

bace all-pairs $\Delta\Delta G$ (N = 1260)				cdk2 all-pairs $\Delta\Delta G$ (N = 240)				jnk1 all-pairs $\Delta\Delta G$ (N = 420)				mcl1 all-pairs $\Delta\Delta G$ (N = 1722)				p38a all-pairs $\Delta\Delta G$ (N = 1122)				ptp1b all-pairs $\Delta\Delta G$ (N = 506)				thrombin all-pairs $\Delta\Delta G$ (N = 110)				tyk2 all-pairs $\Delta\Delta G$ (N = 240)				all within-target pairs $\Delta\Delta G$ (N = 5620)			
RMSE: FEP+	1.22	[95%: 1.17, 1.26]	kcal/mol	RMSE: FEP+	1.52	[95%: 1.41, 1.64]	kcal/mol	RMSE: FEP+	1.65	[95%: 1.57, 1.74]	kcal/mol	RMSE: FEP+	1.49	[95%: 1.45, 1.54]	kcal/mol	RMSE: FEP+	1.39	[95%: 1.34, 1.44]	kcal/mol	RMSE: FEP+	1.16	[95%: 1.08, 1.22]	kcal/mol	RMSE: FEP+	0.80	[95%: 0.70, 0.91]	kcal/mol	RMSE: FEP+	0.83	[95%: 0.76, 0.91]	kcal/mol	RMSE: FEP+	1.37	[95%: 1.34, 1.39]	kcal/mol
RMSE: AMBER TI	1.90	[95%: 1.81, 1.98]	kcal/mol	RMSE: AMBER TI	1.58	[95%: 1.46, 1.68]	kcal/mol	RMSE: AMBER TI	1.63	[95%: 1.53, 1.73]	kcal/mol	RMSE: AMBER TI	2.11	[95%: 2.05, 2.18]	kcal/mol	RMSE: AMBER TI	2.33	[95%: 2.22, 2.42]	kcal/mol	RMSE: AMBER TI	1.46	[95%: 1.37, 1.55]	kcal/mol	RMSE: AMBER TI	0.75	[95%: 0.64, 0.85]	kcal/mol	RMSE: AMBER TI	1.65	[95%: 1.52, 1.79]	kcal/mol	RMSE: AMBER TI	1.97	[95%: 1.93, 2.01]	kcal/mol
MUE : FEP+	0.98	[95%: 0.94, 1.01]	kcal/mol	MUE : FEP+	1.25	[95%: 1.13, 1.37]	kcal/mol	MUE : FEP+	1.36	[95%: 1.27, 1.45]	kcal/mol	MUE : FEP+	1.20	[95%: 1.16, 1.24]	kcal/mol	MUE : FEP+	1.12	[95%: 1.08, 1.17]	kcal/mol	MUE : FEP+	0.91	[95%: 0.85, 0.97]	kcal/mol	MUE : FEP+	0.64	[95%: 0.56, 0.73]	kcal/mol	MUE : FEP+	0.65	[95%: 0.58, 0.71]	kcal/mol	MUE : FEP+	1.09	[95%: 1.07, 1.11]	kcal/mol
MUE : AMBER TI	1.48	[95%: 1.42, 1.55]	kcal/mol	MUE : AMBER TI	1.32	[95%: 1.20, 1.43]	kcal/mol	MUE : AMBER TI	1.33	[95%: 1.24, 1.42]	kcal/mol	MUE : AMBER TI	1.68	[95%: 1.62, 1.74]	kcal/mol	MUE : AMBER TI	1.86	[95%: 1.77, 1.94]	kcal/mol	MUE : AMBER TI	1.14	[95%: 1.07, 1.22]	kcal/mol	MUE : AMBER TI	0.57	[95%: 0.48, 0.66]	kcal/mol	MUE : AMBER TI	1.35	[95%: 1.24, 1.47]	kcal/mol	MUE : AMBER TI	1.55	[95%: 1.51, 1.58]	kcal/mol
R2 : FEP+	-0.23	[95%: -0.36, -0.11]	kcal/mol	R2 : FEP+	0.22	[95%: 0.10, 0.32]	kcal/mol	R2 : FEP+	-0.84	[95%: -1.13, -0.59]	kcal/mol	R2 : FEP+	0.02	[95%: -0.08, 0.10]	kcal/mol	R2 : FEP+	0.05	[95%: -0.05, 0.14]	kcal/mol	R2 : FEP+	0.62	[95%: 0.56, 0.67]	kcal/mol	R2 : FEP+	-0.08	[95%: -0.57, 0.24]	kcal/mol	R2 : FEP+	0.79	[95%: 0.74, 0.83]	kcal/mol	R2 : FEP+	0.10	[95%: 0.05, 0.15]	kcal/mol
R2 : AMBER TI	-1.98	[95%: -2.36, -1.63]	kcal/mol	R2 : AMBER TI	0.16	[95%: 0.03, 0.27]	kcal/mol	R2 : AMBER TI	-0.80	[95%: -1.14, -0.50]	kcal/mol	R2 : AMBER TI	-0.97	[95%: -1.14, -0.82]	kcal/mol	R2 : AMBER TI	-1.66	[95%: -1.99, -1.37]	kcal/mol	R2 : AMBER TI	0.39	[95%: 0.29, 0.47]	kcal/mol	R2 : AMBER TI	0.04	[95%: -0.33, 0.32]	kcal/mol	R2 : AMBER TI	0.19	[95%: -0.00, 0.34]	kcal/mol	R2 : AMBER TI	-0.87	[95%: -0.97, -0.77]	kcal/mol
rho : FEP+	0.78	[95%: 0.76, 0.80]	kcal/mol	rho : FEP+	0.48	[95%: 0.38, 0.56]	kcal/mol	rho : FEP+	0.84	[95%: 0.75, 0.87]	kcal/mol	rho : FEP+	0.77	[95%: 0.74, 0.79]	kcal/mol	rho : FEP+	0.65	[95%: 0.62, 0.68]	kcal/mol	rho : FEP+	0.80	[95%: 0.77, 0.83]	kcal/mol	rho : FEP+	0.71	[95%: 0.62, 0.79]	kcal/mol	rho : FEP+	0.89	[95%: 0.86, 0.91]	kcal/mol	rho : FEP+	0.73	[95%: 0.72, 0.74]	kcal/mol
rho : AMBER TI	0.43	[95%: 0.39, 0.48]	kcal/mol	rho : AMBER TI	0.47	[95%: 0.39, 0.54]	kcal/mol	rho : AMBER TI	0.47	[95%: 0.40, 0.54]	kcal/mol	rho : AMBER TI	0.65	[95%: 0.62, 0.68]	kcal/mol	rho : AMBER TI	0.38	[95%: 0.34, 0.43]	kcal/mol	rho : AMBER TI	0.71	[95%: 0.67, 0.75]	kcal/mol	rho : AMBER TI	0.76	[95%: 0.68, 0.81]	kcal/mol	rho : AMBER TI	0.57	[95%: 0.49, 0.65]	kcal/mol	rho : AMBER TI	0.53	[95%: 0.51, 0.55]	kcal/mol

