	0.81	1.7	1.2	0.7	1.3
		EF 5%	1.6	0.96	0.91	1.4	1.3	0.77	1.3
XIAP	1TFT	EF 1%	42	31	31	20	30	31	29
		EF 5%	15	12	11	9.8	11	10	11
	5C3H	EF 1%	33	9.3	23	24	33	29	35
		EF 5%	14	6.8	9.7	9.5	12	11	12
Mcl-1	5FC4	EF 1%	6.1	8.3	11	12	11	9.4	10
		EF 5%	2.8	3.9	4.4	3.6	4.2	4	4.1
	5MES	EF 1%	3.3	7.4	5.5	3.6	5.4	3.9	5.8
		EF 5%	2.5	3.5	2.7	2.5	2.6	2.2	2.8
Mdm2	4ODF	EF 1%	3	3	2.8	2.9	2.8	2.8	2.8
		EF 5%	2.9	2.9	2.7	2.7	2.7	2.2	2.8
	4ZFI	EF 1%	2.5	2.8	1.4	2	1.3	0.67	1.7
		EF 5%	1.9	2.4	1.4	1.6	1.2	0.7	1.5
Menin	5DB2	EF 1%	3.4	6	2	5.3	5.3	1.6	6
		EF 5%	1.9	2.4	1.9	2.2	2.1	1.7	2.3
	6B41	EF 1%	1	3.3	1.7	3	3.1	1.1	2.4
		EF 5%	1.2	1.9	1.1	1.7	1.6	0.94	1.2

Table S2. The AUC values for the PPI datasets screened using **32 protein SASA descriptors**: SASA receptor total unbound (T_{RU}), SASA receptor total bound (T_{RB}), SASA receptor total delta (ΔT_R), relative SASA receptor total (rel. T_R), SASA receptor hydrophobic unbound (H_{RU}), SASA receptor hydrophobic bound (H_{RB}), SASA receptor hydrophobic delta (ΔH_R), relative SASA receptor hydrophobic (rel. H_R), SASA receptor aromatic unbound (Ar_{RU}), SASA receptor aromatic bound (Ar_{RB}), SASA receptor aromatic delta (ΔAr_R), relative SASA receptor aromatic (rel. Ar_R), SASA receptor donor unbound (D_{RU}), SASA receptor donor bound (D_{RB}), SASA receptor donor delta (ΔD_R), relative SASA receptor donor (rel. D_R), SASA receptor acceptor unbound (Ac_{RU}), SASA receptor acceptor bound (Ac_{RB}), SASA receptor acceptor delta (ΔAc_R), relative SASA receptor acceptor (rel. Ac_R), SASA receptor positive unbound (P_{RU}), SASA receptor positive bound (P_{RB}), SASA receptor positive delta (ΔP_R), relative SASA receptor positive (rel. P_R), SASA receptor negative unbound (N_{RU}), SASA receptor negative bound (N_{RB}), SASA receptor negative delta (ΔN_R), relative SASA receptor negative (rel. N_R), SASA receptor other unbound (O_{RU}), SASA receptor other bound (O_{RB}), SASA receptor other delta (ΔO_R), relative SASA receptor other (rel. O_R); **32 ligand SASA descriptors**: SASA ligand total unbound (T_{LU}), SASA ligand total bound (T_{LB}), SASA ligand total delta (ΔT_L), relative SASA ligand total (rel. T_L), SASA ligand hydrophobic unbound (H_{LU}), SASA ligand hydrophobic bound (H_{LB}), SASA ligand hydrophobic delta (ΔH_L), relative SASA ligand hydrophobic (rel. H_L), SASA ligand aromatic unbound (Ar_{LU}), SASA ligand aromatic bound (Ar_{LB}), SASA ligand aromatic delta (ΔAr_L), relative SASA ligand aromatic (rel. Ar_L), SASA ligand donor unbound (D_{LU}), SASA ligand donor bound (D_{LB}), SASA ligand donor delta (ΔD_L), relative SASA ligand donor (rel. D_L), SASA ligand acceptor unbound (Ac_{LU}), SASA ligand acceptor bound (Ac_{LB}), SASA ligand acceptor delta (ΔAc_L), relative SASA ligand acceptor (rel. Ac_L), SASA ligand positive unbound (P_{LU}), SASA ligand positive bound (P_{LB}), SASA ligand positive delta (ΔP_L), relative SASA ligand positive (rel. P_L), SASA negative unbound (N_{LU}), SASA ligand negative bound (N_{LB}), SASA ligand negative delta (ΔN_L), relative SASA ligand negative (rel. N_L), SASA ligand other unbound (O_{LU}), SASA ligand other bound (O_{LB}), SASA ligand other delta (ΔO_L), relative SASA ligand other (rel. O_L); and **16 protein-ligand SASA descriptors**: SASA receptor ligand total delta (ΔT_{RL}), relative SASA receptor ligand total (rel. T_{RL}), SASA receptor ligand hydrophobic delta (ΔH_{RL}), relative SASA receptor ligand hydrophobic (rel. H_{RL}), SASA receptor ligand aromatic delta (ΔAr_{RL}), relative SASA receptor ligand aromatic (rel. Ar_{RL}), SASA receptor ligand donor delta (ΔD_{RL}), relative SASA receptor ligand donor (rel. D_{RL}), SASA receptor ligand acceptor delta (ΔAc_{RL}),

relative SASA receptor ligand acceptor (rel. Ac_{RL}), SASA receptor ligand positive delta (ΔP_{RL}), relative SASA receptor ligand positive (rel. P_{RL}), SASA receptor ligand negative delta (ΔN_{RL}), relative SASA receptor ligand negative (rel. N_{RL}), SASA receptor ligand other delta (ΔO_{RL}), relative SASA receptor ligand other (rel. O_{RL}). The best AUC score corresponding to each target protein (across columns) is indicated in bold and highlighted in green.

SASA descriptors	BAZ2B		BCL2		BCLXL		BRD4-1		CREBBP		HIV-IN		XIAP		MCL1		MDM2		Menin	
	4XUA	5E73	2O21	4LVT	3INQ	3WIZ	5D3L	5KU3	5EIC	5MMG	4CFD	4CHO	1TFT	5C3H	5FC4	5MES	4ODF	4ZFI	5DB2	6B41
Surflex	0.491	0.482	0.857	0.886	0.844	0.823	0.696	0.426	0.604	0.662	0.627	0.631	0.888	0.892	0.585	0.59	0.64	0.57	0.548	0.517
T_{RU}	0.485	0.485	0.965	0.966	0.944	0.950	0.810	0.738	0.594	0.639	0.605	0.613	0.857	0.835	0.647	0.625	0.733	0.746	0.535	0.531
T_{RB}	0.486	0.484	0.898	0.896	0.868	0.892	0.742	0.606	0.520	0.608	0.582	0.590	0.777	0.758	0.562	0.567	0.621	0.664	0.519	0.502
DT_R	0.488	0.489	0.976	0.977	0.960	0.963	0.805	0.789	0.662	0.632	0.606	0.619	0.872	0.869	0.675	0.670	0.830	0.805	0.544	0.542
rel. T_R	0.491	0.487	0.159	0.127	0.167	0.311	0.550	0.393	0.392	0.503	0.475	0.497	0.360	0.348	0.364	0.418	0.396	0.458	0.486	0.467
H_{RU}	0.487	0.486	0.955	0.959	0.938	0.941	0.790	0.718	0.580	0.628	0.642	0.634	0.804	0.843	0.654	0.608	0.723	0.744	0.528	0.533
H_{RB}	0.487	0.486	0.858	0.818	0.862	0.881	0.648	0.579	0.487	0.590	0.570	0.596	0.667	0.731	0.563	0.563	0.509	0.666	0.506	0.518
DH_R	0.489	0.491	0.968	0.962	0.945	0.946	0.821	0.781	0.665	0.628	0.661	0.626	0.851	0.896	0.679	0.618	0.832	0.793	0.542	0.538
rel. H_R	0.490	0.487	0.306	0.343	0.340	0.307	0.432	0.435	0.386	0.509	0.457	0.509	0.246	0.352	0.395	0.486	0.344	0.551	0.480	0.500
Ar_{RU}	0.487	0.494	0.824	0.911	0.772	0.821	0.804	0.760	0.604	0.559	0.555	0.544	0.646	0.667	0.570	0.550	0.649	0.672	0.547	0.510
Ar_{RB}	0.486	0.490	0.463	0.638	0.461	0.594	0.599	0.490	0.530	0.542	0.539	0.545	0.582	0.384	0.477	0.512	0.521	0.593	0.481	0.514
DAr_R	0.495	0.502	0.927	0.936	0.896	0.868	0.801	0.799	0.545	0.542	0.551	0.548	0.656	0.681	0.617	0.587	0.781	0.704	0.527	0.496
rel. Ar_R	0.490	0.487	0.202	0.318	0.208	0.375	0.353	0.283	0.502	0.503	0.508	0.475	0.409	0.336	0.434	0.437	0.459	0.463	0.479	0.509
D_{RU}	0.496	0.493	0.845	0.897	0.838	0.820	0.758	0.621	0.515	0.635	0.553	0.516	0.746	0.777	0.570	0.608	0.667	0.616	0.548	0.537
D_{RB}	0.500	0.499	0.628	0.580	0.501	0.617	0.743	0.606	0.498	0.528	0.539	0.504	0.659	0.584	0.495	0.546	0.655	0.469	0.507	0.469
DD_R	0.489	0.490	0.881	0.928	0.872	0.874	0.488	0.519	0.522	0.649	0.518	0.527	0.758	0.708	0.584	0.624	0.623	0.745	0.551	0.555
rel. D_R	0.503	0.500	0.298	0.198	0.175	0.332	0.711	0.582	0.486	0.431	0.515	0.503	0.535	0.454	0.436	0.417	0.496	0.358	0.479	0.449
Ac_{RU}	0.497	0.494	0.912	0.833	0.774	0.832	0.489	0.498	0.626	0.584	0.548	0.586	0.704	0.689	0.601	0.570	0.670	0.633	0.521	0.552
Ac_{RB}	0.501	0.500	0.849	0.734	0.732	0.651	0.519	0.462	0.598	0.559	0.519	0.534	0.393	0.565	0.566	0.508	0.631	0.608	0.519	0.535
DAc_R	0.494	0.490	0.918	0.826	0.794	0.821	0.459	0.553	0.634	0.592	0.550	0.595	0.856	0.771	0.599	0.604	0.602	0.612	0.510	0.540
rel. Ac_R	0.504	0.504	0.729	0.488	0.549	0.469	0.556	0.430	0.542	0.509	0.460	0.467	0.309	0.483	0.484	0.459	0.571	0.563	0.512	0.514

P _{RU}	0.500	0.500	0.735	0.776	0.699	0.808	0.502	0.501	0.474	0.531	0.535	0.534	0.767	0.679	0.502	0.599	0.593	0.503	0.506	0.508
P _{RB}	0.500	0.500	0.629	0.642	0.619	0.761	0.502	0.501	0.480	0.532	0.544	0.534	0.785	0.644	0.515	0.538	0.588	0.503	0.502	0.509
DP _R	0.500	0.500	0.831	0.834	0.731	0.803	0.502	0.501	0.462	0.507	0.518	0.524	0.648	0.631	0.508	0.646	0.588	0.504	0.506	0.500
rel. P _R	0.500	0.500	0.492	0.345	0.503	0.529	0.501	0.501	0.522	0.524	0.542	0.533	0.537	0.455	0.513	0.488	0.558	0.503	0.503	0.509
N _{RU}	0.497	0.496	0.911	0.810	0.833	0.796	0.728	0.587	0.500	0.521	0.524	0.526	0.524	0.740	0.527	0.561	0.505	0.502	0.515	0.498
N _{RB}	0.497	0.497	0.814	0.759	0.775	0.765	0.726	0.583	0.500	0.521	0.539	0.541	0.503	0.720	0.520	0.541	0.505	0.502	0.524	0.490
DN _R	0.499	0.498	0.927	0.844	0.797	0.814	0.623	0.582	0.497	0.515	0.492	0.504	0.541	0.689	0.532	0.584	0.505	0.502	0.505	0.509
rel. N _R	0.497	0.497	0.331	0.277	0.518	0.521	0.660	0.576	0.500	0.520	0.541	0.559	0.497	0.567	0.520	0.540	0.505	0.501	0.519	0.485
O _{RU}	0.489	0.490	0.738	0.804	0.762	0.746	0.537	0.540	0.563	0.549	0.533	0.531	0.529	0.609	0.533	0.500	0.589	0.624	0.514	0.502
O _{RB}	0.493	0.494	0.614	0.556	0.637	0.498	0.426	0.465	0.496	0.522	0.501	0.475	0.360	0.560	0.522	0.500	0.472	0.525	0.485	0.492
DO _R	0.487	0.489	0.732	0.789	0.734	0.705	0.639	0.583	0.614	0.550	0.535	0.559	0.735	0.648	0.521	0.500	0.623	0.658	0.524	0.510
rel. O _R	0.498	0.497	0.611	0.539	0.515	0.461	0.426	0.465	0.461	0.510	0.501	0.475	0.282	0.526	0.522	0.500	0.469	0.453	0.485	0.491
T _{LU}	0.487	0.486	0.977	0.978	0.970	0.968	0.752	0.744	0.638	0.641	0.607	0.616	0.942	0.944	0.691	0.697	0.840	0.844	0.547	0.543
T _{LB}	0.498	0.499	0.970	0.969	0.961	0.952	0.710	0.777	0.622	0.597	0.537	0.532	0.880	0.926	0.670	0.682	0.646	0.759	0.521	0.530
DT _L	0.480	0.478	0.964	0.966	0.950	0.958	0.711	0.580	0.605	0.616	0.638	0.651	0.927	0.873	0.661	0.653	0.842	0.809	0.551	0.543
rel. T _L	0.505	0.508	0.686	0.721	0.833	0.734	0.667	0.762	0.588	0.544	0.499	0.468	0.688	0.833	0.619	0.626	0.504	0.624	0.466	0.494
H _{LU}	0.510	0.509	0.900	0.899	0.840	0.843	0.543	0.532	0.634	0.634	0.499	0.504	0.556	0.558	0.671	0.674	0.705	0.709	0.448	0.445
H _{LB}	0.508	0.511	0.863	0.789	0.840	0.798	0.665	0.724	0.608	0.622	0.544	0.539	0.613	0.719	0.633	0.656	0.457	0.579	0.438	0.448
DH _L	0.508	0.505	0.820	0.863	0.757	0.798	0.472	0.380	0.612	0.602	0.469	0.478	0.460	0.361	0.643	0.638	0.723	0.664	0.461	0.453
rel. H _L	0.502	0.507	0.619	0.505	0.677	0.568	0.689	0.777	0.545	0.554	0.555	0.550	0.644	0.813	0.550	0.568	0.352	0.469	0.465	0.478
Ar _{LU}	0.522	0.521	0.836	0.829	0.877	0.890	0.510	0.501	0.652	0.650	0.471	0.478	0.554	0.562	0.725	0.727	0.292	0.307	0.422	0.417
Ar _{LB}	0.510	0.513	0.788	0.767	0.852	0.861	0.578	0.630	0.586	0.604	0.495	0.489	0.621	0.720	0.679	0.695	0.371	0.422	0.412	0.427
DAr _L	0.522	0.520	0.769	0.788	0.805	0.826	0.489	0.436	0.649	0.640	0.475	0.481	0.459	0.365	0.683	0.685	0.320	0.299	0.440	0.427
rel. Ar _L	0.496	0.501	0.562	0.533	0.671	0.549	0.582	0.646	0.535	0.556	0.512	0.511	0.643	0.801	0.564	0.574	0.470	0.560	0.458	0.472
D _{LU}	0.487	0.487	0.731	0.730	0.640	0.645	0.524	0.530	0.421	0.421	0.481	0.499	0.905	0.898	0.584	0.586	0.520	0.521	0.456	0.456
D _{LB}	0.497	0.491	0.712	0.742	0.705	0.680	0.516	0.562	0.458	0.451	0.477	0.491	0.750	0.543	0.589	0.595	0.519	0.516	0.455	0.477
DD _L	0.487	0.489	0.683	0.654	0.579	0.590	0.510	0.485	0.420	0.419	0.489	0.511	0.909	0.921	0.555	0.558	0.493	0.494	0.463	0.454
rel. D _L	0.495	0.489	0.666	0.698	0.699	0.661	0.510	0.557	0.461	0.454	0.485	0.498	0.632	0.458	0.572	0.585	0.477	0.481	0.463	0.479
Ac _{LU}	0.496	0.496	0.871	0.869	0.731	0.737	0.675	0.680	0.528	0.525	0.518	0.515	0.502	0.511	0.586	0.583	0.563	0.572	0.493	0.491
Ac _{LB}	0.495	0.498	0.870	0.870	0.739	0.766	0.569	0.633	0.589	0.549	0.464	0.468	0.528	0.530	0.580	0.586	0.595	0.617	0.475	0.502

DAc _L	0.499	0.496	0.740	0.723	0.646	0.629	0.659	0.630	0.491	0.518	0.550	0.548	0.477	0.498	0.539	0.538	0.529	0.512	0.505	0.491
rel. Ac _L	0.497	0.500	0.754	0.724	0.655	0.700	0.523	0.570	0.593	0.545	0.458	0.470	0.540	0.528	0.548	0.556	0.575	0.597	0.476	0.513
P _{LU}	0.511	0.510	0.688	0.686	0.618	0.611	0.495	0.494	0.491	0.492	0.459	0.459	0.542	0.577	0.539	0.539	0.504	0.503	0.481	0.482
P _{LB}	0.503	0.505	0.608	0.599	0.549	0.585	0.496	0.498	0.498	0.497	0.474	0.480	0.497	0.491	0.526	0.536	0.512	0.486	0.485	0.493
DP _L	0.510	0.509	0.610	0.609	0.585	0.550	0.496	0.494	0.491	0.491	0.461	0.462	0.546	0.581	0.524	0.511	0.487	0.507	0.482	0.482
rel. P _L	0.503	0.505	0.615	0.605	0.552	0.589	0.496	0.498	0.498	0.497	0.474	0.480	0.497	0.491	0.527	0.537	0.514	0.485	0.485	0.493
N _{LU}	0.500	0.500	0.519	0.519	0.665	0.665	0.493	0.493	0.476	0.476	0.492	0.495	0.501	0.501	0.599	0.599	0.595	0.595	0.492	0.492
N _{LB}	0.500	0.500	0.518	0.520	0.666	0.664	0.493	0.495	0.477	0.476	0.492	0.492	0.503	0.504	0.594	0.593	0.594	0.591	0.492	0.496
DN _L	0.500	0.500	0.519	0.518	0.664	0.666	0.493	0.493	0.476	0.476	0.492	0.492	0.499	0.499	0.597	0.598	0.594	0.591	0.492	0.491
rel. N _L	0.500	0.500	0.518	0.520	0.667	0.664	0.493	0.495	0.477	0.476	0.493	0.493	0.504	0.504	0.594	0.593	0.594	0.591	0.492	0.496
O _{LU}	0.477	0.477	0.953	0.952	0.897	0.897	0.645	0.633	0.555	0.559	0.604	0.609	0.931	0.933	0.507	0.505	0.657	0.655	0.611	0.608
O _{LB}	0.494	0.494	0.906	0.923	0.885	0.858	0.680	0.698	0.589	0.567	0.556	0.550	0.893	0.932	0.546	0.541	0.623	0.635	0.598	0.583
DO _L	0.472	0.471	0.942	0.940	0.865	0.885	0.576	0.543	0.528	0.548	0.611	0.615	0.901	0.850	0.483	0.478	0.628	0.623	0.602	0.604
rel. O _L	0.509	0.512	0.517	0.659	0.730	0.632	0.657	0.679	0.574	0.534	0.498	0.460	0.693	0.806	0.570	0.570	0.564	0.572	0.532	0.509
DT _{RL}	0.483	0.482	0.971	0.973	0.957	0.962	0.775	0.696	0.638	0.635	0.629	0.645	0.918	0.880	0.674	0.668	0.860	0.822	0.549	0.543
rel. T _{RL}	0.498	0.498	0.365	0.388	0.567	0.556	0.696	0.714	0.502	0.536	0.471	0.468	0.578	0.781	0.548	0.565	0.456	0.581	0.469	0.477
DH _{RL}	0.501	0.499	0.960	0.954	0.922	0.941	0.652	0.545	0.675	0.647	0.545	0.539	0.697	0.633	0.699	0.662	0.830	0.775	0.483	0.472
rel. H _{RL}	0.491	0.492	0.415	0.377	0.504	0.381	0.569	0.657	0.413	0.507	0.523	0.544	0.485	0.679	0.436	0.529	0.307	0.525	0.460	0.486
DA _{rRL}	0.520	0.519	0.903	0.914	0.912	0.906	0.638	0.588	0.651	0.640	0.496	0.508	0.567	0.484	0.706	0.700	0.415	0.416	0.454	0.486
rel. A _{rRL}	0.482	0.488	0.339	0.401	0.397	0.457	0.492	0.528	0.477	0.481	0.527	0.526	0.572	0.611	0.496	0.475	0.453	0.575	0.455	0.490
DD _{RL}	0.487	0.490	0.868	0.903	0.845	0.806	0.521	0.498	0.437	0.481	0.500	0.514	0.928	0.934	0.595	0.628	0.605	0.669	0.511	0.501
rel. D _{RL}	0.502	0.500	0.323	0.268	0.245	0.407	0.694	0.605	0.532	0.500	0.522	0.496	0.391	0.320	0.465	0.440	0.549	0.404	0.484	0.468
DAC _{RL}	0.497	0.493	0.821	0.813	0.708	0.695	0.650	0.634	0.533	0.541	0.553	0.575	0.563	0.584	0.552	0.558	0.547	0.543	0.506	0.500
rel. AC _{RL}	0.501	0.503	0.803	0.672	0.653	0.695	0.495	0.508	0.588	0.523	0.459	0.460	0.449	0.517	0.569	0.550	0.593	0.612	0.478	0.514
DP _{RL}	0.510	0.509	0.833	0.835	0.740	0.802	0.499	0.495	0.458	0.506	0.511	0.492	0.649	0.632	0.514	0.646	0.586	0.509	0.494	0.481
rel. P _{RL}	0.503	0.505	0.492	0.345	0.495	0.534	0.498	0.499	0.524	0.524	0.542	0.519	0.535	0.454	0.520	0.486	0.556	0.486	0.494	0.501
DN _{RL}	0.499	0.498	0.923	0.837	0.863	0.848	0.613	0.573	0.473	0.489	0.493	0.490	0.532	0.674	0.625	0.658	0.596	0.589	0.498	0.502
rel. N _{RL}	0.497	0.496	0.332	0.282	0.481	0.499	0.662	0.575	0.481	0.501	0.521	0.553	0.509	0.569	0.589	0.564	0.597	0.583	0.526	0.497
DO _{RL}	0.472	0.471	0.942	0.940	0.867	0.886	0.577	0.544	0.532	0.550	0.611	0.615	0.901	0.851	0.483	0.478	0.630	0.632	0.602	0.604
rel. O _{RL}	0.509	0.513	0.516	0.658	0.724	0.617	0.657	0.679	0.573	0.531	0.498	0.460	0.693	0.811	0.570	0.570	0.562	0.565	0.532	0.510

Table S3. The percent improvement or depreciation in the AUC values with respect to the Surflex scoring function for the 10 PPI targets (20 protein structures) using different SASA scoring methods. The positive value indicates a percent increase in the AUC, while the negative value indicates a percent decrease in the AUC. The AUC values with an improvement greater than 10% are shown in bold and are highlighted in green.

SASA descriptor	BAZ2B		BCL2		BCLXL		BRD4-1		CREBBP		HIV-IN		XIAP		MCL1		MDM2		Menin	
	4XUA	5E73	2021	4LVT	3INQ	3WIZ	5D3L	5KU3	5EIC	5MMG	4CFD	4CHO	1TFT	5C3H	5FC4	5MES	4ODF	4ZFI	5DB2	6B41
T _{RU}	-1.19	0.57	12.59	9.02	11.89	15.43	16.33	73.29	-1.61	-3.47	-3.44	-2.85	-3.52	-6.44	10.58	5.88	14.54	30.94	-2.38	2.63
T _{RB}	-1.07	0.48	4.74	1.08	2.89	8.35	6.64	42.23	-13.99	-8.21	-7.13	-6.45	-12.56	-15.05	-3.88	-3.84	-3.01	16.54	-5.38	-2.97
ΔT _R	-0.57	1.52	13.92	10.32	13.77	16.97	15.73	85.31	9.64	-4.50	-3.39	-1.93	-1.83	-2.62	15.33	13.58	29.64	41.23	-0.70	4.79
rel. T _R	-0.07	0.99	-81.47	-85.64	-80.23	-62.23	-21.03	-7.64	-35.07	-23.99	-24.28	-21.28	-59.47	-61.02	-37.75	-29.21	-38.06	-19.71	-11.31	-9.64
H _{RU}	-0.89	0.79	11.43	8.27	11.15	14.30	13.48	68.65	-3.93	-5.11	2.43	0.53	-9.50	-5.54	11.79	3.06	12.94	30.45	-3.68	3.13
H _{RB}	-0.76	0.76	0.15	-7.70	2.12	7.10	-6.95	35.80	-19.32	-10.92	-9.06	-5.49	-24.94	-18.10	-3.77	-4.54	-20.43	16.92	-7.67	0.16
ΔH _R	-0.42	1.85	12.90	8.59	11.92	15.00	17.94	83.23	10.06	-5.19	5.38	-0.78	-4.19	0.42	16.10	4.75	29.94	39.06	-1.09	4.01
rel. H _R	-0.26	1.11	-64.30	-61.25	-59.75	-62.69	-37.89	2.15	-36.07	-23.06	-27.06	-19.36	-72.29	-60.58	-32.53	-17.55	-46.18	-3.28	-12.34	-3.31
Ar _{RU}	-0.85	2.44	-3.84	2.84	-8.58	-0.28	15.48	78.29	0.07	-15.55	-11.50	-13.77	-27.24	-25.21	-2.64	-6.77	1.40	17.97	-0.10	-1.27
Ar _{RB}	-1.08	1.70	-45.95	-28.04	-45.38	-27.86	-14.01	15.06	-12.31	-18.06	-14.11	-13.58	-34.43	-56.99	-18.48	-13.23	-18.53	4.03	-12.17	-0.53
ΔAr _R	0.78	4.15	8.12	5.67	6.21	5.46	15.11	87.47	-9.78	-18.06	-12.04	-13.12	-26.13	-23.64	5.45	-0.49	22.04	23.57	-3.78	-4.10
rel. Ar _R	-0.27	1.11	-76.42	-64.07	-75.37	-54.49	-49.22	-33.50	-16.90	-24.00	-18.90	-24.72	-53.90	-62.34	-25.75	-25.94	-28.29	-18.80	-12.55	-1.58
D _{RU}	0.92	2.37	-1.37	1.21	-0.71	-0.31	8.86	45.72	-14.66	-4.06	-11.84	-18.20	-15.98	-12.84	-2.63	3.03	4.22	8.05	0.04	3.81
D _{RB}	1.82	3.43	-26.68	-34.56	-40.65	-25.03	6.79	42.22	-17.56	-20.28	-14.02	-20.11	-25.77	-34.53	-15.41	-7.42	2.37	-17.65	-7.50	-9.32
ΔD _R	-0.35	1.66	2.81	4.71	3.32	6.17	-29.94	21.93	-13.63	-1.95	-17.34	-16.46	-14.60	-20.68	-0.10	5.78	-2.65	30.70	0.47	7.44
rel. D _R	2.38	3.64	-65.25	-77.68	-79.23	-59.68	2.10	36.54	-19.59	-34.89	-17.86	-20.29	-39.77	-49.08	-25.55	-29.39	-22.56	-37.16	-12.53	-13.25
Ac _{RU}	1.28	2.49	6.43	-5.95	-8.33	1.05	-29.75	17.00	3.67	-11.71	-12.60	-7.12	-20.77	-22.74	2.79	-3.33	4.74	11.08	-4.99	6.80
Ac _{RB}	2.10	3.67	-0.96	-17.16	-13.29	-20.91	-25.44	8.53	-0.96	-15.61	-17.24	-15.37	-55.75	-36.62	-3.19	-13.83	-1.38	6.71	-5.22	3.38
ΔAc _R	0.67	1.74	7.12	-6.76	-5.97	-0.24	-34.05	29.86	5.05	-10.51	-12.27	-5.73	-3.57	-13.54	2.46	2.30	-6.01	7.30	-7.00	4.41
rel. Ac _R	2.74	4.57	-14.89	-44.89	-34.94	-43.03	-20.10	0.87	-10.21	-23.05	-26.59	-26.05	-65.18	-45.89	-17.29	-22.18	-10.73	-1.28	-6.66	-0.64
P _{RU}	1.86	3.72	-14.21	-12.40	-17.14	-1.87	-27.88	17.67	-21.46	-19.79	-14.74	-15.42	-13.63	-23.92	-14.24	1.59	-7.31	-11.71	-7.73	-1.70
P _{RB}	1.86	3.72	-26.61	-27.59	-26.66	-7.54	-27.91	17.67	-20.51	-19.58	-13.16	-15.39	-11.65	-27.81	-11.90	-8.79	-8.06	-11.71	-8.44	-1.63

ΔP_R	1.85	3.73	-3.03	-5.84	-13.38	-2.39	-27.93	17.53	-23.45	-23.47	-17.36	-16.92	-27.05	-29.27	-13.22	9.43	-8.20	-11.57	-7.66	-3.33
rel. P_R	1.86	3.72	-42.64	-61.10	-40.46	-35.69	-27.95	17.67	-13.60	-20.89	-13.63	-15.46	-39.51	-48.94	-12.35	-17.23	-12.79	-11.72	-8.24	-1.63
N_{RU}	1.20	2.93	6.31	-8.62	-1.33	-3.31	4.62	37.71	-17.27	-21.25	-16.47	-16.69	-41.05	-17.00	-9.95	-4.85	-21.09	-11.99	-5.95	-3.59
N_{RB}	1.21	3.02	-5.02	-14.35	-8.15	-7.04	4.33	36.95	-17.17	-21.24	-14.06	-14.24	-43.33	-19.25	-11.18	-8.39	-21.09	-12.01	-4.32	-5.20
ΔN_R	1.69	3.24	8.22	-4.73	-5.53	-1.14	-10.54	36.69	-17.74	-22.24	-21.61	-20.17	-39.03	-22.74	-9.11	-1.06	-21.11	-11.87	-7.80	-1.47
rel. N_R	1.21	3.04	-61.40	-68.73	-38.61	-36.67	-5.21	35.29	-17.16	-21.47	-13.78	-11.46	-43.98	-36.48	-11.18	-8.41	-21.09	-12.02	-5.33	-6.17
O_{RU}	-0.49	1.67	-13.89	-9.28	-9.77	-9.37	-22.78	26.71	-6.78	-17.13	-14.96	-15.88	-40.41	-31.68	-8.93	-15.26	-7.99	9.51	-6.17	-2.87
O_{RB}	0.36	2.41	-28.40	-37.24	-24.51	-39.45	-38.78	9.19	-17.81	-21.14	-20.08	-24.78	-59.46	-37.20	-10.82	-15.26	-26.32	-7.96	-11.46	-4.88
ΔO_R	-0.84	1.46	-14.64	-10.98	-13.06	-14.39	-8.16	36.86	1.65	-16.87	-14.63	-11.44	-17.21	-27.32	-10.90	-15.25	-2.60	15.36	-4.40	-1.27
rel. O_R	1.33	3.11	-28.67	-39.15	-38.94	-43.99	-38.78	9.19	-23.73	-23.04	-20.09	-24.78	-68.29	-40.98	-10.80	-15.26	-26.79	-20.57	-11.50	-5.00
T_{LU}	-0.83	0.87	13.99	10.34	14.88	17.65	8.08	74.70	5.55	-3.10	-3.20	-2.38	6.11	5.84	18.07	18.07	31.22	48.00	-0.17	4.93
T_{LB}	1.46	3.57	13.23	9.40	13.81	15.71	1.99	82.28	3.06	-9.76	-14.37	-15.65	-0.93	3.77	14.47	15.62	0.99	33.15	-4.86	2.45
ΔT_L	-2.18	-0.78	12.48	8.98	12.54	16.35	2.10	36.17	0.22	-6.98	1.79	3.19	4.42	-2.10	13.06	10.75	31.52	41.88	0.47	5.06
rel. T_L	2.91	5.38	-19.99	-18.62	-1.25	-10.82	-4.22	78.76	-2.66	-17.87	-20.49	-25.82	-22.55	-6.59	5.89	6.12	-21.25	9.41	-14.97	-4.50
H_{LU}	3.84	5.67	5.03	1.42	-0.43	2.37	-22.02	24.82	4.93	-4.22	-20.47	-20.12	-37.41	-37.45	14.75	14.17	10.15	24.38	-18.25	-13.99
H_{LB}	3.48	6.10	0.75	-10.92	-0.49	-3.03	-4.43	70.00	0.74	-6.02	-13.29	-14.56	-30.95	-19.40	8.18	11.24	-28.64	1.65	-20.15	-13.28
ΔH_L	3.51	4.73	-4.35	-2.63	-10.28	-3.05	-32.14	-10.88	1.24	-9.03	-25.15	-24.32	-48.25	-59.57	9.99	8.10	12.93	16.51	-15.84	-12.47
rel. H_L	2.22	5.23	-27.78	-43.01	-19.83	-31.02	-1.06	82.46	-9.85	-16.26	-11.48	-12.81	-27.48	-8.86	-5.92	-3.68	-44.93	-17.68	-15.20	-7.56
Ar_{LU}	6.37	8.18	-2.40	-6.46	3.88	8.08	-26.72	17.64	8.01	-1.78	-24.87	-24.18	-37.58	-36.97	23.89	23.29	-54.39	-46.23	-23.02	-19.32
Ar_{LB}	3.87	6.45	-8.01	-13.39	1.01	4.61	-16.97	47.96	-2.91	-8.69	-21.11	-22.58	-30.01	-19.26	16.06	17.80	-42.04	-26.01	-24.75	-17.38
ΔAr_L	6.30	7.84	-10.27	-11.05	-4.65	0.30	-29.78	2.40	7.45	-3.32	-24.27	-23.73	-48.35	-59.03	16.69	16.11	-49.97	-47.47	-19.63	-17.42
rel. Ar_L	1.04	3.88	-34.44	-39.79	-20.55	-33.32	-16.36	51.74	-11.42	-15.97	-18.29	-19.01	-27.61	-10.22	-3.64	-2.70	-26.51	-1.71	-16.46	-8.66
D_{LU}	-0.77	1.06	-14.70	-17.60	-24.16	-21.60	-24.66	24.46	-30.26	-36.46	-23.23	-20.87	1.93	0.71	-0.22	-0.65	-18.76	-8.53	-16.72	-11.86
D_{LB}	1.29	1.85	-16.93	-16.22	-16.52	-17.33	-25.87	31.99	-24.12	-31.85	-23.87	-22.17	-15.53	-39.10	0.69	0.81	-18.85	-9.46	-17.04	-7.66
ΔD_L	-0.75	1.52	-20.30	-26.23	-31.42	-28.34	-26.71	13.93	-30.53	-36.76	-21.95	-18.99	2.39	3.26	-5.18	-5.49	-22.92	-13.29	-15.48	-12.24
rel. D_L	0.78	1.38	-22.34	-21.21	-17.14	-19.66	-26.69	30.67	-23.59	-31.41	-22.72	-21.11	-28.83	-48.71	-2.27	-0.92	-25.54	-15.67	-15.57	-7.38
Ac_{LU}	1.09	2.89	1.62	-1.91	-13.34	-10.41	-3.05	59.57	-12.51	-20.70	-17.39	-18.41	-43.52	-42.75	0.16	-1.19	-12.08	0.29	-9.99	-5.04
Ac_{LB}	0.88	3.35	1.47	-1.78	-12.46	-6.95	-18.26	48.59	-2.41	-17.02	-26.07	-25.79	-40.57	-40.62	-0.84	-0.66	-7.11	8.21	-13.34	-2.96
ΔAc_L	1.58	2.93	-13.63	-18.36	-23.49	-23.59	-5.30	47.84	-18.71	-21.82	-12.31	-13.12	-46.33	-44.19	-7.85	-8.84	-17.39	-10.21	-7.87	-4.99
rel. Ac_L	1.15	3.66	-11.99	-18.32	-22.40	-14.91	-24.87	33.78	-1.75	-17.61	-27.03	-25.45	-39.17	-40.79	-6.35	-5.84	-10.22	4.69	-13.12	-0.79

P _{LU}	4.07	5.90	-19.67	-22.53	-26.74	-25.71	-28.86	15.88	-18.64	-25.75	-26.75	-27.29	-39.00	-35.32	-7.90	-8.62	-21.28	-11.78	-12.30	-6.82
P _{LB}	2.50	4.76	-29.07	-32.39	-34.92	-28.86	-28.74	16.95	-17.61	-24.87	-24.41	-23.96	-44.05	-44.99	-10.07	-9.18	-20.03	-14.82	-11.55	-4.61
ΔP _L	3.79	5.62	-28.84	-31.22	-30.72	-33.12	-28.78	15.99	-18.67	-25.76	-26.51	-26.77	-38.52	-34.91	-10.35	-13.43	-23.93	-11.03	-12.01	-6.73
rel. P _L	2.52	4.78	-28.22	-31.71	-34.65	-28.39	-28.74	16.95	-17.61	-24.87	-24.41	-23.98	-44.04	-45.00	-9.92	-8.95	-19.72	-14.83	-11.57	-4.60
N _{LU}	1.81	3.70	-39.39	-41.38	-21.19	-19.15	-29.20	15.68	-21.14	-28.05	-21.54	-21.53	-43.53	-43.79	2.44	1.47	-7.02	4.39	-10.28	-4.92
N _{LB}	1.88	3.68	-39.58	-41.31	-21.08	-19.30	-29.12	16.27	-20.95	-28.04	-21.55	-21.97	-43.30	-43.51	1.47	0.45	-7.13	3.64	-10.26	-4.04
ΔN _L	1.78	3.66	-39.40	-41.48	-21.36	-19.11	-29.20	15.67	-21.16	-28.07	-21.50	-22.01	-43.81	-44.06	2.08	1.36	-7.17	3.68	-10.26	-5.08
rel. N _L	1.88	3.68	-39.57	-41.30	-21.01	-19.28	-29.12	16.27	-20.95	-28.04	-21.38	-21.92	-43.29	-43.50	1.48	0.49	-7.13	3.64	-10.25	-4.03
O _{LU}	-2.90	-1.11	11.17	7.47	6.22	9.01	-7.35	48.70	-8.18	-15.49	-3.74	-3.43	4.81	4.61	-13.37	-14.46	2.72	14.93	11.57	17.65
O _{LB}	0.54	2.45	5.72	4.14	4.89	4.22	-2.36	63.75	-2.55	-14.35	-11.25	-12.91	0.59	4.46	-6.71	-8.39	-2.72	11.38	9.14	12.67
ΔO _L	-3.80	-2.21	9.97	6.10	2.50	7.48	-17.22	27.55	-12.55	-17.18	-2.52	-2.58	1.45	-4.74	-17.43	-18.90	-1.80	9.29	9.77	16.82
rel. O _L	3.59	6.18	-39.62	-25.59	-13.50	-23.27	-5.57	59.43	-4.89	-19.41	-20.58	-27.04	-21.91	-9.64	-2.52	-3.33	-11.86	0.42	-2.92	-1.54
ΔT _{RL}	-1.66	-0.07	13.35	9.87	13.39	16.88	11.30	63.37	5.67	-4.14	0.30	2.18	3.39	-1.36	15.24	13.20	34.39	44.29	0.15	5.04
rel. T _{RL}	1.40	3.28	-57.41	-56.23	-32.81	-32.42	0.02	67.58	-16.95	-19.11	-24.89	-25.78	-34.94	-12.46	-6.31	-4.22	-28.82	1.96	-14.44	-7.77
ΔH _{RL}	2.02	3.62	12.07	7.70	9.24	14.35	-6.27	27.89	11.80	-2.33	-13.10	-14.57	-21.45	-29.04	19.41	12.23	29.68	36.05	-11.93	-8.73
rel. H _{RL}	-0.09	2.17	-51.61	-57.41	-40.25	-53.70	-18.27	54.21	-31.62	-23.43	-16.59	-13.72	-45.36	-23.84	-25.55	-10.30	-51.97	-7.93	-16.13	-5.95
ΔA _{RL}	5.87	7.71	5.39	3.17	8.11	10.06	-8.34	38.08	7.74	-3.39	-20.82	-19.57	-36.14	-45.75	20.74	18.71	-35.14	-27.10	-17.24	-5.95
rel. A _{RL}	-1.81	1.18	-60.47	-54.72	-52.97	-44.53	-29.34	23.93	-20.98	-27.30	-15.96	-16.64	-35.54	-31.55	-15.18	-19.53	-29.15	0.84	-16.91	-5.26
ΔD _{RL}	-0.89	1.67	1.26	1.89	0.13	-2.03	-25.15	16.84	-27.60	-27.30	-20.19	-18.61	4.49	4.68	1.77	6.52	-5.43	17.34	-6.71	-3.18
rel. D _{RL}	2.28	3.68	-62.27	-69.77	-70.96	-50.59	-0.30	42.12	-11.89	-24.52	-16.67	-21.46	-55.96	-64.08	-20.44	-25.46	-14.16	-29.15	-11.64	-9.39
ΔA _{CRL}	1.20	2.38	-4.21	-8.25	-16.07	-15.58	-6.55	48.82	-11.80	-18.22	-11.73	-8.91	-36.55	-34.55	-5.60	-5.46	-14.60	-4.77	-7.64	-3.28
rel. A _{CRL}	2.04	4.37	-6.34	-24.19	-22.61	-15.58	-28.86	19.24	-2.71	-20.94	-26.82	-27.09	-49.46	-41.99	-2.65	-6.86	-7.39	7.28	-12.71	-0.52
ΔP _{RL}	3.80	5.63	-2.81	-5.71	-12.33	-2.56	-28.37	16.15	-24.13	-23.60	-18.48	-22.04	-26.91	-29.16	-12.14	9.49	-8.42	-10.66	-9.93	-6.94
rel. P _{RL}	2.54	4.77	-42.65	-61.05	-41.39	-35.17	-28.42	17.25	-13.31	-20.85	-13.59	-17.74	-39.79	-49.07	-11.07	-17.60	-13.12	-14.80	-9.93	-3.11
ΔN _{RL}	1.65	3.22	7.73	-5.50	2.30	3.03	-11.90	34.47	-21.66	-26.11	-21.42	-22.41	-40.11	-24.47	6.81	11.57	-6.81	3.40	-9.12	-2.82
rel. N _{RL}	1.24	2.99	-61.30	-68.22	-42.95	-39.36	-4.84	35.09	-20.43	-24.29	-16.93	-12.42	-42.64	-36.20	0.66	-4.43	-6.78	2.29	-4.11	-3.96
ΔO _{RL}	-3.79	-2.19	9.95	6.15	2.68	7.65	-17.10	27.59	-11.85	-16.85	-2.51	-2.55	1.45	-4.63	-17.41	-18.90	-1.50	10.81	9.79	16.81
rel. O _{RL}	3.65	6.35	-39.84	-25.78	-14.27	-25.07	-5.67	59.41	-5.20	-19.81	-20.58	-27.11	-21.92	-9.10	-2.54	-3.33	-12.14	-0.89	-2.92	-1.44

Table S4. The BEDROC values ($\alpha = 20$) for the datasets screened using SASA descriptors. The best BEDROC score corresponding to each target protein (across columns) is indicated in bold and highlighted in green.

SASA descriptor	BAZ2B		BCL2		BCLXL		BRD4-1		CREBBP		HIV-IN		XIAP		MCL1		MDM2		Menin	
	4XUA	5E73	2O21	4LVT	3INQ	3WIZ	5D3L	5KU3	5EIC	5MMG	4CFD	4CHO	1TFT	5C3H	5FC4	5MES	4ODF	4ZFI	5DB2	6B41
Surflex	0.120	0.120	0.641	0.701	0.523	0.500	0.672	0.254	0.100	0.160	0.604	0.639	0.767	0.704	0.170	0.150	0.842	0.600	0.104	0.065
T _{RU}	0.125	0.131	0.882	0.872	0.792	0.809	0.753	0.596	0.093	0.119	0.398	0.443	0.431	0.385	0.260	0.223	0.689	0.662	0.111	0.108
T _{RB}	0.123	0.132	0.640	0.582	0.543	0.592	0.766	0.479	0.076	0.117	0.450	0.530	0.300	0.288	0.128	0.143	0.498	0.579	0.084	0.076
DT _R	0.127	0.132	0.932	0.927	0.864	0.864	0.721	0.677	0.120	0.107	0.370	0.381	0.410	0.425	0.290	0.283	0.742	0.699	0.126	0.136
rel. T _R	0.133	0.142	0.002	0.003	0.006	0.006	0.385	0.143	0.031	0.051	0.327	0.302	0.016	0.012	0.039	0.048	0.095	0.246	0.047	0.049
H _{RU}	0.125	0.132	0.847	0.864	0.740	0.767	0.754	0.565	0.089	0.125	0.468	0.436	0.261	0.367	0.236	0.204	0.635	0.648	0.100	0.104
H _{RB}	0.123	0.132	0.450	0.368	0.466	0.536	0.593	0.434	0.072	0.125	0.504	0.475	0.156	0.259	0.104	0.139	0.315	0.535	0.078	0.091
DH _R	0.128	0.132	0.911	0.872	0.801	0.786	0.767	0.646	0.120	0.101	0.412	0.403	0.346	0.492	0.280	0.226	0.744	0.714	0.116	0.112
rel. H _R	0.125	0.132	0.004	0.006	0.026	0.009	0.135	0.166	0.035	0.047	0.323	0.307	0.002	0.019	0.043	0.063	0.071	0.299	0.052	0.067
Ar _{RU}	0.102	0.124	0.362	0.656	0.152	0.396	0.701	0.649	0.104	0.077	0.325	0.344	0.113	0.076	0.125	0.125	0.574	0.530	0.101	0.082
Ar _{RB}	0.124	0.128	0.042	0.049	0.010	0.189	0.346	0.334	0.093	0.080	0.332	0.364	0.072	0.013	0.092	0.085	0.378	0.350	0.066	0.076
DAr _R	0.132	0.134	0.677	0.759	0.588	0.453	0.752	0.727	0.071	0.076	0.362	0.354	0.156	0.178	0.199	0.171	0.671	0.613	0.093	0.084
rel. Ar _R	0.125	0.137	0.006	0.008	0.005	0.028	0.089	0.108	0.054	0.046	0.377	0.274	0.013	0.004	0.042	0.038	0.174	0.180	0.064	0.058
D _{RU}	0.097	0.103	0.556	0.584	0.522	0.428	0.866	0.527	0.066	0.108	0.396	0.412	0.293	0.150	0.136	0.173	0.559	0.487	0.084	0.106
D _{RB}	0.145	0.140	0.356	0.072	0.044	0.108	0.849	0.531	0.065	0.070	0.366	0.431	0.160	0.091	0.068	0.089	0.479	0.363	0.066	0.050
DD _R	0.123	0.128	0.483	0.654	0.489	0.510	0.434	0.604	0.062	0.144	0.398	0.404	0.259	0.171	0.160	0.167	0.487	0.644	0.096	0.139
rel. D _R	0.147	0.142	0.006	0.003	0.003	0.005	0.697	0.542	0.046	0.032	0.357	0.413	0.035	0.021	0.029	0.026	0.159	0.095	0.052	0.051
Ac _{RU}	0.129	0.123	0.672	0.453	0.330	0.350	0.473	0.484	0.121	0.092	0.492	0.581	0.246	0.269	0.195	0.131	0.650	0.612	0.068	0.102
Ac _{RB}	0.130	0.125	0.563	0.276	0.249	0.128	0.478	0.470	0.103	0.077	0.516	0.444	0.039	0.143	0.153	0.102	0.612	0.579	0.064	0.068
DAC _R	0.137	0.136	0.721	0.426	0.393	0.471	0.405	0.476	0.121	0.110	0.403	0.499	0.279	0.207	0.212	0.173	0.480	0.518	0.067	0.105
rel. Ac _R	0.145	0.138	0.180	0.027	0.023	0.021	0.368	0.327	0.065	0.050	0.287	0.297	0.006	0.044	0.046	0.043	0.436	0.402	0.059	0.063
P _{RU}	0.001	0.002	0.088	0.100	0.120	0.287	0.404	0.101	0.052	0.074	0.483	0.596	0.167	0.115	0.020	0.114	0.479	0.108	0.068	0.076
P _{RB}	0.001	0.002	0.070	0.080	0.101	0.256	0.400	0.101	0.058	0.083	0.412	0.595	0.177	0.059	0.092	0.114	0.536	0.108	0.054	0.078

DP _R	0.001	0.002	0.421	0.419	0.241	0.310	0.386	0.091	0.063	0.063	0.348	0.563	0.187	0.175	0.021	0.217	0.460	0.103	0.085	0.068
rel. P _R	0.001	0.002	0.022	0.010	0.008	0.035	0.391	0.101	0.088	0.068	0.446	0.569	0.067	0.008	0.078	0.041	0.316	0.104	0.060	0.078
N _{RU}	0.054	0.047	0.665	0.419	0.500	0.408	0.774	0.631	0.053	0.091	0.408	0.457	0.042	0.135	0.011	0.003	0.075	0.157	0.089	0.086
N _{RB}	0.060	0.054	0.297	0.268	0.367	0.354	0.824	0.624	0.057	0.094	0.487	0.494	0.089	0.156	0.056	0.069	0.075	0.154	0.078	0.071
DN _R	0.028	0.033	0.805	0.519	0.370	0.500	0.565	0.654	0.042	0.080	0.380	0.401	0.151	0.234	0.123	0.129	0.073	0.161	0.091	0.098
rel. N _R	0.055	0.043	0.007	0.007	0.015	0.017	0.384	0.545	0.056	0.073	0.410	0.455	0.038	0.026	0.056	0.068	0.075	0.147	0.071	0.061
O _{RU}	0.021	0.069	0.090	0.503	0.435	0.220	0.084	0.088	0.096	0.065	0.454	0.400	0.076	0.132	0.028	0.000	0.281	0.463	0.075	0.075
O _{RB}	0.131	0.132	0.074	0.112	0.082	0.046	0.108	0.125	0.091	0.048	0.407	0.342	0.072	0.143	0.080	0.000	0.355	0.420	0.054	0.067
DO _R	0.126	0.125	0.121	0.477	0.183	0.120	0.529	0.255	0.125	0.076	0.462	0.429	0.067	0.220	0.000	0.000	0.206	0.562	0.076	0.078
rel. O _R	0.130	0.138	0.039	0.037	0.025	0.004	0.108	0.125	0.036	0.047	0.401	0.342	0.000	0.018	0.084	0.000	0.274	0.166	0.051	0.066
T _{LU}	0.128	0.130	0.936	0.933	0.879	0.880	0.627	0.590	0.111	0.114	0.362	0.379	0.666	0.673	0.313	0.312	0.742	0.746	0.138	0.129
T _{LB}	0.138	0.140	0.899	0.897	0.846	0.820	0.589	0.612	0.113	0.095	0.352	0.377	0.506	0.633	0.299	0.288	0.624	0.700	0.107	0.109
DT _L	0.121	0.118	0.895	0.881	0.817	0.845	0.585	0.513	0.085	0.097	0.419	0.490	0.614	0.412	0.257	0.244	0.863	0.793	0.144	0.127
rel. T _L	0.141	0.144	0.193	0.238	0.386	0.279	0.539	0.673	0.090	0.058	0.354	0.400	0.298	0.403	0.173	0.155	0.422	0.556	0.072	0.078
H _{LU}	0.146	0.144	0.537	0.530	0.453	0.475	0.514	0.494	0.103	0.104	0.341	0.345	0.105	0.108	0.205	0.204	0.630	0.636	0.055	0.051
H _{LB}	0.137	0.144	0.515	0.367	0.427	0.448	0.593	0.766	0.114	0.131	0.454	0.460	0.223	0.249	0.192	0.194	0.488	0.705	0.048	0.052
DH _L	0.144	0.138	0.417	0.505	0.359	0.345	0.415	0.281	0.092	0.085	0.312	0.260	0.017	0.014	0.148	0.142	0.809	0.700	0.062	0.052
rel. H _L	0.128	0.134	0.193	0.112	0.188	0.128	0.691	0.848	0.069	0.090	0.615	0.615	0.203	0.312	0.075	0.077	0.385	0.573	0.060	0.064
Ar _{LU}	0.154	0.152	0.332	0.303	0.556	0.602	0.406	0.375	0.143	0.139	0.428	0.429	0.109	0.121	0.274	0.268	0.082	0.083	0.039	0.040
Ar _{LB}	0.145	0.146	0.363	0.305	0.535	0.506	0.480	0.532	0.100	0.098	0.392	0.440	0.244	0.307	0.246	0.230	0.163	0.177	0.040	0.042
DAr _L	0.159	0.155	0.273	0.248	0.361	0.462	0.301	0.253	0.149	0.135	0.367	0.329	0.023	0.010	0.216	0.207	0.090	0.073	0.046	0.045
rel. Ar _L	0.128	0.134	0.144	0.085	0.170	0.103	0.424	0.588	0.035	0.045	0.464	0.457	0.206	0.282	0.066	0.063	0.422	0.555	0.068	0.070
D _{LU}	0.157	0.159	0.134	0.135	0.105	0.109	0.475	0.498	0.038	0.039	0.365	0.375	0.322	0.312	0.085	0.086	0.506	0.484	0.054	0.055
D _{LB}	0.146	0.137	0.184	0.225	0.153	0.153	0.554	0.697	0.047	0.050	0.373	0.360	0.201	0.160	0.105	0.111	0.554	0.508	0.058	0.066
DD _L	0.150	0.154	0.117	0.104	0.092	0.095	0.452	0.413	0.039	0.041	0.314	0.333	0.327	0.339	0.080	0.078	0.434	0.461	0.054	0.055
rel. D _L	0.124	0.121	0.107	0.120	0.145	0.094	0.506	0.612	0.059	0.061	0.392	0.388	0.024	0.011	0.085	0.088	0.302	0.286	0.070	0.071
Ac _{LU}	0.159	0.158	0.581	0.569	0.387	0.408	0.621	0.645	0.035	0.036	0.445	0.445	0.077	0.086	0.191	0.191	0.500	0.505	0.032	0.030
Ac _{LB}	0.132	0.139	0.635	0.591	0.402	0.466	0.533	0.615	0.072	0.047	0.470	0.430	0.130	0.136	0.193	0.176	0.539	0.624	0.048	0.053
DAc _L	0.162	0.156	0.289	0.272	0.218	0.198	0.619	0.511	0.032	0.039	0.454	0.510	0.029	0.026	0.133	0.121	0.412	0.332	0.036	0.028
rel. Ac _L	0.137	0.138	0.218	0.153	0.135	0.172	0.337	0.401	0.079	0.052	0.419	0.481	0.059	0.049	0.098	0.077	0.393	0.410	0.061	0.054

P _{LU}	0.112	0.112	0.210	0.212	0.168	0.151	0.140	0.139	0.035	0.035	0.226	0.228	0.085	0.103	0.091	0.091	0.298	0.277	0.043	0.045
P _{LB}	0.061	0.074	0.162	0.152	0.110	0.142	0.076	0.098	0.040	0.039	0.260	0.302	0.032	0.025	0.079	0.090	0.296	0.162	0.044	0.054
DP _L	0.107	0.106	0.162	0.178	0.151	0.104	0.142	0.138	0.034	0.034	0.233	0.228	0.096	0.118	0.077	0.059	0.220	0.283	0.046	0.044
rel. P _L	0.063	0.076	0.254	0.210	0.132	0.161	0.076	0.098	0.040	0.039	0.260	0.294	0.033	0.024	0.088	0.092	0.348	0.150	0.042	0.055
N _{LU}	0.074	0.074	0.072	0.071	0.261	0.264	0.104	0.104	0.027	0.027	0.373	0.445	0.034	0.033	0.192	0.184	0.716	0.714	0.050	0.049
N _{LB}	0.069	0.068	0.076	0.078	0.292	0.282	0.105	0.106	0.027	0.025	0.343	0.405	0.051	0.044	0.189	0.184	0.711	0.705	0.051	0.060
DN _L	0.072	0.072	0.074	0.071	0.271	0.284	0.099	0.101	0.024	0.024	0.431	0.435	0.025	0.030	0.196	0.201	0.709	0.694	0.051	0.046
rel. N _L	0.069	0.068	0.078	0.079	0.300	0.283	0.105	0.106	0.027	0.026	0.393	0.445	0.053	0.046	0.190	0.188	0.710	0.705	0.051	0.061
O _{LU}	0.114	0.115	0.878	0.873	0.706	0.710	0.475	0.453	0.076	0.080	0.377	0.381	0.612	0.614	0.157	0.157	0.519	0.521	0.136	0.133
O _{LB}	0.134	0.129	0.668	0.741	0.649	0.599	0.573	0.548	0.096	0.075	0.381	0.402	0.522	0.620	0.168	0.166	0.590	0.581	0.127	0.122
DO _L	0.108	0.113	0.823	0.805	0.569	0.619	0.392	0.403	0.057	0.072	0.313	0.310	0.484	0.368	0.106	0.117	0.422	0.462	0.131	0.129
rel. O _L	0.146	0.149	0.085	0.123	0.216	0.138	0.505	0.575	0.089	0.060	0.372	0.395	0.210	0.249	0.130	0.128	0.510	0.517	0.068	0.069
DT _{RL}	0.121	0.123	0.918	0.911	0.853	0.862	0.643	0.578	0.106	0.108	0.391	0.426	0.563	0.438	0.282	0.274	0.813	0.753	0.140	0.133
rel. T _{RL}	0.141	0.144	0.028	0.040	0.129	0.095	0.466	0.591	0.059	0.042	0.364	0.414	0.185	0.294	0.085	0.098	0.296	0.471	0.051	0.055
DH _{RL}	0.142	0.139	0.848	0.813	0.684	0.741	0.675	0.468	0.137	0.113	0.412	0.340	0.124	0.149	0.271	0.224	0.896	0.813	0.099	0.085
rel. H _{RL}	0.131	0.137	0.015	0.020	0.060	0.016	0.395	0.601	0.036	0.050	0.543	0.608	0.042	0.144	0.041	0.079	0.131	0.468	0.053	0.057
DAr _{RL}	0.157	0.153	0.518	0.562	0.630	0.604	0.550	0.423	0.151	0.132	0.358	0.348	0.091	0.047	0.245	0.227	0.142	0.186	0.053	0.057
rel. Ar _{RL}	0.127	0.132	0.017	0.034	0.038	0.059	0.289	0.390	0.028	0.027	0.445	0.403	0.090	0.082	0.044	0.033	0.280	0.384	0.064	0.070
DD _{RL}	0.150	0.155	0.395	0.506	0.380	0.236	0.445	0.420	0.042	0.027	0.345	0.360	0.434	0.454	0.109	0.122	0.478	0.575	0.061	0.076
rel. D _{RL}	0.142	0.138	0.009	0.003	0.005	0.014	0.643	0.644	0.068	0.047	0.382	0.403	0.005	0.008	0.037	0.031	0.259	0.167	0.054	0.056
DAC _{RL}	0.161	0.156	0.441	0.421	0.325	0.248	0.588	0.534	0.043	0.047	0.450	0.524	0.055	0.063	0.139	0.139	0.432	0.376	0.038	0.036
rel. AC _{RL}	0.133	0.138	0.287	0.125	0.094	0.248	0.380	0.465	0.071	0.040	0.416	0.471	0.061	0.064	0.097	0.077	0.489	0.444	0.069	0.061
DP _{RL}	0.108	0.107	0.423	0.420	0.251	0.310	0.401	0.154	0.062	0.063	0.342	0.463	0.188	0.176	0.070	0.218	0.461	0.321	0.083	0.045
rel. P _{RL}	0.063	0.077	0.022	0.012	0.008	0.034	0.388	0.126	0.092	0.068	0.443	0.502	0.067	0.008	0.076	0.040	0.303	0.173	0.060	0.070
DN _{RL}	0.084	0.087	0.673	0.384	0.467	0.479	0.476	0.546	0.025	0.035	0.422	0.418	0.091	0.160	0.230	0.242	0.719	0.713	0.065	0.063
rel. N _{RL}	0.069	0.051	0.006	0.005	0.006	0.012	0.388	0.551	0.055	0.073	0.422	0.479	0.041	0.031	0.077	0.066	0.709	0.581	0.071	0.065
DO _{RL}	0.108	0.113	0.822	0.807	0.577	0.619	0.393	0.403	0.059	0.072	0.313	0.310	0.484	0.382	0.106	0.117	0.426	0.475	0.132	0.129
rel. O _{RL}	0.146	0.148	0.084	0.121	0.210	0.127	0.504	0.576	0.087	0.058	0.372	0.396	0.210	0.254	0.130	0.128	0.505	0.501	0.068	0.070

Table S5. Enrichment Factors at 1% subsetting for protein structures of ten PPI targets obtained using post docking derivatized SASA descriptors.

The best enrichment score corresponding to each target protein (across columns) is shown in bold and highlighted in green.

SASA descriptor	BAZ2B		BCL2		BCLXL		BRD4-1		CREBBP		HIV-IN		XIAP		MCL1		MDM2		Menin	
	4XUA	5E73	2021	4LVT	3INQ	3WIZ	5D3L	5KU3	5EIC	5MMG	4CFD	4CHO	1TFT	5C3H	5FC4	5MES	4ODF	4ZFI	5DB2	6B41
Surflex	0.77	0.86	25	28	26	27	0.96	0.72	1.8	5.1	1.4	1.5	42	33	6.1	3.3	3	2.5	3.4	1
T _{RU}	0.96	1.2	28	27	44	45	1.8	1.6	1.4	1.5	1.5	1.6	16	16	11	8.9	2.5	2.6	3.3	3.3
T _{RB}	0.98	1.2	23	18	29	28	1.9	0.96	1.3	1.4	0.91	1.3	7.8	9.1	4	4.4	1.8	2.3	3	2
ΔT _R	1.1	1.1	28	27	47	46	1.3	1.6	1.5	1.4	1.7	1.3	19	20	16	14	2.5	2.6	3.1	4.1
rel. T _R	1.1	1.3	0	0.057	0	0.1	0.48	0.12	0.15	0.077	0.57	0.46	0.18	0	0.91	0.63	0.13	0.36	0.71	0.85
H _{RU}	0.96	1.1	27	27	41	41	1.7	1.4	1.2	1.7	1.4	1.5	9.1	13	11	7	2.5	2.4	3	3
H _{RB}	0.93	1.1	16	11	19	22	1.1	0.6	1	2.1	1.4	0.91	2.9	7.8	2.4	3.9	0.89	1.7	1.8	2.8
ΔH _R	1.2	1.1	28	27	44	45	1.7	1.4	1.5	1.2	1.7	1.4	15	19	14	8.9	2.5	2.7	2.8	3.3
rel. H _R	0.92	0.99	0	0.11	0.42	0.1	0	0.12	0.54	0.15	0.69	0.34	0	0.088	0.77	1.4	0	0.94	0.71	1
Ar _{RU}	0.86	0.93	11	22	6.7	26	1.2	1.6	1.6	0.77	0.57	1.1	2.6	4.4	4.6	1.4	2.3	1.8	1.8	1.8
Ar _{RB}	0.9	1	0.28	0.62	0.1	6.9	0.12	0.6	1.5	0.62	0.46	1	2.1	0.35	3.1	1.3	1.1	0.54	0.71	1.7
ΔAr _R	0.99	1.1	22	26	27	22	1.7	1.2	0.62	1.4	1	1.4	6.7	8.3	7.7	5.1	2.4	2.5	2.3	2.3
rel. Ar _R	0.92	1.1	0.057	0.057	0.1	0.42	0	0.12	0.23	0.46	0.34	0.57	0.18	0	0.77	0.35	0.13	0.22	0.43	0.85
D _{RU}	1	1.1	20	19	23	22	1.8	0.96	1.3	1.7	1	1.6	7.6	4.1	5.6	6	2	1.9	2.1	2.4
D _{RB}	1.2	1.2	13	1.8	1.2	5.3	1.6	1.1	1.2	0.92	0.23	1.4	1.1	3.2	1.3	1.7	1.4	0.98	0.71	1.3
ΔD _R	0.88	0.99	14	22	21	22	1.1	1.3	1.1	2.5	1.3	1.4	11	6.3	5.6	5.1	2.4	2.5	2.8	4.6
rel. D _R	1.2	1.2	0.057	0	0.1	0	1.3	1.1	0.69	0.23	0.57	0.46	0.18	0.088	0.21	0	0.22	0.18	1.3	1.6
Ac _{RU}	0.88	0.79	25	22	23	7.4	1.2	0.84	1.6	1.1	1.1	1.4	7.7	11	7.8	4.3	2.1	2.5	1.8	3.1
Ac _{RB}	0.9	0.77	21	11	14	4.1	1.4	0.84	1.4	0.77	1.4	0.69	2.6	5	5.1	2.6	2.1	2.1	1.3	1.7
ΔAc _R	0.83	1	26	14	20	21	0.84	1.1	1.9	1.8	1.4	1	8.6	7.2	7.5	6.4	2.2	2.3	1.7	3.8
rel. Ac _R	1.3	1.2	2	0.057	0	0.1	0.12	0.6	0.62	0.38	0.11	0.8	0.088	0.79	0.14	0.56	0.63	0.98	0.71	1
P _{RU}	0.044	0.073	5.7	5.9	6.8	20	0.72	0.48	1.1	0.69	1.4	1.7	3.4	2.1	1.5	0.14	1.6	1.6	2	1
P _{RB}	0.044	0.073	2	0.62	4.5	12	0.6	0.48	1.1	0.92	1.1	1.6	3.8	0.88	2.3	1.2	2.1	1.4	1	1.1

ΔP_R	0.029	0.073	13	13	10	12	1.2	0.36	0.85	1.3	1.4	1.6	11	6.3	1.2	7.5	2.2	1.6	2.1	1.1
rel. P_R	0.044	0.073	0.057	0.23	0	0	0.84	0.48	0.54	1	1.1	1.4	0.18	0	1.3	0	0.8	1.1	0.57	1.4
N_{RU}	0.54	0.77	15	9.3	19	19	1.7	0.84	0.77	1.1	1.1	1.3	3.4	7.1	0	0.21	1.2	1.3	2.4	2.8
N_{RB}	0.54	0.77	3.8	3.4	13	15	1.7	0.96	0.77	1.8	0.69	1.4	4.6	4.9	0.84	0.77	1.2	1.1	2.3	1.3
ΔN_R	0.95	0.67	28	18	20	25	1.1	1.3	0.62	1.6	1.6	0.8	8	9.8	3.6	2.7	1.1	1.4	2.1	3.3
rel. N_R	0	0	0	0.17	0.21	0	0	0.72	0.46	0.54	0.91	0.69	0.62	0	0.84	0.63	1.2	0.72	1	1.3
O_{RU}	0	0.015	6.6	25	22	1.9	0.12	0.12	1.2	1.2	1.3	0.8	4.9	2.5	0	0	0.67	1.7	1.7	1.6
O_{RB}	0.8	0.98	2.8	2.3	1.9	1.8	0.24	0.12	0.77	0.31	1	1	4.5	0.79	0.99	0	0.8	1.4	1.7	1.3
ΔO_R	0.86	0.88	2.8	21	4.9	3.6	0.36	0.24	2.2	0.85	1.3	0.8	3.4	7.4	0	0	1.5	2.6	2.1	1.3
rel. O_R	0.77	0.99	0	0	0	0	0.24	0.12	0.46	0.38	0.8	0.91	0	0	1.9	0	0	0.045	1	1
T_{LU}	1.1	1.1	27	27	46	46	1.1	0.96	1.9	1.9	2.4	2.4	29	30	17	17	2.6	2.6	4.8	3.7
T_{LB}	1.2	1.3	27	27	45	46	0.84	1.1	1.8	1.2	2.4	2.4	25	29	14	13	2.6	2.6	2.7	2.8
ΔT_L	1	0.88	27	28	46	47	1.2	0.84	0.85	1.8	1.5	1.1	25	18	13	10	2.7	2.7	5	3.8
rel. T_L	1.2	1.1	5.3	4.5	15	12	1.2	1.6	1.6	0.85	2.3	2.3	17	19	4.6	3.1	2.4	2.6	1.7	1.3
H_{LU}	1.1	1.1	17	17	23	25	1.1	1.1	1.5	1.2	1.9	2.1	2.7	3.2	6.6	6.2	1.5	1.6	0.85	0.71
H_{LB}	1	0.98	17	13	20	23	1.4	1.7	1.5	2.5	2.1	2.2	10	10	6.8	6.6	2.1	2.5	1	0.85
ΔH_L	0.99	1	14	16	15	14	0.72	0.6	1	0.62	0.23	0	0.088	0	2.9	3.9	2.3	1.9	0.43	0.85
rel. H_L	0.8	0.9	3.6	2.1	4.7	3.1	1.9	2.2	0.77	2.5	1.9	1.9	4.9	11	0.7	0.99	1.7	2.1	1.4	0.43
Ar_{LU}	1.2	1.2	9	8.5	24	25	0.72	0.6	3.2	3.5	1.7	1.6	4	4.1	9.6	9.1	0.13	0.22	1	1
Ar_{LB}	1.2	1.2	11	8.7	28	23	0.6	1.2	1.4	1.8	2.2	2.2	11	14	7.6	6.8	0.85	1	0.43	0.28
ΔAr_L	1.4	1.3	8.8	7.5	14	24	0.36	0.24	3	2.4	1.1	0.8	0.18	0.26	5.5	7.2	0.18	0.13	0.71	0.71
rel. Ar_L	0.93	1.1	2.8	0.45	3.6	1.5	0.6	1.2	0.54	0.46	0.8	1.5	5.6	6.3	0.56	0.63	1.7	2.1	1.6	1.3
D_{LU}	1.8	1.8	1.5	1.6	4.4	4.4	0.84	0.84	0.54	0.62	1.7	1.8	7.1	6.9	1.6	1.6	2.5	2.6	1.6	1.7
D_{LB}	1.4	1.2	2.9	4	5	5	1.3	1.4	0.38	0.92	1.8	2.1	6.4	4.8	1.2	1.8	2.5	2.5	1.1	1.4
ΔD_L	1.4	1.4	1.1	1.5	4.4	4.3	0.6	0.84	0.46	0.54	0.57	0.57	5.8	5.6	0.84	0.99	1.9	2.1	1.6	1.7
rel. D_L	1.1	0.12	0	0.057	0.1	0	1.3	1.2	0.77	1.2	0.57	0.8	0.18	0.088	0.14	0	0.045	0.089	1.3	1.3
Ac_{LU}	1.7	1.5	15	15	14	16	1.4	1.6	0.31	0.38	2.4	2.4	1.9	2.4	6.8	7.7	2.1	2	0.43	0.28
Ac_{LB}	0.99	0.96	22	21	20	24	1.6	1.6	0.69	0.54	2.4	2.4	4.8	5.2	7.2	6.1	2.3	2.4	0.85	0.71
ΔAc_L	1.8	1.6	7	6.6	6.7	5.5	1.6	0.96	0.38	0.38	2.1	2.2	0.26	0.44	3.8	3.9	0.94	0.94	0.71	0.28
rel. Ac_L	1.2	1.2	1.5	0.68	1.1	0.83	0.24	0.84	0.62	0.69	0.91	1.3	0.088	0	1.6	1.5	0.98	1.2	1.4	0.28

P _{LU}	1	1	0.68	0.62	3.9	4.2	0.96	0.84	0.38	0.38	0.34	0.46	0.88	0.71	1.5	1.5	1.4	1.2	0.71	0.57
P _{LB}	1.1	0.92	0.51	0.85	4.5	4.7	0.24	0.48	0.46	0.38	0.34	0.69	0.71	0.88	1.9	1.8	1.3	0.76	0.57	0.43
ΔP _L	0.98	1.1	1.3	1.1	3.2	3.2	0.96	0.84	0.23	0.23	0.46	0.46	0.97	0.53	1.7	1.7	0.98	1.3	0.57	0.71
rel. P _L	1.3	1.4	0	0	0	0	0.24	0.48	0.46	0.38	0.34	0.46	0	0.44	0	0	0	0	0.28	1
N _{LU}	1.2	1.2	1.6	1.7	6.4	6.9	0.6	0.48	0.15	0.23	0.8	0.91	0.53	0.35	4.1	3.7	2.7	2.8	0.85	0.57
N _{LB}	1	1	3.2	2.3	8.4	7.6	0.6	0.48	0.46	0.23	0.34	0.57	3.5	1.6	4.8	4.3	2.7	3	0.85	1.3
ΔN _L	1.3	1.1	2.6	1.4	6.3	6.3	0.36	0.36	0.23	0.31	0.91	0.91	0.088	0.35	3.6	5.9	2.6	2.7	0.57	0.43
rel. N _L	0.99	0.99	3.5	2.7	11	6.4	0.6	0.48	0.54	0.31	1.7	2.3	4.3	2.4	5	5.1	2.7	2.9	0.85	1.4
O _{LU}	0.9	1.1	26	26	40	40	0.72	0.72	1.8	2	1.7	0.91	26	26	7.2	7.2	2.4	2.4	3.7	3.6
O _{LB}	1.1	1.1	23	25	34	33	0.96	1.1	1.9	1.3	2.1	1.9	24	26	7.2	6.5	2.5	2.5	3.4	3
ΔO _L	0.83	0.89	27	27	29	32	0.72	0.6	1.2	1.8	0.23	0.23	18	13	3	3.9	1.1	1.4	3.6	3.8
rel. O _L	1.2	1.2	1.5	1.6	6.3	4.9	0.24	1.4	1.5	0.92	2.2	2.1	11	8.7	2.8	2.3	2.2	2.2	1	0.85
ΔT _{RL}	1	0.92	27	27	47	47	1.3	1.2	1.5	1.8	1.5	1.1	23	21	16	13	2.7	2.7	4.1	4
rel. T _{RL}	1.2	1.3	0.57	0.85	5.5	4.2	0.96	1.3	0.85	0.38	2.2	2.1	11	14	1.7	1.3	1.7	2.3	1.1	0.85
ΔH _{RL}	1.2	1.1	28	28	38	40	1.8	1.2	1.3	1.1	1.1	1	3.5	6	11	8.3	2.5	2.7	2	1.8
rel. H _{RL}	1.1	1.1	0.057	0.17	0.52	0.1	0.84	1.3	0.38	0.15	1.8	1.9	0.88	2.8	0.28	1.3	0.49	1.8	0.85	0.71
ΔAr _{RL}	1.4	1.4	16	17	30	31	1.2	0.96	3.1	2.2	0.8	0.69	2.6	1.7	7.4	7.3	0.36	0.85	0.71	0.71
rel. Ar _{RL}	1	1	0	0.28	0.83	0.73	0.12	0.84	0.23	0.077	1	0.91	1.8	1.4	0.42	0.56	0.8	1.2	1.3	0.85
ΔD _{RL}	1.4	1.5	5.8	9.1	10	6	0.72	0.96	0.54	0.077	1	1	12	12	1.8	2.2	2.6	2.5	1.6	2.6
rel. D _{RL}	1	1.1	0	0	0	0.1	1.2	1.4	0.77	0.54	0.57	1.3	0.088	0	0.49	0	0.36	0.13	1.3	1.1
ΔAc _{RL}	1.7	1.6	13	13	14	8.7	1.6	1.3	0.15	0.38	2.2	2.2	0.79	0.97	4.4	4.2	1.5	1.4	0.71	0.43
rel. Ac _{RL}	0.93	1	4.9	1.5	0.52	8.7	0.48	0.84	0.38	0.38	1	2.1	1.1	1.1	0.91	0.77	1.3	1.3	1.7	0.85
ΔP _{RL}	0.98	1.1	13	13	10	12	1.2	0.84	0.85	1.3	1.3	1.3	11	6.4	2.3	7.3	2.2	1.7	2.1	1
rel. P _{RL}	1.3	1.3	0.057	0.4	0	0	0.72	0.84	0.54	1	1.1	0.69	0.088	0	1.1	0	0	0	0.71	1
ΔN _{RL}	1.3	1.1	15	6.1	17	19	0.36	0.36	0.23	0.31	0.69	1	0.44	3	3.7	5.8	2.6	2.7	1.3	1.4
rel. N _{RL}	0	0	0	0.057	0	0	0	0.72	0.54	0.69	0.69	0.8	0.71	0.26	1.5	0.28	2.5	1.5	1	1.3
ΔO _{RL}	0.89	0.89	27	27	30	31	0.6	0.6	1.3	1.9	0.23	0.23	18	14	3	3.9	1.2	1.5	3.6	3.8
rel. O _{RL}	1.1	1.2	1.5	1.6	6.4	4.8	0.24	1.4	1.4	1.1	2.2	2.1	11	8.9	2.7	2.3	2.2	2.2	1	1

Table S6. Enrichment Factors at 5% subsetting for protein structures of ten PPI targets obtained using post docking derivatized SASA descriptors.

The best enrichment score corresponding to each target protein (across columns) is shown in bold and highlighted in green.

SASA descriptor	BAZ2B		BCL2		BCLXL		BRD4-1		CREBBP		HIV-IN		XIAP		MCL1		MDM2		Menin	
	4XUA	5E73	2021	4LVT	3INQ	3WIZ	5D3L	5KU3	5EIC	5MMG	4CFD	4CHO	1TFT	5C3H	5FC4	5MES	4ODF	4ZFI	5DB2	6B41
Surflex	0.88	0.89	11	12	10	9.7	1.4	0.43	1.6	2.7	1.6	1.6	15	14	2.8	2.5	2.9	1.9	1.9	1.2
T _{RU}	0.98	1	17	16	16	16	1.6	1.2	1.4	2	0.82	0.87	8.2	7.2	4.5	3.8	2.1	1.9	1.9	1.9
T _{RB}	0.92	0.98	11	10	10	12	1.7	1	1.2	1.9	0.98	1.3	6	5.7	2.1	2.3	1.5	1.7	1.3	1.2
ΔT _R	0.94	0.99	18	18	17	17	1.6	1.4	1.9	1.7	0.8	0.82	7.3	7.4	4.9	4.8	2.2	2	2.2	2.5
rel. T _R	1	1.1	0.011	0.023	0.062	0.062	0.78	0.24	0.52	0.8	0.75	0.66	0.19	0.11	0.63	0.7	0.21	0.74	0.66	0.88
H _{RU}	0.94	1	16	16	15	16	1.6	1.2	1.4	2.1	1	0.87	4.4	7.2	4	3.5	2	1.9	1.7	1.8
H _{RB}	0.94	0.98	7.4	6.2	9.3	11	1.3	0.83	1.2	2.1	1.2	1.1	2.8	5	1.7	2.2	0.93	1.6	1.3	1.6
ΔH _R	0.97	1	17	16	16	16	1.6	1.4	1.9	1.6	0.82	0.87	6	9.2	4.7	3.8	2.1	2.1	2.1	2.1
rel. H _R	0.9	0.99	0.034	0.068	0.48	0.12	0.26	0.17	0.48	0.52	0.78	0.69	0	0.16	0.63	0.84	0.18	0.81	0.74	1.3
Ar _{RU}	0.66	0.72	6	12	2.6	6.9	1.6	1.4	1.7	1.4	0.59	0.75	2.2	1.4	2.5	2.2	1.8	1.6	1.4	1.4
Ar _{RB}	0.93	0.97	0.63	0.7	0.083	3.7	0.47	0.74	1.5	1.3	0.71	0.91	1.1	0.19	1.5	1.4	1.1	1	1.1	1.2
ΔAr _R	1	1	12	14	12	8.2	1.5	1.5	1.1	1.2	0.78	0.71	2.7	2.9	3.2	2.9	2	1.9	1.5	1.5
rel. Ar _R	0.88	1	0.1	0.079	0.042	0.42	0.095	0.19	0.77	0.54	0.96	0.57	0.12	0.018	0.58	0.56	0.42	0.41	1.1	0.77
D _{RU}	0.25	0.7	10	10	11	7	2	1.1	1	1.4	0.87	0.96	5.4	2.3	2.1	3	1.6	1.5	1.4	1.7
D _{RB}	1.1	1.1	6.5	0.93	0.71	1.8	1.9	1.1	0.94	1.2	0.87	0.98	3.3	1.3	1.1	1.4	1.5	1.3	1.1	0.68
ΔD _R	0.91	0.98	8.2	12	9.7	10	0.9	1.3	0.91	2.5	0.87	0.98	4.7	2.8	2.7	2.8	1.4	2	1.5	2.5
rel. D _R	1.1	1.1	0.045	0.045	0.021	0.021	1.4	1.1	0.71	0.45	0.71	1	0.28	0.25	0.32	0.49	0.39	0.18	0.8	0.77
Ac _{RU}	0.98	0.85	12	6.6	5.4	8.9	0.95	1.1	2	1.4	1.1	1.5	5.5	5.4	3.3	2.1	2.2	2	1.1	1.8
Ac _{RB}	0.96	0.94	10	4.5	4.1	2.2	0.85	1.1	1.7	1.2	1.3	1.1	0.58	2.6	2.6	1.4	2	1.9	1.1	1.1
ΔAc _R	1.1	1	13	7.1	7.5	9.6	0.83	1.1	1.9	1.7	0.94	1.1	3.7	3.9	3.7	3	1.4	1.6	1.1	1.8
rel. Ac _R	1.1	1	2.6	0.29	0.29	0.27	0.76	0.62	1	0.69	0.59	0.55	0.088	0.9	0.65	0.68	1.3	1.3	1	1.1
P _{RU}	0.0088	0.015	1.1	1.2	1.3	4	1.2	0.21	0.83	1.4	1.4	1.6	3	1.8	0.31	2.2	2	0.36	1.1	1.3
P _{RB}	0.0088	0.015	0.68	0.82	1.6	4.7	1	0.21	0.97	1.3	1.1	1.6	2	0.81	1.5	2	1.9	0.36	0.83	1.4

ΔP_R	0.0058	0.015	7.1	7.1	4.3	6	1	0.19	0.98	0.95	0.78	1.5	3.2	3	0.24	3.8	1.4	0.33	1.5	1.1
rel. P_R	0.0088	0.015	0.18	0.09	0	0.6	0.97	0.21	1.7	0.92	1.2	1.5	1.8	0	1.3	0.56	0.91	0.36	1.2	1.4
N_{RU}	0.11	0.15	13	8.1	10	7.3	1.7	1.4	0.74	1.7	0.82	1.1	0.69	2.3	0	0.042	0.23	0.59	1.5	1.5
N_{RB}	0.11	0.15	4.2	5.4	6.5	6.7	1.9	1.4	0.91	1.7	1.3	1.3	1.4	2.3	0.73	1	0.23	0.59	1.3	1.2
ΔN_R	0.24	0.31	15	9.1	6.7	10	1.2	1.5	0.57	1.5	0.87	1	2.7	4.2	2.3	2.1	0.22	0.58	1.7	1.7
rel. N_R	0	0	0.09	0.11	0.17	0	0.62	1.1	0.82	1.4	0.96	1.1	0.49	0.088	0.73	0.97	0.23	0.59	1.2	0.88
O_{RU}	0	0.0029	1.3	8.7	9.3	4.9	0.12	0.14	1.7	0.8	1.3	1.1	1.2	0.49	0.72	0	1.3	1	1.3	1.2
O_{RB}	0.99	0.97	0.56	2	1.4	0.89	0.14	0.24	1.3	0.71	1	0.82	1	3.1	1.3	0	1.2	1.4	0.91	1.2
ΔO_R	0.97	0.92	0.56	8.5	3.1	1.7	1.1	0.21	2.1	1.3	1.4	1.2	1.2	4.6	0	0	0.61	1.7	1.2	1.4
rel. O_R	0.98	1.1	0	0.32	0.48	0	0.14	0.24	0.35	0.65	1	0.85	0	0	1.3	0	0.93	0.32	0.77	1.3
T_{LU}	0.96	0.97	18	18	18	18	1.4	1.3	1.8	1.9	0.78	0.8	13	13	5.4	5.2	2.1	2.1	2.4	2.3
T_{LB}	1	1.1	17	17	17	16	1.3	1.1	2	1.4	0.82	0.82	9.3	12	5.2	5.2	2	2.1	1.9	2.1
ΔT_L	0.93	0.89	17	17	16	17	1.3	1	1.3	1.5	0.82	1.1	12	7.6	4.3	4.3	2.6	2.4	2.7	2.4
rel. T_L	1	1.1	3	3.9	7.4	5.2	1.1	1.4	1.4	0.91	0.85	0.8	5.2	7.1	3	2.6	1.3	1.7	1.2	1.4
H_{LU}	1.1	1.1	9.3	9.1	8.5	9.2	1.1	1.1	1.6	1.6	0.69	0.64	1.8	1.9	3.3	3.5	1.8	1.9	0.68	0.74
H_{LB}	0.98	1.1	8.9	6.2	8.2	8.6	1.2	1.6	1.8	2.3	1.1	1.1	4	4.4	3.3	3.3	1.6	2.4	0.77	0.83
ΔH_L	1.1	1	6.9	8.8	7.1	6.5	0.85	0.57	1.4	1.3	0.75	0.55	0.21	0.16	2.5	2.2	2.4	2.2	0.97	0.71
rel. H_L	0.98	0.96	3.2	1.8	3.8	2.4	1.6	1.8	1.1	1.5	1.5	1.4	3.8	5.8	1.1	1.3	1.3	1.9	1	1.2
Ar_{LU}	1.2	1.1	5.3	4.7	11	12	0.9	0.81	2.2	2.2	1.1	1	1.7	2.1	4.7	4.5	0.27	0.24	0.57	0.6
Ar_{LB}	1.1	1.1	6.1	5.2	11	10	1.1	1.1	1.6	1.6	0.82	1.1	4.5	5.6	4.3	3.9	0.43	0.49	0.68	0.68
ΔAr_L	1.2	1.2	4.5	3.8	6.8	9	0.64	0.43	2.5	2.3	0.94	0.8	0.3	0.16	3.9	3.4	0.21	0.19	0.63	0.77
rel. Ar_L	0.92	1	2.4	1.3	3.2	2	0.9	1.3	0.34	0.57	1.1	1.1	3.8	5	0.94	0.84	1.4	1.8	1.1	1.2
D_{LU}	1.2	1.3	1.3	1.4	1.6	1.6	1	1	0.48	0.46	0.78	0.78	5.4	5.5	1.1	1.1	1.5	1.5	0.77	0.8
D_{LB}	1.1	1	3	3.5	2.5	2.6	1.3	1.6	0.72	0.71	0.89	0.87	3.8	3	1.6	1.8	1.7	1.5	0.97	1
ΔD_L	1.2	1.2	1.5	1.2	1.4	1.4	0.88	0.78	0.52	0.57	0.66	0.64	4.7	4.9	1.3	1.1	1.3	1.4	0.77	0.91
rel. D_L	0.88	0.98	1.5	1.5	2.6	2.4	1.2	1.4	1	1	1.1	1.1	0.19	0.053	1.3	1.4	1	0.81	1.3	1.3
Ac_{LU}	1.3	1.2	11	11	7.9	8.4	1.3	1.4	0.38	0.43	1.1	1.1	1.2	1.4	3.3	3.3	1.4	1.4	0.37	0.43
Ac_{LB}	1	1.1	12	10	7.7	9	1.2	1.4	1.1	0.62	1.2	1	2.4	2.5	3.3	2.9	1.6	2	0.71	0.83
ΔAc_L	1.3	1.2	4.8	4.6	4.4	3.8	1.3	0.97	0.42	0.55	1.1	1.2	0.44	0.34	2.3	1.9	1.2	0.94	0.43	0.26
rel. Ac_L	1.1	1	3.6	2.2	2.7	3.2	0.55	0.78	1.1	0.72	1.1	1.3	0.79	0.65	1.5	1.2	1.2	1.1	1	0.74

P _{LU}	1.3	1.3	2.5	2.5	3.3	1.9	0.36	0.36	0.43	0.43	0.39	0.39	2.6	2.6	1.5	1.5	0.91	0.88	0.57	0.66
P _{LB}	0.59	0.77	3.6	3.3	2.8	2.7	0.17	0.21	0.66	0.65	0.37	0.48	0.88	0.56	2	2.1	0.87	0.65	0.43	0.74
ΔP _L	1.3	1.3	2.8	4.2	3.3	2.8	0.36	0.36	0.42	0.42	0.37	0.32	2.4	2.5	1.6	1.4	0.9	0.89	0.74	0.51
rel. P _L	0.59	0.77	4.7	4.4	2.9	4	0.17	0.21	0.66	0.65	0.37	0.48	0.88	0.58	2	2.4	1.5	0.63	0.4	0.74
N _{LU}	0.77	0.77	1.7	1.7	7.6	7.6	0.24	0.24	0.35	0.34	0.82	1.3	0.95	0.95	4.5	4.4	2.8	2.8	0.63	0.68
N _{LB}	0.72	0.71	1.6	1.7	7.5	7.4	0.24	0.24	0.26	0.25	0.78	1.1	0.94	0.95	4.5	4.4	2.8	2.8	0.66	0.83
ΔN _L	0.76	0.76	1.7	1.6	7.5	7.5	0.24	0.24	0.2	0.28	1.2	1.1	0.86	0.85	4.4	4.5	2.8	2.8	0.66	0.54
rel. N _L	0.72	0.71	1.6	1.7	7.5	7.4	0.24	0.24	0.26	0.25	0.8	1.2	0.94	0.95	4.6	4.5	2.8	2.8	0.66	0.83
O _{LU}	0.78	0.82	17	17	14	14	1	0.9	1.2	1.3	0.69	0.69	12	12	2.7	2.7	1.6	1.6	2.3	2.3
O _{LB}	1	0.94	12	14	13	12	1.2	1.1	1.6	1.1	0.69	0.71	9.7	12	2.9	2.8	1.9	1.8	2.2	2.1
ΔO _L	0.76	0.85	15	15	11	12	0.88	0.85	0.88	1.1	0.57	0.5	9.4	6.9	1.9	2.1	1.3	1.4	2.3	2.3
rel. O _L	1.1	1.1	1.2	1.8	4	2.5	1	1.2	1.4	0.88	0.82	0.85	3.6	4.2	2.2	2.1	1.6	1.6	1.1	1.2
ΔT _{RL}	0.89	0.93	18	18	17	17	1.4	1.2	1.7	1.8	0.78	0.94	11	7.9	4.8	4.6	2.4	2.2	2.5	2.5
rel. T _{RL}	1.1	1.1	0.36	0.55	2.3	1.7	0.83	1.3	0.92	0.58	0.94	0.94	3	5	1.3	1.5	0.83	1.5	0.83	1
ΔH _{RL}	1.1	1	16	15	13	15	1.4	1.1	2.3	1.7	0.91	0.64	1.9	2.5	4.5	3.9	2.8	2.4	1.8	1.6
rel. H _{RL}	0.95	1	0.11	0.24	1	0.27	0.76	1.4	0.45	0.65	1.3	1.5	0.56	2.5	0.65	1.2	0.35	1.5	0.85	0.94
ΔAr _{RL}	1.2	1.1	8.6	9.7	13	12	1.2	0.85	2.5	2.2	0.87	0.8	1.5	0.74	4.3	3.8	0.35	0.54	0.88	0.94
rel. Ar _{RL}	1	1	0.15	0.44	0.62	1.1	0.66	0.76	0.34	0.31	1	0.94	1.5	1.4	0.59	0.25	0.8	1.1	1	1.2
ΔD _{RL}	1.2	1.3	6.9	9.2	7.7	3.7	0.88	0.85	0.55	0.31	0.75	0.78	7.4	8.3	1.8	1.9	1.4	1.8	1	1.2
rel. D _{RL}	1.1	1	0.068	0	0.021	0.25	1.4	1.3	1.1	0.69	0.87	0.87	0.071	0.11	0.51	0.46	0.65	0.39	0.8	0.91
ΔAc _{RL}	1.2	1.2	7.7	7.2	6.5	4.8	1.2	1	0.57	0.66	1	1.3	0.86	0.99	2.4	2.4	1.3	1.1	0.48	0.43
rel. Ac _{RL}	0.97	1	4.8	1.8	1.6	4.8	0.83	0.93	0.94	0.48	1	1.2	1	1.1	1.4	1.2	1.5	1.3	1.1	0.97
ΔP _{RL}	1.3	1.3	7.1	7.1	4.5	6.1	0.97	0.4	0.97	0.95	0.75	1.3	3.1	3.1	1.4	3.9	1.4	1	1.5	0.54
rel. P _{RL}	0.6	0.78	0.19	0.12	0.042	0.64	0.97	0.28	1.7	0.94	1.2	1.3	1.9	0	1.2	0.52	0.87	0.72	1.1	1.3
ΔN _{RL}	0.94	0.91	13	6	9.6	10	1	1.1	0.2	0.28	1	1.1	1.9	2.8	4.4	4.6	2.8	2.7	0.85	0.77
rel. N _{RL}	0	0	0.079	0.079	0	0	0.64	1.1	0.82	1.4	1	1.3	0.53	0.18	0.96	0.94	2.7	2	1.2	0.97
ΔO _{RL}	0.77	0.83	15	15	11	12	0.85	0.85	0.94	1.1	0.57	0.5	9.4	7.3	1.9	2.1	1.3	1.4	2.4	2.3
rel. O _{RL}	1.1	1.1	1.2	1.8	3.9	2.2	1	1.2	1.3	0.8	0.82	0.82	3.6	4.3	2.2	2.1	1.5	1.5	1.1	1.2

Table S7. 10-fold Cross-Validation TN, FP, FN, TP, Total, Sensitivity, Specificity, Precision, Concordance (Accuracy), J, MCC, F₁, k, ROC score, EF 1%, and EF 5% values for the different machine learning models obtained on 10 PPI targets with a total of 20 protein structures.

Target	PDB ID	ML techniques	TN	FP	FN	TP	Total	Sensitivity	Specificity	Precision	Concordance	J	MCC	F ₁	k	ROC score	EF 1%	EF 5%
BAZ2B	4XUA	Tree	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.543	2.127	1.633
		Bagged forest	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.500	1.000	1.000
		Random forest	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.601	3.931	2.345
		Bayesian	34543	55	4722	72	39392	0.015	0.998	0.567	0.879	0.013	0.077	0.029	0.023	0.602	3.136	2.032
		SVM	34492	106	4181	613	39392	0.128	0.997	0.853	0.891	0.125	0.305	0.222	0.197	0.758	7.464	5.125
		Logistic regression	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.550	1.296	1.081
		Neural net	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.543	1.066	1.181
		Neural net (bagging)	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.651	3.952	2.667
	5E73	Tree	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.534	1.922	1.490
		Bagged forest	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.500	1.000	1.000
		Random forest	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.631	3.617	2.391
		Bayesian	34499	99	4699	95	39392	0.020	0.997	0.490	0.878	0.017	0.079	0.038	0.029	0.602	3.178	2.070
		SVM	34492	106	4065	729	39392	0.152	0.997	0.873	0.894	0.149	0.338	0.259	0.231	0.772	7.569	5.738
		Logistic regression	34598	0	4793	1	39392	0.000	1.000	1.000	0.878	0.000	0.014	0.000	0.000	0.535	1.443	1.089
		Neural net	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.542	1.422	1.294
		Neural net (bagging)	34598	0	4794	0	39392	0.000	1.000	N/A	0.878	0.000	N/A	N/A	0.000	0.671	4.286	2.942
Bcl-2	2O21	Tree	34305	38	166	1074	35583	0.866	0.999	0.966	0.994	0.865	0.912	0.913	0.910	0.965	28.557	18.313
		Bagged forest	34262	81	147	1093	35583	0.881	0.998	0.931	0.994	0.879	0.903	0.906	0.902	0.943	27.496	17.798
		Random forest	34305	38	152	1088	35583	0.877	0.999	0.966	0.995	0.876	0.918	0.920	0.917	0.999	28.696	19.663
		Bayesian	33822	521	124	1116	35583	0.900	0.985	0.682	0.982	0.885	0.775	0.776	0.767	0.984	28.546	18.066
		SVM	34322	21	99	1141	35583	0.920	0.999	0.982	0.997	0.920	0.949	0.950	0.948	0.990	28.696	19.292
		Logistic regression	34318	25	418	822	35583	0.663	0.999	0.970	0.988	0.662	0.797	0.788	0.782	0.973	27.483	18.098
		Neural net	34307	36	170	1070	35583	0.863	0.999	0.967	0.994	0.862	0.911	0.912	0.909	0.992	28.696	18.937

	4LVT	Neural net (bagging)	34341	2	27	1213	35583	0.978	1.000	0.998	0.999	0.978	0.988	0.988	0.988	1.000	28.696	20.002
		Tree	34311	32	173	1067	35583	0.860	0.999	0.971	0.994	0.860	0.911	0.912	0.909	0.948	28.581	17.984
		Bagged forest	34259	84	155	1085	35583	0.875	0.998	0.928	0.993	0.873	0.898	0.901	0.897	0.940	27.278	17.687
		Random forest	34310	33	151	1089	35583	0.878	0.999	0.971	0.995	0.877	0.921	0.922	0.919	0.998	28.696	19.469
		Bayesian	33886	457	125	1115	35583	0.899	0.987	0.709	0.984	0.886	0.791	0.793	0.785	0.984	28.516	18.227
		SVM	34324	19	117	1123	35583	0.906	0.999	0.983	0.996	0.905	0.942	0.943	0.941	0.988	28.696	19.292
		Logistic regression	34316	27	451	789	35583	0.636	0.999	0.967	0.987	0.636	0.779	0.768	0.761	0.979	27.079	18.195
		Neural net	34299	44	164	1076	35583	0.868	0.999	0.961	0.994	0.866	0.910	0.912	0.909	0.989	28.615	18.889
		Neural net (bagging)	34341	2	16	1224	35583	0.987	1.000	0.998	0.999	0.987	0.992	0.993	0.992	1.000	28.696	20.002
Bcl-xL	3INQ	Tree	34382	38	131	543	35094	0.806	0.999	0.935	0.995	0.805	0.865	0.865	0.863	0.971	51.306	18.616
		Bagged forest	34346	74	141	533	35094	0.791	0.998	0.878	0.994	0.789	0.830	0.832	0.829	0.907	46.798	16.444
		Random forest	34401	19	129	545	35094	0.809	0.999	0.966	0.996	0.808	0.882	0.880	0.878	0.997	52.068	19.563
		Bayesian	33764	656	72	602	35094	0.893	0.981	0.479	0.979	0.874	0.645	0.623	0.614	0.983	49.688	18.405
		SVM	34404	16	72	602	35094	0.893	1.000	0.974	0.997	0.893	0.932	0.932	0.931	0.991	51.771	19.266
		Logistic regression	34402	18	511	163	35094	0.242	0.999	0.901	0.985	0.241	0.462	0.381	0.376	0.980	46.861	18.494
		Neural net	34379	41	123	551	35094	0.818	0.999	0.931	0.995	0.816	0.870	0.870	0.868	0.987	51.919	19.028
		Neural net (bagging)	34418	2	7	667	35094	0.990	1.000	0.997	1.000	0.990	0.993	0.993	0.993	1.000	52.068	20.008
	3WIZ	Tree	34399	21	159	515	35094	0.764	0.999	0.961	0.995	0.763	0.854	0.851	0.849	0.973	50.892	18.713
		Bagged forest	34352	68	148	526	35094	0.780	0.998	0.886	0.994	0.778	0.828	0.830	0.827	0.906	46.432	16.415
		Random forest	34396	24	128	546	35094	0.810	0.999	0.958	0.996	0.809	0.879	0.878	0.876	0.998	52.068	19.622
		Bayesian	31015	3405	43	631	35094	0.936	0.901	0.156	0.902	0.837	0.360	0.268	0.243	0.977	50.581	17.663
		SVM	34420	0	14	660	35094	0.979	1.000	1.000	1.000	0.979	0.989	0.990	0.989	1.000	52.068	19.949
		Logistic regression	34405	15	577	97	35094	0.144	1.000	0.866	0.983	0.143	0.349	0.247	0.243	0.975	47.456	18.405
		Neural net	34397	23	127	547	35094	0.812	0.999	0.960	0.996	0.811	0.880	0.879	0.877	0.988	44.641	15.979
		Neural net (bagging)	34420	0	13	661	35094	0.981	1.000	1.000	1.000	0.981	0.990	0.990	0.990	1.000	52.068	20.008
BRD4-1	5D3L	Tree	624	63	73	519	1279	0.877	0.908	0.892	0.894	0.785	0.786	0.884	0.786	0.962	2.155	2.150
		Bagged forest	638	49	66	526	1279	0.889	0.929	0.915	0.910	0.817	0.819	0.901	0.819	0.972	2.160	2.160
		Random forest	614	73	59	533	1279	0.900	0.894	0.880	0.897	0.794	0.793	0.890	0.793	0.968	2.160	2.160
		Bayesian	585	102	69	523	1279	0.883	0.852	0.837	0.866	0.735	0.733	0.859	0.732	0.936	2.160	2.160

CREBBP	5KU3	SVM	619	68	74	518	1279	0.875	0.901	0.884	0.889	0.776	0.777	0.879	0.777	0.952	1.980	2.126
		Logistic regression	629	58	139	453	1279	0.765	0.916	0.886	0.846	0.681	0.693	0.821	0.687	0.917	2.160	2.092
		Neural net	600	87	79	513	1279	0.867	0.873	0.855	0.870	0.740	0.739	0.861	0.739	0.947	2.160	2.160
		Neural net (bagging)	687	0	0	592	1279	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	2.160	2.160
		Tree	635	52	42	550	1279	0.929	0.924	0.914	0.927	0.853	0.852	0.921	0.852	0.972	2.160	2.160
		Bagged forest	614	73	50	542	1279	0.916	0.894	0.881	0.904	0.809	0.808	0.898	0.807	0.966	2.160	2.160
		Random forest	581	106	55	537	1279	0.907	0.846	0.835	0.874	0.753	0.751	0.870	0.748	0.957	2.160	2.160
		Bayesian	540	147	65	527	1279	0.890	0.786	0.782	0.834	0.676	0.675	0.833	0.670	0.924	2.160	2.160
	5EIC	SVM	591	96	88	504	1279	0.851	0.860	0.840	0.856	0.712	0.711	0.846	0.711	0.927	2.160	2.126
		Logistic regression	611	76	139	453	1279	0.765	0.889	0.856	0.832	0.655	0.663	0.808	0.659	0.900	2.160	2.126
		Neural net	581	106	88	504	1279	0.851	0.846	0.826	0.848	0.697	0.696	0.839	0.696	0.928	2.160	2.160
		Neural net (bagging)	687	0	1	591	1279	0.998	1.000	1.000	0.999	0.998	0.998	0.999	0.998	1.000	2.160	2.160
		Tree	32425	0	910	0	33335	0.000	1.000	N/A	0.973	0.000	N/A	N/A	0.000	0.635	5.140	3.225
		Bagged forest	32425	0	910	0	33335	0.000	1.000	N/A	0.973	0.000	N/A	N/A	0.000	0.500	1.000	1.000
		Random forest	32425	0	910	0	33335	0.000	1.000	N/A	0.973	0.000	N/A	N/A	0.000	0.887	24.531	10.356
		Bayesian	31019	1406	677	233	33335	0.256	0.957	0.142	0.938	0.213	0.160	0.183	0.153	0.794	9.020	5.211
HIV IN	5MMG	SVM	32392	33	535	375	33335	0.412	0.999	0.919	0.983	0.411	0.609	0.569	0.562	0.938	34.872	13.545
		Logistic regression	32425	0	910	0	33335	0.000	1.000	N/A	0.973	0.000	N/A	N/A	0.000	0.766	6.820	4.683
		Neural net	32425	0	910	0	33335	0.000	1.000	N/A	0.973	0.000	N/A	N/A	0.000	0.766	7.810	4.683
		Neural net (bagging)	32425	0	901	9	33335	0.010	1.000	1.000	0.973	0.010	0.098	0.020	0.019	0.938	26.951	12.489
		Tree	32425	0	910	0	33335	0.000	1.000	N/A	0.973	0.000	N/A	N/A	0.000	0.714	6.344	3.832
		Bagged forest	32425	0	910	0	33335	0.000	1.000	N/A	0.973	0.000	N/A	N/A	0.000	0.500	1.000	1.000
		Random forest	32425	0	910	0	33335	0.000	1.000	N/A	0.973	0.000	N/A	N/A	0.000	0.883	20.131	10.224
		Bayesian	29632	2793	636	274	33335	0.301	0.914	0.089	0.897	0.215	0.121	0.138	0.100	0.746	4.840	3.980
	4CFD	SVM	32398	27	467	443	33335	0.487	0.999	0.943	0.985	0.486	0.672	0.642	0.635	0.946	36.412	14.138
		Logistic regression	32425	0	910	0	33335	0.000	1.000	N/A	0.973	0.000	N/A	N/A	0.000	0.734	5.500	4.486
		Neural net	32425	0	910	0	33335	0.000	1.000	N/A	0.973	0.000	N/A	N/A	0.000	0.760	6.710	4.617
		Neural net (bagging)	32425	0	904	6	33335	0.007	1.000	1.000	0.973	0.007	0.080	0.013	0.013	0.934	23.981	11.829
		Tree	829	26	93	517	1465	0.848	0.970	0.952	0.919	0.817	0.834	0.897	0.830	0.970	2.402	2.402

			Bagged forest	801	54	134	476	1465	0.780	0.937	0.898	0.872	0.717	0.736	0.835	0.731	0.920	2.402	2.374
			Random forest	771	84	114	496	1465	0.813	0.902	0.855	0.865	0.715	0.721	0.834	0.720	0.936	2.402	2.402
			Bayesian	625	230	122	488	1465	0.800	0.731	0.680	0.760	0.531	0.524	0.735	0.518	0.827	2.402	2.171
			SVM	720	135	119	491	1465	0.805	0.842	0.784	0.827	0.647	0.645	0.794	0.645	0.895	2.230	2.237
			Logistic regression	807	48	431	179	1465	0.293	0.944	0.789	0.673	0.237	0.323	0.428	0.261	0.781	2.230	1.941
			Neural net	719	136	209	401	1465	0.657	0.841	0.747	0.765	0.498	0.510	0.699	0.507	0.831	2.402	2.303
			Neural net (bagging)	855	0	0	610	1465	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	2.402	2.402
		4CHO	Tree	782	73	172	438	1465	0.718	0.915	0.857	0.833	0.633	0.654	0.781	0.648	0.931	2.402	2.402
			Bagged forest	794	61	146	464	1465	0.761	0.929	0.884	0.859	0.689	0.709	0.818	0.703	0.928	2.402	2.402
			Random forest	808	47	165	445	1465	0.730	0.945	0.904	0.855	0.675	0.704	0.808	0.694	0.929	2.402	2.402
			Bayesian	608	247	135	475	1465	0.779	0.711	0.658	0.739	0.490	0.483	0.713	0.477	0.832	2.402	2.369
			SVM	734	121	141	469	1465	0.769	0.858	0.795	0.821	0.627	0.631	0.782	0.630	0.896	2.402	2.336
			Logistic regression	805	50	411	199	1465	0.326	0.942	0.799	0.685	0.268	0.351	0.463	0.293	0.770	2.402	2.336
			Neural net	744	111	232	378	1465	0.620	0.870	0.773	0.766	0.490	0.512	0.688	0.504	0.833	2.402	2.303
			Neural net (bagging)	855	0	0	610	1465	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	2.402	2.402
XIAP		1TFT	Tree	34425	103	263	530	35321	0.668	0.997	0.837	0.990	0.665	0.743	0.743	0.738	0.972	38.484	17.750
			Bagged forest	34385	143	237	556	35321	0.701	0.996	0.795	0.989	0.697	0.741	0.745	0.740	0.974	37.172	17.453
			Random forest	34509	19	206	587	35321	0.740	0.999	0.969	0.994	0.740	0.844	0.839	0.836	0.998	44.541	19.849
			Bayesian	29963	4565	21	772	35321	0.974	0.868	0.145	0.870	0.841	0.348	0.252	0.221	0.981	36.213	17.478
			SVM	34479	49	99	694	35321	0.875	0.999	0.934	0.996	0.874	0.902	0.904	0.902	0.997	43.532	19.471
			Logistic regression	34514	14	683	110	35321	0.139	1.000	0.887	0.980	0.138	0.346	0.240	0.235	0.984	36.592	18.260
			Neural net	34462	66	159	634	35321	0.799	0.998	0.906	0.994	0.798	0.848	0.849	0.846	0.994	43.658	19.294
			Neural net (bagging)	34524	4	8	785	35321	0.990	1.000	0.995	1.000	0.990	0.992	0.992	0.992	1.000	44.541	20.001
		5C3H	Tree	34409	119	214	579	35321	0.730	0.997	0.830	0.991	0.727	0.774	0.777	0.772	0.985	42.323	18.547
			Bagged forest	34357	171	208	585	35321	0.738	0.995	0.774	0.989	0.733	0.750	0.755	0.750	0.984	38.358	18.386
			Random forest	34509	19	221	572	35321	0.721	0.999	0.968	0.993	0.721	0.832	0.827	0.823	0.998	44.541	19.849
			Bayesian	32991	1537	85	708	35321	0.893	0.955	0.315	0.954	0.848	0.515	0.466	0.448	0.981	36.339	17.024
			SVM	34476	52	104	689	35321	0.869	0.998	0.930	0.996	0.867	0.897	0.898	0.896	0.998	43.910	19.698
			Logistic regression	34513	15	670	123	35321	0.155	1.000	0.891	0.981	0.155	0.367	0.264	0.259	0.987	36.844	17.983

		Neural net	34435	93	144	649	35321	0.818	0.997	0.875	0.993	0.816	0.843	0.846	0.842	0.997	43.532	19.673
		Neural net (bagging)	34522	6	9	784	35321	0.989	1.000	0.992	1.000	0.988	0.990	0.991	0.990	1.000	44.541	20.001
Mcl-1	5FC4	Tree	34065	82	856	139	35142	0.140	0.998	0.629	0.973	0.137	0.288	0.229	0.221	0.752	22.055	8.207
		Bagged forest	34074	73	862	133	35142	0.134	0.998	0.646	0.973	0.132	0.286	0.221	0.214	0.578	16.208	3.915
		Random forest	34144	3	822	173	35142	0.174	1.000	0.983	0.977	0.174	0.408	0.295	0.289	0.930	29.583	13.227
		Bayesian	31061	3086	493	502	35142	0.505	0.910	0.140	0.898	0.414	0.227	0.219	0.183	0.811	19.420	7.619
		SVM	34082	65	712	283	35142	0.284	0.998	0.813	0.978	0.283	0.473	0.421	0.413	0.835	28.476	11.538
		Logistic regression	34144	3	989	6	35142	0.006	1.000	0.667	0.972	0.006	0.062	0.012	0.011	0.817	20.023	8.704
		Neural net	34145	2	984	11	35142	0.011	1.000	0.846	0.972	0.011	0.095	0.022	0.021	0.842	22.238	9.448
		Neural net (bagging)	34138	9	743	252	35142	0.253	1.000	0.966	0.979	0.253	0.489	0.401	0.394	0.956	32.602	14.131
	5MES	Tree	34048	99	845	150	35142	0.151	0.997	0.602	0.973	0.148	0.292	0.241	0.232	0.780	21.735	9.548
		Bagged forest	34051	96	848	147	35142	0.148	0.997	0.605	0.973	0.145	0.290	0.237	0.229	0.583	17.077	4.082
		Random forest	34145	2	881	114	35142	0.115	1.000	0.983	0.975	0.115	0.331	0.205	0.200	0.921	27.269	12.463
		Bayesian	32781	1366	605	390	35142	0.392	0.960	0.222	0.944	0.352	0.268	0.284	0.257	0.819	20.125	7.840
		SVM	34089	58	628	367	35142	0.369	0.998	0.864	0.980	0.367	0.557	0.517	0.509	0.877	31.897	13.428
		Logistic regression	34147	0	993	2	35142	0.002	1.000	1.000	0.972	0.002	0.044	0.004	0.004	0.817	18.213	8.583
		Neural net	34147	0	993	2	35142	0.002	1.000	1.000	0.972	0.002	0.044	0.004	0.004	0.843	21.835	9.548
		Neural net (bagging)	34139	8	768	227	35142	0.228	1.000	0.966	0.978	0.228	0.464	0.369	0.362	0.957	31.998	14.393
Mdm2	4ODF	Tree	2941	99	229	1330	4599	0.853	0.967	0.931	0.929	0.821	0.839	0.890	0.838	0.943	2.950	2.950
		Bagged forest	2903	137	233	1326	4599	0.851	0.955	0.906	0.920	0.805	0.819	0.878	0.818	0.938	2.950	2.924
		Random forest	2972	68	266	1293	4599	0.829	0.978	0.950	0.927	0.807	0.837	0.886	0.833	0.977	2.950	2.950
		Bayesian	2656	384	198	1361	4599	0.873	0.874	0.780	0.873	0.747	0.728	0.824	0.726	0.932	2.950	2.937
		SVM	2947	93	170	1389	4599	0.891	0.969	0.937	0.943	0.860	0.871	0.914	0.871	0.966	2.950	2.937
		Logistic regression	2931	109	369	1190	4599	0.763	0.964	0.916	0.896	0.727	0.765	0.833	0.758	0.942	2.884	2.924
		Neural net	2870	170	220	1339	4599	0.859	0.944	0.887	0.915	0.803	0.810	0.873	0.809	0.952	2.884	2.937
		Neural net (bagging)	3029	11	60	1499	4599	0.962	0.996	0.993	0.985	0.958	0.966	0.977	0.965	0.999	2.949	2.950
	4ZFI	Tree	2941	99	255	1304	4599	0.836	0.967	0.929	0.923	0.804	0.826	0.880	0.824	0.952	2.950	2.950
		Bagged forest	2925	115	303	1256	4599	0.806	0.962	0.916	0.909	0.768	0.795	0.857	0.791	0.937	2.950	2.926
		Random forest	2987	53	297	1262	4599	0.809	0.983	0.960	0.924	0.792	0.830	0.878	0.823	0.977	2.950	2.950

Menin		Bayesian	2671	369	249	1310	4599	0.840	0.879	0.780	0.866	0.719	0.707	0.809	0.706	0.926	2.950	2.950
		SVM	2925	115	198	1361	4599	0.873	0.962	0.922	0.932	0.835	0.847	0.897	0.846	0.962	2.950	2.950
		Logistic regression	2942	98	327	1232	4599	0.790	0.968	0.926	0.908	0.758	0.791	0.853	0.786	0.942	2.950	2.950
		Neural net	2881	159	227	1332	4599	0.854	0.948	0.893	0.916	0.802	0.811	0.873	0.811	0.956	2.950	2.950
		Neural net (bagging)	3034	6	56	1503	4599	0.964	0.998	0.996	0.987	0.962	0.970	0.980	0.970	0.999	2.950	2.950
	5DB2	Tree	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.500	1.000	1.000
		Bagged forest	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.500	1.000	1.000
		Random forest	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.823	14.060	6.928
		Bayesian	21903	117	448	43	22511	0.088	0.995	0.269	0.975	0.082	0.143	0.132	0.123	0.758	10.800	5.013
		SVM	22017	3	333	158	22511	0.322	1.000	0.981	0.985	0.322	0.558	0.485	0.479	0.903	41.772	12.267
		Logistic regression	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.662	6.928	3.790
		Neural net	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.680	4.483	3.219
		Neural net (bagging)	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.969	34.640	15.242
	6B41	Tree	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.538	3.663	2.449
		Bagged forest	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.500	1.000	1.000
		Random forest	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.828	11.207	5.339
		Bayesian	21938	82	457	34	22511	0.069	0.996	0.293	0.976	0.066	0.134	0.112	0.105	0.760	9.781	4.809
		SVM	22016	4	341	150	22511	0.305	1.000	0.974	0.985	0.305	0.541	0.465	0.459	0.897	42.179	11.900
		Logistic regression	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.617	1.223	0.652
		Neural net	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.679	3.668	2.527
		Neural net (bagging)	22020	0	491	0	22511	0.000	1.000	N/A	0.978	0.000	N/A	N/A	0.000	0.971	37.085	16.342

Table S8: External Statistics for the machine learning models attained on 10 PPI targets and the corresponding protein structures. The best value(s) corresponding to each target protein (across rows) is shown in bold and highlighted in green.

Target	PDB ID	External statistics	Tree	Bagged forest	Random forest	Bayesian	SVM	Logistic regression	Neural net	Neural net (bagging)
BAZ2B	4XUA	ROC score	0.534	0.5	0.537	0.53	0.521	0.532	0.53	0.54
		Sensitivity	0	0	0	0.002	0.047	0	0	0
		Specificity	1.000	1.000	1.000	0.997	0.974	1.000	1.000	1.000
		Precision	N/A	N/A	N/A	0.116	0.204	0	N/A	N/A
		Concordance	0.878	0.878	0.878	0.876	0.862	0.878	0.878	0.878
	5.00E+73	ROC score	0.524	0.5	0.546	0.525	0.54	0.52	0.538	0.553
		Sensitivity	0	0	0	0.006	0.057	0	0	0
		Specificity	1.000	1.000	1.000	0.995	0.97	1.000	1.000	1.000
		Precision	N/A	N/A	N/A	0.141	0.206	N/A	N/A	N/A
		Concordance	0.878	0.878	0.878	0.874	0.858	0.878	0.878	0.878
Bcl-2	2021	ROC score	0.966	0.949	0.987	0.978	0.979	0.972	0.981	0.985
		Sensitivity	0.868	0.893	0.894	0.906	0.896	0.661	0.851	0.896
		Specificity	0.999	0.998	0.999	0.985	0.999	0.999	0.999	0.999
		Precision	0.966	0.939	0.976	0.681	0.956	0.978	0.964	0.981
		Concordance	0.994	0.994	0.995	0.982	0.995	0.988	0.994	0.996
	4LVT	ROC score	0.948	0.948	0.992	0.982	0.976	0.974	0.988	0.991
		Sensitivity	0.861	0.879	0.878	0.895	0.898	0.612	0.872	0.898
		Specificity	0.999	0.998	0.999	0.986	0.998	1.000	0.999	0.999
		Precision	0.968	0.949	0.969	0.704	0.95	0.982	0.955	0.962
		Concordance	0.994	0.994	0.995	0.983	0.995	0.986	0.994	0.995
Bcl-xL	3INQ	ROC score	0.964	0.91	0.989	0.982	0.983	0.985	0.99	0.986
		Sensitivity	0.772	0.792	0.765	0.889	0.865	0.249	0.792	0.824
		Specificity	0.998	0.997	0.999	0.982	0.999	1.000	0.999	0.999
		Precision	0.896	0.854	0.94	0.491	0.923	0.923	0.935	0.944
		Concordance	0.994	0.993	0.995	0.98	0.996	0.985	0.995	0.996
	3WIZ	ROC score	0.979	0.916	0.989	0.975	0.981	0.986	0.988	0.993
		Sensitivity	0.782	0.799	0.817	0.931	0.875	0.145	0.817	0.858
		Specificity	1.000	0.998	1.000	0.901	0.991	1.000	0.999	0.999
		Precision	0.983	0.906	0.971	0.156	0.661	0.875	0.959	0.969
		Concordance	0.996	0.995	0.996	0.902	0.989	0.983	0.996	0.997
BRD4-1	5D3L	ROC score	0.926	0.926	0.918	0.897	0.915	0.893	0.917	0.918
		Sensitivity	0.826	0.83	0.818	0.834	0.846	0.779	0.842	0.846
		Specificity	0.881	0.891	0.861	0.823	0.854	0.874	0.854	0.861
		Precision	0.857	0.868	0.835	0.802	0.833	0.842	0.832	0.839
		Concordance	0.856	0.863	0.841	0.828	0.85	0.83	0.848	0.854

	5KU3	ROC score	0.901	0.901	0.911	0.886	0.908	0.887	0.906	0.927
		Sensitivity	0.87	0.858	0.881	0.889	0.866	0.794	0.866	0.866
		Specificity	0.786	0.796	0.741	0.752	0.806	0.847	0.789	0.854
		Precision	0.777	0.783	0.746	0.755	0.793	0.817	0.779	0.836
		Concordance	0.824	0.824	0.806	0.815	0.834	0.823	0.824	0.859
CREBBP	5EIC	ROC score	0.631	0.5	0.769	0.726	0.724	0.744	0.75	0.772
		Sensitivity	0	0	0	0.205	0.179	0	0	0.003
		Specificity	1.000	1.000	1.000	0.958	0.98	1.000	1.000	1.000
		Precision	N/A	N/A	N/A	0.12	0.203	N/A	N/A	1.000
		Concordance	0.973	0.973	0.973	0.937	0.958	0.973	0.973	0.973
	5MMG	ROC score	0.689	0.5	0.691	0.712	0.732	0.721	0.746	0.788
		Sensitivity	0	0	0	0.279	0.162	0	0	0.003
		Specificity	1.000	1.000	1.000	0.916	0.976	1.000	1.000	1.000
		Precision	N/A	N/A	N/A	0.086	0.157	N/A	N/A	1.000
		Concordance	0.973	0.973	0.973	0.899	0.953	0.973	0.973	0.973
HIV IN	4CFD	ROC score	0.822	0.827	0.801	0.74	0.805	0.742	0.784	0.832
		Sensitivity	0.598	0.613	0.632	0.667	0.713	0.261	0.567	0.713
		Specificity	0.863	0.869	0.806	0.678	0.779	0.934	0.822	0.822
		Precision	0.757	0.769	0.699	0.596	0.697	0.739	0.695	0.741
		Concordance	0.753	0.762	0.734	0.673	0.751	0.654	0.716	0.777
	4CHO	ROC score	0.792	0.807	0.791	0.73	0.816	0.714	0.753	0.824
		Sensitivity	0.544	0.579	0.544	0.663	0.655	0.261	0.506	0.67
		Specificity	0.828	0.861	0.831	0.683	0.811	0.915	0.809	0.817
		Precision	0.693	0.748	0.696	0.599	0.713	0.687	0.653	0.723
		Concordance	0.71	0.743	0.711	0.675	0.746	0.643	0.683	0.756
XIAP	1TFT	ROC score	0.97	0.972	0.996	0.979	0.99	0.981	0.994	0.997
		Sensitivity	0.644	0.674	0.626	0.962	0.782	0.162	0.762	0.838
		Specificity	0.997	0.995	0.999	0.866	0.997	1.000	0.998	0.999
		Precision	0.836	0.774	0.926	0.142	0.864	0.948	0.912	0.928
		Concordance	0.989	0.988	0.99	0.869	0.992	0.981	0.993	0.995
	5C3H	ROC score	0.973	0.976	0.994	0.974	0.994	0.985	0.995	0.995
		Sensitivity	0.709	0.718	0.571	0.862	0.788	0.141	0.776	0.862
		Specificity	0.995	0.994	0.999	0.952	0.996	1.000	0.997	0.997
		Precision	0.777	0.744	0.907	0.292	0.838	0.96	0.86	0.888
		Concordance	0.989	0.988	0.989	0.95	0.992	0.981	0.992	0.994
Mcl-1	5FC4	ROC score	0.742	0.586	0.854	0.783	0.776	0.813	0.843	0.859
		Sensitivity	0.141	0.131	0.127	0.458	0.23	0.005	0.005	0.167
		Specificity	0.997	0.998	1.000	0.907	0.997	1.000	1.000	0.999
		Precision	0.6	0.609	0.947	0.125	0.671	0.5	0.667	0.78
		Concordance	0.973	0.973	0.975	0.894	0.975	0.972	0.972	0.975
	5MES	ROC score	0.755	0.573	0.845	0.786	0.715	0.809	0.835	0.846
		Sensitivity	0.138	0.134	0.073	0.359	0.258	0	0	0.148
		Specificity	0.997	0.997	1.000	0.957	0.994	1.000	1.000	0.999
		Precision	0.578	0.576	0.939	0.196	0.547	N/A	0	0.797

		Concordance	0.973	0.973	0.974	0.94	0.973	0.972	0.972	0.975
Mdm2	4ODF	ROC score	0.947	0.947	0.958	0.922	0.957	0.946	0.95	0.963
		Sensitivity	0.84	0.849	0.801	0.867	0.891	0.765	0.861	0.879
		Specificity	0.968	0.951	0.975	0.853	0.952	0.97	0.943	0.961
		Precision	0.93	0.899	0.944	0.751	0.904	0.929	0.886	0.92
		Concordance	0.924	0.916	0.916	0.857	0.931	0.901	0.915	0.933
	4ZFI	ROC score	0.941	0.94	0.949	0.919	0.954	0.943	0.951	0.961
		Sensitivity	0.847	0.825	0.798	0.847	0.888	0.798	0.88	0.889
		Specificity	0.951	0.957	0.965	0.875	0.952	0.954	0.94	0.955
		Precision	0.898	0.908	0.922	0.776	0.904	0.899	0.883	0.91
		Concordance	0.916	0.912	0.909	0.866	0.93	0.901	0.92	0.933
Menin	5DB2	ROC score	0.5	0.5	0.674	0.622	0.614	0.62	0.646	0.646
		Sensitivity	0	0	0	0.033	0.071	0	0	0
		Specificity	1.000	1.000	1.000	0.994	0.982	1.000	1.000	1.000
		Precision	N/A	N/A	N/A	0.117	0.083	N/A	N/A	N/A
		Concordance	0.978	0.978	0.978	0.973	0.962	0.978	0.978	0.978
	6B41	ROC score	0.536	0.5	0.669	0.601	0.608	0.633	0.656	0.637
		Sensitivity	0	0	0	0.009	0.076	0	0	0
		Specificity	1.000	1.000	1.000	0.994	0.983	1.000	1.000	1.000
		Precision	N/A	N/A	N/A	0.037	0.09	N/A	N/A	N/A
		Concordance	0.978	0.978	0.978	0.973	0.963	0.978	0.978	0.978

Table S9. Confusion matrices generated when the machine learning models were applied to the test sets of the different PPI targets.

Target	PDB ID	ML techniques	TN	FP	FN	TP	Total
BAZ2B	4XUA	Tree	14827	0	2055	0	16882
		Bagged forest	14827	0	2055	0	16882
		Random forest	14827	0	2055	0	16882
		Bayesian	14789	38	2050	5	16882
		SVM	14448	379	1958	97	16882
		Logistic regression	14825	2	2055	0	16882
		Neural net	14827	0	2055	0	16882
		Neural net (bagging)	14827	0	2055	0	16882
	5E73	Tree	14827	0	2055	0	16882
		Bagged forest	14827	0	2055	0	16882
		Random forest	14827	0	2055	0	16882
		Bayesian	14748	79	2042	13	16882
		SVM	14376	451	1938	117	16882
		Logistic regression	14827	0	2055	0	16882
		Neural net	14827	0	2055	0	16882
		Neural net (bagging)	14827	0	2055	0	16882
Bcl-2	2021	Tree	14702	16	70	461	15249

		Bagged forest	14687	31	57	474	15249
		Random forest	14704	14	67	564	15349
		Bayesian	14493	225	50	481	15249
		SVM	14696	22	55	476	15249
		Logistic regression	14710	8	180	351	15249
		Neural net	14701	17	79	452	15249
		Neural net (bagging)	14709	9	55	476	15249
	4LVT	Tree	14703	15	74	457	15249
		Bagged forest	14693	25	64	467	15249
		Random forest	14703	15	65	466	15249
		Bayesian	14518	200	56	475	15249
		SVM	14693	25	54	477	15249
		Logistic regression	14712	6	206	325	15249
		Neural net	14696	22	68	463	15249
		Neural net (bagging)	14699	19	54	477	15249
Bcl-xL	3INQ	Tree	14725	26	66	223	15040
		Bagged forest	14712	39	60	229	15040
		Random forest	14737	14	68	221	15040
		Bayesian	14485	266	32	257	15040
		SVM	14730	21	39	250	15040
		Logistic regression	14745	6	217	72	15040
		Neural net	14735	16	60	229	15040
		Neural net (bagging)	14737	14	51	238	15040
	3WIZ	Tree	14747	4	63	226	15040
		Bagged forest	14727	24	58	231	15040
		Random forest	14744	7	53	236	15040
		Bayesian	13295	1456	20	269	15040
		SVM	14621	130	36	253	15040
		Logistic regression	14745	6	247	42	15040
		Neural net	14741	10	53	236	15040
		Neural net (bagging)	14743	8	41	248	15040
BRD4-1	5D3L	Tree	259	35	44	209	547
		Bagged forest	262	32	43	210	547
		Random forest	253	41	46	207	547
		Bayesian	242	52	42	211	547
		SVM	251	43	39	214	547
		Logistic regression	257	37	56	197	547
		Neural net	251	43	40	213	547
		Neural net (bagging)	253	41	39	214	547
	5KU3	Tree	231	63	33	220	547
		Bagged forest	234	60	36	217	547
		Random forest	218	76	30	223	547
		Bayesian	221	73	28	225	547

		SVM	237	57	34	219	547
		Logistic regression	249	45	52	201	547
		Neural net	232	62	34	219	547
		Neural net (bagging)	251	43	34	219	547
CREBBP	5EIC	Tree	13896	0	390	0	14286
		Bagged forest	13896	0	390	0	14286
		Random forest	13896	0	390	0	14286
		Bayesian	13311	585	310	80	14286
		SVM	13621	275	320	70	14286
		Logistic regression	13896	0	390	0	14286
		Neural net	13896	0	390	0	14286
		Neural net (bagging)	13896	0	389	1	14286
	5MMG	Tree	13897	0	390	0	14287
		Bagged forest	13897	0	390	0	14287
		Random forest	13896	0	390	0	14286
		Bayesian	12736	1161	281	109	14287
		SVM	13559	338	327	63	14287
		Logistic regression	13897	0	390	0	14287
		Neural net	13897	0	390	0	14287
		Neural net (bagging)	13897	0	389	1	14287
HIV IN	4CFD	Tree	316	50	105	156	627
		Bagged forest	318	48	101	160	627
		Random forest	295	71	96	165	627
		Bayesian	248	118	87	174	627
		SVM	285	81	75	186	627
		Logistic regression	342	24	193	68	627
		Neural net	301	65	113	148	627
		Neural net (bagging)	301	65	75	186	627
	4CHO	Tree	303	63	119	142	627
		Bagged forest	315	51	110	151	627
		Random forest	304	62	119	142	627
		Bayesian	250	116	88	173	627
		SVM	297	69	90	171	627
		Logistic regression	335	31	193	68	627
		Neural net	296	70	129	132	627
		Neural net (bagging)	299	67	86	175	627
XIAP	1TFT	Tree	14755	43	121	219	15138
		Bagged forest	14731	67	111	229	15138
		Random forest	14781	17	127	213	15138
		Bayesian	12821	1977	13	327	15138
		SVM	14756	42	74	266	15138
		Logistic regression	14795	3	285	55	15138
		Neural net	14773	25	81	259	15138

		Neural net (bagging)	14776	22	55	285	15138
		Tree	14729	69	99	241	15138
		Bagged forest	14714	84	96	244	15138
		Random forest	14778	20	146	194	15138
		Bayesian	14088	710	47	293	15138
		SVM	14746	52	72	268	15138
		Logistic regression	14796	2	292	48	15138
		Neural net	14755	43	76	264	15138
		Neural net (bagging)	14761	37	47	293	15138
Mcl-1	5FC4	Tree	14595	40	366	60	15061
		Bagged forest	14599	36	370	56	15061
		Random forest	14632	3	372	54	15061
		Bayesian	13273	1362	231	195	15061
		SVM	14587	48	328	98	15061
		Logistic regression	14633	2	424	2	15061
		Neural net	14634	1	424	2	15061
		Neural net (bagging)	14615	20	355	71	15061
	5MES	Tree	14592	43	367	59	15061
		Bagged forest	14593	42	369	57	15061
		Random forest	14633	2	395	31	15061
		Bayesian	14009	626	273	153	15061
		SVM	14544	91	316	110	15061
		Logistic regression	14635	0	426	0	15061
		Neural net	14634	1	426	0	15061
		Neural net (bagging)	14619	16	363	63	15061
Mdm2	4ODF	Tree	1261	42	107	561	1971
		Bagged forest	1239	64	101	567	1971
		Random forest	1271	32	133	535	1971
		Bayesian	1111	192	89	579	1971
		SVM	1240	63	73	595	1971
		Logistic regression	1264	39	157	511	1971
		Neural net	1229	74	93	575	1971
		Neural net (bagging)	1252	51	81	587	1971
	4ZFI	Tree	1239	64	102	566	1971
		Bagged forest	1247	56	117	551	1971
		Random forest	1258	45	135	533	1971
		Bayesian	1140	163	102	566	1971
		SVM	1240	63	75	593	1971
		Logistic regression	1243	60	135	533	1971
		Neural net	1225	78	80	588	1971
		Neural net (bagging)	1244	59	74	594	1971
Menin	5DB2	Tree	9437	0	211	0	9648

		Bagged forest	9437	0	211	0	9648
		Random forest	9437	0	211	0	9648
		Bayesian	9384	53	204	7	9648
		SVM	9271	166	196	15	9648
		Logistic regression	9437	0	211	0	9648
		Neural net	9437	0	211	0	9648
		Neural net (bagging)	9437	0	211	0	9648
	6B41	Tree	9437	0	211	0	9648
		Bagged forest	9437	0	211	0	9648
		Random forest	9437	0	211	0	9648
		Bayesian	9385	52	209	2	9648
		SVM	9276	161	195	16	9648
		Logistic regression	9437	0	211	0	9648
		Neural net	9437	0	211	0	9648
		Neural net (bagging)	9437	0	211	0	9648

Table S10. External enrichment factors (EF1% and EF5%) for the machine learning models for the different PPI targets. The best enrichment score(s) corresponding to each target protein (across rows) is shown in bold and highlighted in green.

Target	PDB ID	Enrichment factors	Tree	Bagged forest	Random forest	Bayesian	SVM	Logistic regression	Neural net	Neural net (bagging)
BAZ2B	4XUA	EF 1%	1.706	1.000	1.565	1.222	1.907	1.271	1.467	2.005
		EF 5%	1.526	1.000	1.431	1.265	1.518	1.236	1.256	1.479
	5E73	EF 1%	1.530	1.000	1.956	1.320	2.200	0.880	1.467	1.858
		EF 5%	1.397	1.000	1.450	1.139	1.489	1.119	1.363	1.489
Bcl-2	2021	EF 1%	28.459	27.752	28.718	28.602	28.718	27.584	28.718	28.718
		EF 5%	18.399	18.048	19.107	18.241	18.730	18.278	18.806	18.844
	4LVT	EF 1%	28.583	27.736	28.718	28.718	28.718	28.151	28.718	28.718
		EF 5%	17.970	17.974	18.806	18.090	18.730	18.165	18.693	18.957
Bcl-xL	3INQ	EF 1%	49.757	45.272	51.695	49.960	51.348	48.225	51.695	52.042
		EF 5%	18.033	16.581	18.893	18.408	18.893	18.547	18.824	18.824
	3WIZ	EF 1%	51.794	47.425	52.042	49.960	50.654	48.572	52.042	52.042
		EF 5%	18.738	16.784	19.239	17.509	18.478	18.270	19.170	19.308
BRD4-1	5D3L	EF 1%	2.162	2.162	2.162	1.730	2.162	2.162	2.162	2.162
		EF 5%	2.137	2.115	2.082	2.082	2.162	2.002	2.162	2.162
	5KU3	EF 1%	2.162	2.162	2.162	2.162	2.162	2.162	2.162	2.162
		EF 5%	2.082	2.162	2.162	2.002	2.082	2.082	2.162	2.162
CREBBP	5EIC	EF 1%	2.992	1.000	12.124	8.771	9.803	4.901	6.965	12.382
		EF 5%	2.454	1.000	5.695	4.258	4.874	4.053	4.412	5.900
	5MMG	EF 1%	4.161	1.000	1.548	4.128	8.513	5.160	5.676	9.029

		EF 5%	2.659	1.000	2.155	2.976	4.720	4.002	3.540	6.054
HIV IN	4CFD	EF 1%	2.402	2.402	2.402	2.402	2.402	2.402	2.402	2.402
		EF 5%	2.325	2.247	2.247	2.092	2.092	2.247	2.247	2.325
	4CHO	EF 1%	2.002	2.402	2.402	1.602	1.602	2.002	2.402	2.402
		EF 5%	2.170	2.092	2.247	2.015	2.015	1.627	2.015	2.247
XIAP	1TFT	EF 1%	38.037	38.184	43.934	34.498	42.165	37.152	42.165	43.344
		EF 5%	17.374	17.079	19.435	17.727	18.846	17.845	19.082	19.553
	5C3H	EF 1%	40.690	38.332	43.049	33.909	42.754	36.857	43.344	43.934
		EF 5%	17.939	17.842	19.082	15.901	19.140	18.080	19.317	19.435
Mcl-1	5FC4	EF 1%	19.798	17.694	23.570	18.856	23.805	17.913	17.206	23.098
		EF 5%	7.175	4.191	9.954	7.043	9.156	8.451	9.296	10.329
	5MES	EF 1%	18.856	15.130	22.627	16.734	22.155	18.149	21.920	23.570
		EF 5%	9.045	3.701	9.531	7.137	8.639	8.123	9.296	9.437
Mdm2	4ODF	EF 1%	2.951	2.951	2.951	2.795	2.951	2.795	2.951	2.951
		EF 5%	2.951	2.951	2.951	2.860	2.920	2.920	2.920	2.951
	4ZFI	EF 1%	2.816	2.795	2.951	2.640	2.951	2.951	2.951	2.795
		EF 5%	2.899	2.885	2.920	2.800	2.890	2.890	2.890	2.890
Menin	5DB2	EF 1%	1.000	1.000	6.192	3.810	6.668	5.716	3.810	5.716
		EF 5%	1.000	1.000	3.036	2.751	2.277	2.941	2.846	3.131
	6B41	EF 1%	3.045	1.000	3.334	1.905	6.668	1.905	2.382	3.334
		EF 5%	2.403	1.000	2.751	2.751	3.036	1.138	2.467	2.561