

Supporting Information

DeepAtom: A Framework for Protein-Ligand Binding Affinity Prediction

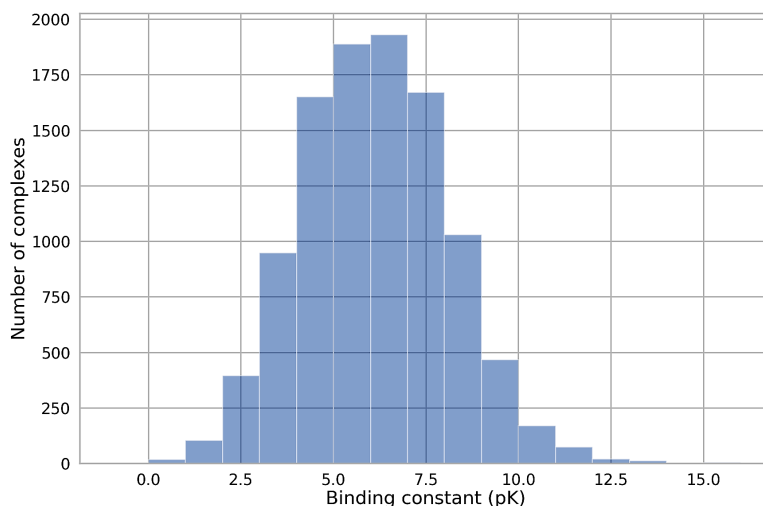


Figure S1. Binding score distribution of the full proposed benchmark data set (10,383 complexes), including the “training set-2” (9,383 complexes) and validation (1,000 complexes).

Table S1. Validation (377 complexes) results with the “training set-1”.

	RMSE	MAE	SD	R
DeepAtom	1.348 (0.003)	0.996 (0.015)	1.340 (0.028)	0.740 (0.013)
RF-Score	1.403 (0.003)	1.064 (0.002)	1.405 (0.003)	0.709 (0.001)
Pafnucy	1.542 (0.008)	1.192 (0.006)	1.534 (0.009)	0.638 (0.006)

Table S2. Validation (1000 complexes) results with the “training set-2”.

	RMSE	MAE	SD	R
DeepAtom	1.230 (0.012)	0.891 (0.013)	1.223 (0.011)	0.801 (0.004)
RF-Score	1.326 (0.003)	1.041 (0.002)	1.320 (0.003)	0.767 (0.001)
Pafnucy	1.451 (0.021)	1.153 (0.019)	1.452 (0.022)	0.710 (0.008)