

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: OPLS3	1.22	[95%: 1.17, 1.26]	kcal/mol	RMSE: OPLS3	1.52	[95%: 1.41, 1.63]	kcal/mol	RMSE: OPLS3	1.65	[95%: 1.57, 1.73]	kcal/mol	RMSE: OPLS3	1.49	[95%: 1.44, 1.54]	kcal/mol	RMSE: OPLS3	1.39	[95%: 1.34, 1.44]	kcal/mol	RMSE: OPLS3	1.16	[95%: 1.08, 1.24]	kcal/mol	RMSE: OPLS3	0.80	[95%: 0.70, 0.90]	kcal/mol	RMSE: OPLS3	0.83	[95%: 0.76, 0.91]	kcal/mol	RMSE: OPLS3	1.37	[95%: 1.34, 1.39]	kcal/mol
RMSE: GAFF	1.90	[95%: 1.81, 1.98]	kcal/mol	RMSE: GAFF	1.58	[95%: 1.46, 1.69]	kcal/mol	RMSE: GAFF	1.63	[95%: 1.53, 1.73]	kcal/mol	RMSE: GAFF	2.11	[95%: 2.05, 2.18]	kcal/mol	RMSE: GAFF	2.33	[95%: 2.23, 2.42]	kcal/mol	RMSE: GAFF	1.46	[95%: 1.36, 1.55]	kcal/mol	RMSE: GAFF	0.75	[95%: 0.64, 0.86]	kcal/mol	RMSE: GAFF	1.65	[95%: 1.52, 1.78]	kcal/mol	RMSE: GAFF	1.97	[95%: 1.93, 2.01]	kcal/mol
MUE : OPLS3	0.98	[95%: 0.94, 1.01]	kcal/mol	MUE : OPLS3	1.25	[95%: 1.15, 1.37]	kcal/mol	MUE : OPLS3	1.36	[95%: 1.26, 1.45]	kcal/mol	MUE : OPLS3	1.20	[95%: 1.16, 1.24]	kcal/mol	MUE : OPLS3	1.12	[95%: 1.08, 1.17]	kcal/mol	MUE : OPLS3	0.91	[95%: 0.85, 0.98]	kcal/mol	MUE : OPLS3	0.64	[95%: 0.56, 0.73]	kcal/mol	MUE : OPLS3	0.65	[95%: 0.58, 0.72]	kcal/mol	MUE : OPLS3	1.09	[95%: 1.07, 1.11]	kcal/mol
MUE : GAFF	1.48	[95%: 1.42, 1.55]	kcal/mol	MUE : GAFF	1.32	[95%: 1.21, 1.43]	kcal/mol	MUE : GAFF	1.33	[95%: 1.25, 1.42]	kcal/mol	MUE : GAFF	1.68	[95%: 1.62, 1.74]	kcal/mol	MUE : GAFF	1.86	[95%: 1.78, 1.94]	kcal/mol	MUE : GAFF	1.14	[95%: 1.07, 1.22]	kcal/mol	MUE : GAFF	0.57	[95%: 0.48, 0.66]	kcal/mol	MUE : GAFF	1.35	[95%: 1.23, 1.47]	kcal/mol	MUE : GAFF	1.55	[95%: 1.51, 1.58]	kcal/mol
R2 : OPLS3	-0.23	[95%: -0.38, -0.09]	kcal/mol	R2 : OPLS3	0.22	[95%: 0.10, 0.31]	kcal/mol	R2 : OPLS3	-0.84	[95%: -1.15, -0.58]	kcal/mol	R2 : OPLS3	0.02	[95%: -0.08, 0.11]	kcal/mol	R2 : OPLS3	0.05	[95%: -0.06, 0.15]	kcal/mol	R2 : OPLS3	0.62	[95%: 0.54, 0.67]	kcal/mol	R2 : OPLS3	-0.08	[95%: -0.51, 0.24]	kcal/mol	R2 : OPLS3	0.79	[95%: 0.74, 0.83]	kcal/mol	R2 : OPLS3	0.10	[95%: 0.06, 0.15]	kcal/mol
R2 : GAFF	-1.98	[95%: -2.39, -1.63]	kcal/mol	R2 : GAFF	0.16	[95%: 0.03, 0.26]	kcal/mol	R2 : GAFF	-0.80	[95%: -1.14, -0.53]	kcal/mol	R2 : GAFF	-0.97	[95%: -1.16, -0.82]	kcal/mol	R2 : GAFF	-1.66	[95%: -1.99, -1.37]	kcal/mol	R2 : GAFF	0.39	[95%: 0.29, 0.48]	kcal/mol	R2 : GAFF	0.04	[95%: -0.36, 0.35]	kcal/mol	R2 : GAFF	0.19	[95%: 0.02, 0.34]	kcal/mol	R2 : GAFF	-0.87	[95%: -0.97, -0.77]	kcal/mol
rho : OPLS3	0.78	[95%: 0.76, 0.80]	kcal/mol	rho : OPLS3	0.48	[95%: 0.38, 0.56]	kcal/mol	rho : OPLS3	0.84	[95%: 0.75, 0.87]	kcal/mol	rho : OPLS3	0.77	[95%: 0.75, 0.79]	kcal/mol	rho : OPLS3	0.65	[95%: 0.62, 0.68]	kcal/mol	rho : OPLS3	0.80	[95%: 0.77, 0.83]	kcal/mol	rho : OPLS3	0.71	[95%: 0.62, 0.79]	kcal/mol	rho : OPLS3	0.89	[95%: 0.86, 0.91]	kcal/mol	rho : OPLS3	0.73	[95%: 0.72, 0.74]	kcal/mol
rho : GAFF	0.43	[95%: 0.38, 0.48]	kcal/mol	rho : GAFF	0.47	[95%: 0.39, 0.54]	kcal/mol	rho : GAFF	0.47	[95%: 0.40, 0.54]	kcal/mol	rho : GAFF	0.65	[95%: 0.62, 0.68]	kcal/mol	rho : GAFF	0.38	[95%: 0.34, 0.43]	kcal/mol	rho : GAFF	0.71	[95%: 0.67, 0.75]	kcal/mol	rho : GAFF	0.76	[95%: 0.68, 0.81]	kcal/mol	rho : GAFF	0.57	[95%: 0.49, 0.65]	kcal/mol	rho : GAFF	0.53	[95%: 0.51, 0.55]	kcal/mol

