

PPI-Graphomer: Enhanced Protein-Protein Affinity Prediction Using Pretrained and Graph Transformer Models

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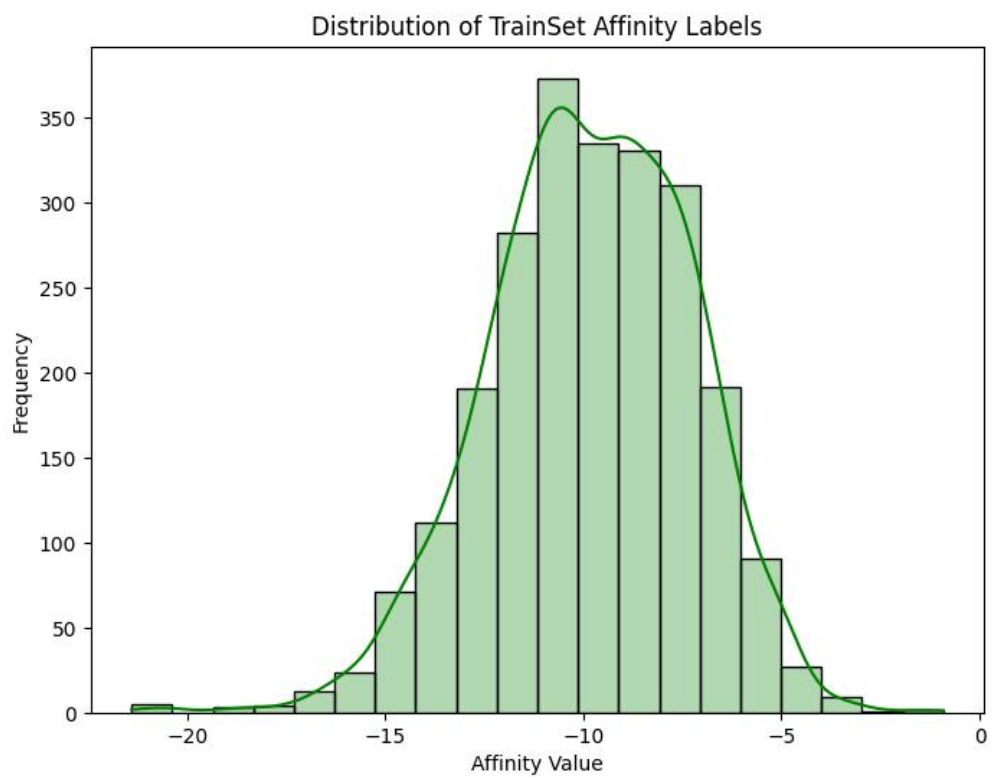


Figure S1: Histogram of affinity labels for the training set, containing 2376 samples.

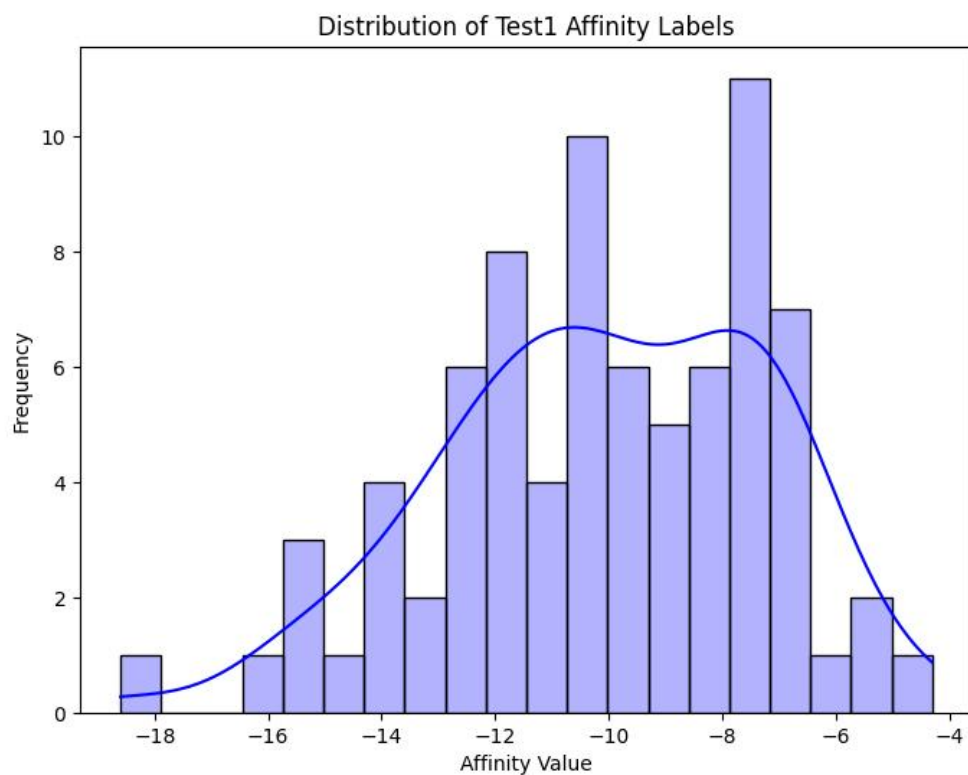


Figure S2: Histogram of affinity labels for the Test1 set, containing 75 samples.

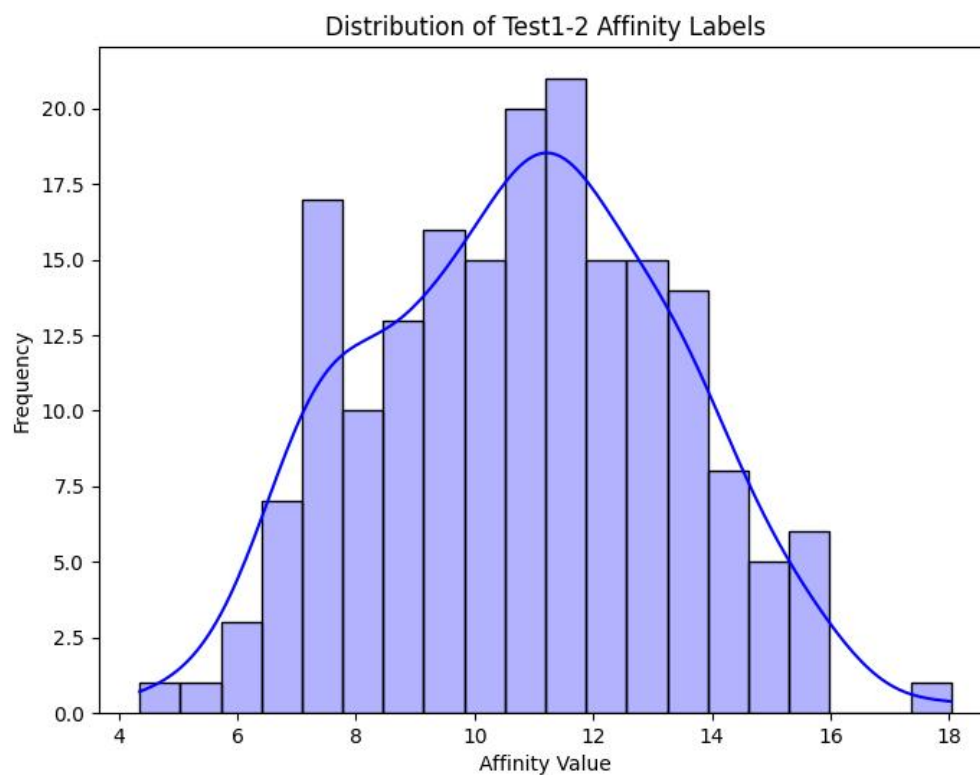


Figure S3: Histogram of affinity labels for the new version of Test1 set, containing 188 samples.

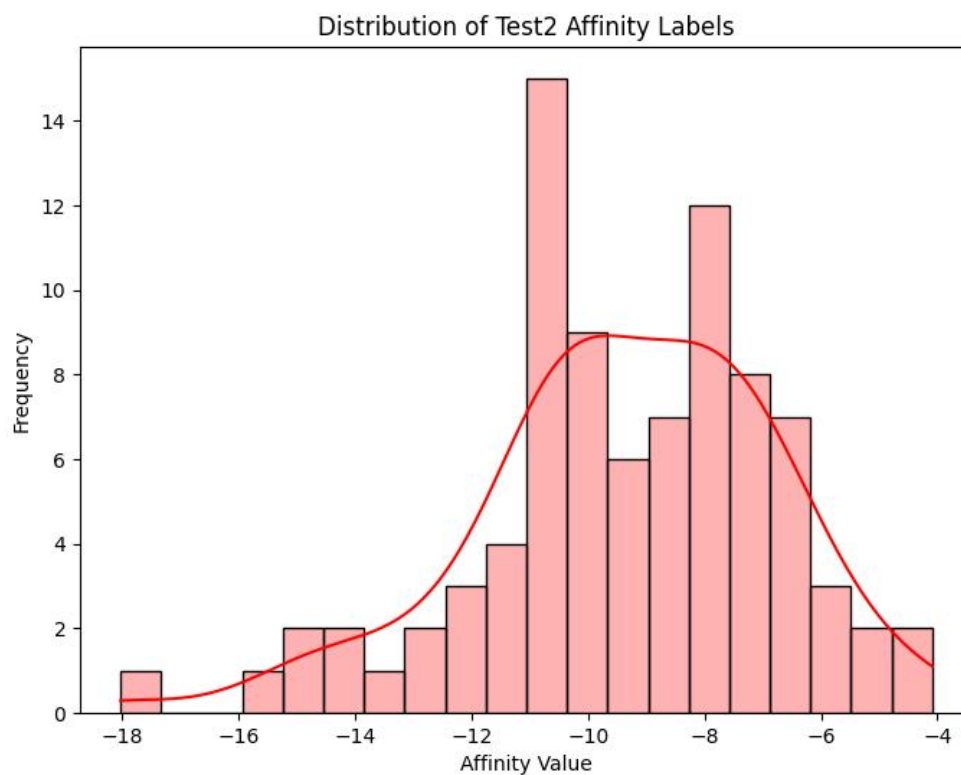


Figure S4: Histogram of affinity labels for the Test2 set, containing 87 samples.

Method	PCC	Method	PCC
CP_BFKV	0.063286	HBOND	-0.04173
CP_BL	0.073562	PI_PI	0.113018
CP_BT	0.119709	CAT_PI	-0.01737
CP_GKS	0.037547	ALIPH	0.121423
CP_HLPL	0.059554	ZRANK	-0.00511
CP_MJPL	0.049929	ZRANK2	0.061387
CP_MJ3h	0.06892	ROT_S	-0.00951
CP_MJ2h	0.076734	TRANS_S	0.017461
CP_MJ1	-0.0439	NSC	-0.04627
CP_MJ2	0.058987	FA_ATR	0.019951
CP_MSBM	0.00232	FA_REP	0.000468
CP_MS	0.047812	LK_SOLV	0.023188
CP_Qa	0.015578	FA_PP	-0.01612
CP_Qm	0.020554	CG_VDW	0.058549
CP_Qp	0.025967	CG_PP	0.029717
CP_RO	0.059292	CG_ENV	-0.0193
CP_SKOb	0.02172	CG_BETA	0.064074
CP_SKOa	0.037035	HBOND2	-0.08019
CP_SJKG	0.072764	AA_PROP	-0.05882
CP_TD	0.01818	ROSETTADOCK	0.039548
CP_TEI	0.011799	NHB	0.076593
CP_TEs	0.003305	ELE	-0.07091
CP_TS	0.054586	DESOLV	0.035199
CP_VD	0.086457	VDW	0.01481
CP_SKOIP	0.064051	PYDOCK_TOT	-0.03704
AP_DCOMPLEX	0.004998	ODA	-0.02298
AP_dDFIRE	0.06425	PROPNTS	-0.15291
AP_DFIRE2	0.067084	SIPPER	-0.06458
CP_RMFCEN1	-0.00049	AP_OPUS_PSP	-0.04461
CP_RMFCEN2	-0.03029	AP_GEOMETRIC	0.06375
CP_RMFCA	0.01474	AP_DARS	0.133078
CP_TB	-0.03513	AP_URS	0.046131
CP_TSC	0.044209	AP_MPS	0.095673
AP_T1	-0.00133	AP_W1	-0.05068
AP_T2	-0.00048	CP_D1	0.034902
AP_DOPE	-0.08167	CP_ZPAIR_CB	-0.00652
AP_DOPE_HR	-0.07411	CP_ZLOCAL_CB	0.014575
AP_ACE	0.018659	CP_ZS3DC_CB	0.055498
INSIDE	0.007175	CP_Z3DC_CB	-0.05494

Method	PCC	Method	PCC
CP_EPAIR_CB	-0.08236	AP_calRWp	0.004547
CP_ELOCAL_CB	-0.0351	AP_GOAP_ALL	0.13229
CP_ES3DC_CB	0.045293	AP_GOAP_DF	0.027171
CP_E3DC_CB	0.00254	AP_GOAP_G	0.103645
CP_E3D_CB	-0.05445	AP_PISA	-0.06087
CP_ZPAIR_MIN	-0.01082	FIREDOCK	0.042978
CP_ZLOCAL_MIN	0.01786	FIREDOCK_AB	0.050236
CP_ZS3DC_MIN	0.046575	FIREDOCK_EI	0.025852
CP_Z3DC_MIN	0.013367	CP_PIE	-0.06239
CP_EPAIR_MIN	-0.11213	CP_DDG_U	-0.00302
CP_ELOCAL_MIN	0.040369	CP_DDG_W	-0.01877
CP_ES3DC_MIN	0.094192	AP_DDG_U	0.002409
CP_E3DC_MIN	-0.07766	AP_DDG_W	-0.01249
CP_E3D_MIN	0.007783	DDG_V	0.048516
AP_calRW	0.006482	PPI-Graphomer	0.686479

Table S1: The Pearson correlation coefficient between the scores of different methods and the affinity labels. The scores come from the website [Computational Characterisation of Protein-Protein Interactions](#).

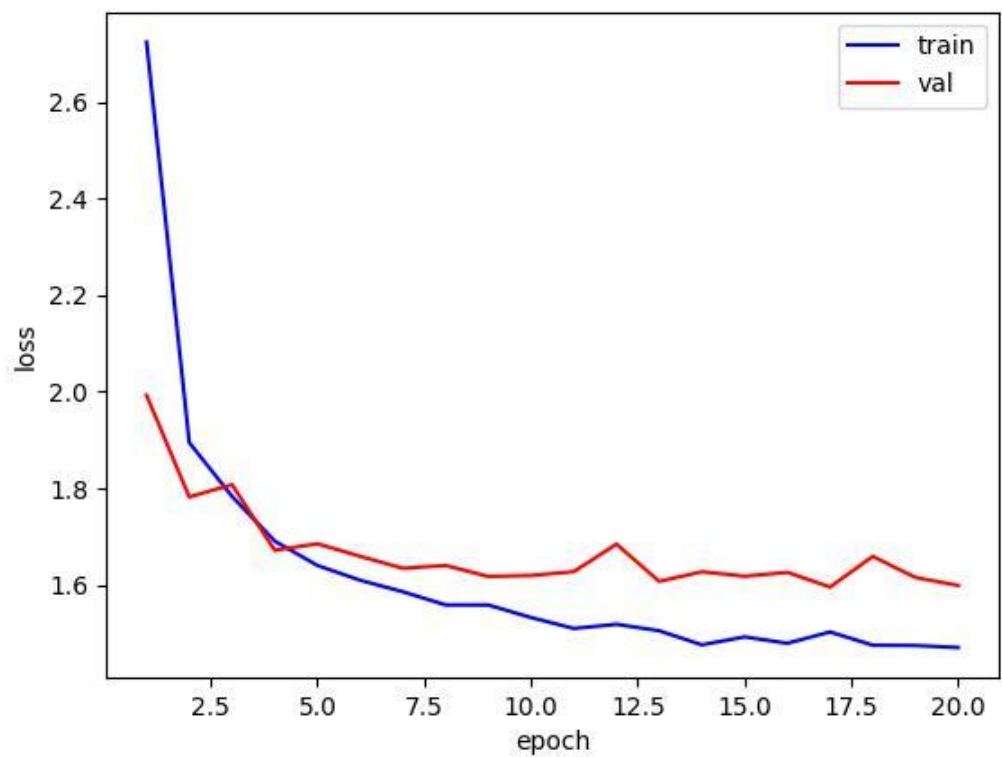


Figure S5: Training history (loss) of the training.