

Table S2a. Best performance of each model on PDBbind v.2016 core set

Test data	RMSE	MAE	SD	R
dataset1	1.43	1.14	1.40	0.77
dataset2	1.45	1.17	1.43	0.75
dataset3	1.40	1.10	1.35	0.78
dataset4	1.37	1.09	1.36	0.78

Each models's best performance among 10 evaluatoins on PDBbind v.2016 core set.

Table S2b. Best performance of each model on PDBbind v.2013 core set

Test data	RMSE	MAE	SD	R
dataset1	1.61	1.27	1.61	0.70
dataset2	1.63	1.33	1.61	0.70
dataset3	1.47	1.19	1.45	0.77
dataset4	1.48	1.22	1.47	0.76

Each models's best performance among 10 evaluatoins on PDBbind v.2013 core set.