

Table 1: Comparison of RMSE on the Leak-Proof PDBBind benchmark for binding affinity prediction.

Model	Train	Validation	Test
AutoDock Vina [?]	2.42	2.29	2.56
InteractionGraphNet (IGN) [?]	1.65	2.00	2.16
Random Forest (RF)-Score [?]	0.68	2.14	2.10
DeepDTA [?]	1.41	2.07	2.29
MPRL [?]	0.48	1.47	1.55
ArkDTA [?]	1.18	1.47	1.48
LINKER (Our)	1.38	1.53	1.47