

bace ΔG (N = 36)				cdk2 ΔG (N = 16)				jnk1 ΔG (N = 21)				mcl1 ΔG (N = 42)				p38a ΔG (N = 34)				ptp1b ΔG (N = 23)				thrombin ΔG (N = 11)				tyk2 ΔG (N = 16)			
RMSE: OPLS3	0.85	[95%: 0.67, 1.02]	kcal/mol	RMSE: OPLS3	1.04	[95%: 0.75, 1.30]	kcal/mol	RMSE: OPLS3	1.14	[95%: 0.96, 1.32]	kcal/mol	RMSE: OPLS3	1.04	[95%: 0.82, 1.26]	kcal/mol	RMSE: OPLS3	0.97	[95%: 0.80, 1.12]	kcal/mol	RMSE: OPLS3	0.80	[95%: 0.52, 1.09]	kcal/mol	RMSE: OPLS3	0.54	[95%: 0.31, 0.77]	kcal/mol	RMSE: OPLS3	0.57	[95%: 0.35, 0.77]	kcal/mol
RMSE: GAFF	1.32	[95%: 0.94, 1.73]	kcal/mol	RMSE: GAFF	1.08	[95%: 0.78, 1.33]	kcal/mol	RMSE: GAFF	1.13	[95%: 0.77, 1.45]	kcal/mol	RMSE: GAFF	1.48	[95%: 1.19, 1.76]	kcal/mol	RMSE: GAFF	1.62	[95%: 1.22, 2.01]	kcal/mol	RMSE: GAFF	1.01	[95%: 0.66, 1.32]	kcal/mol	RMSE: GAFF	0.51	[95%: 0.25, 0.74]	kcal/mol	RMSE: GAFF	1.13	[95%: 0.74, 1.48]	kcal/mol
MUE : OPLS3	0.66	[95%: 0.50, 0.85]	kcal/mol	MUE : OPLS3	0.88	[95%: 0.63, 1.13]	kcal/mol	MUE : OPLS3	1.05	[95%: 0.87, 1.25]	kcal/mol	MUE : OPLS3	0.84	[95%: 0.64, 1.04]	kcal/mol	MUE : OPLS3	0.86	[95%: 0.71, 1.01]	kcal/mol	MUE : OPLS3	0.60	[95%: 0.40, 0.84]	kcal/mol	MUE : OPLS3	0.42	[95%: 0.23, 0.64]	kcal/mol	MUE : OPLS3	0.44	[95%: 0.29, 0.63]	kcal/mol
MUE : GAFF	1.03	[95%: 0.78, 1.31]	kcal/mol	MUE : GAFF	0.90	[95%: 0.62, 1.20]	kcal/mol	MUE : GAFF	0.90	[95%: 0.64, 1.19]	kcal/mol	MUE : GAFF	1.24	[95%: 1.00, 1.51]	kcal/mol	MUE : GAFF	1.28	[95%: 0.96, 1.63]	kcal/mol	MUE : GAFF	0.76	[95%: 0.51, 1.05]	kcal/mol	MUE : GAFF	0.37	[95%: 0.18, 0.58]	kcal/mol	MUE : GAFF	0.89	[95%: 0.56, 1.22]	kcal/mol
R2 : OPLS3	-0.23	[95%: -1.58, 0.39]	kcal/mol	R2 : OPLS3	0.22	[95%: -0.61, 0.51]	kcal/mol	R2 : OPLS3	-0.84	[95%: -3.35, 0.03]	kcal/mol	R2 : OPLS3	0.02	[95%: -0.73, 0.46]	kcal/mol	R2 : OPLS3	0.05	[95%: -0.76, 0.41]	kcal/mol	R2 : OPLS3	0.62	[95%: 0.01, 0.80]	kcal/mol	R2 : OPLS3	-0.08	[95%: -3.25, 0.65]	kcal/mol	R2 : OPLS3	0.79	[95%: 0.48, 0.92]	kcal/mol
R2 : GAFF	-1.98	[95%: -5.95, -0.40]	kcal/mol	R2 : GAFF	0.16	[95%: -0.53, 0.42]	kcal/mol	R2 : GAFF	-0.80	[95%: -3.47, 0.11]	kcal/mol	R2 : GAFF	-0.97	[95%: -2.32, -0.21]	kcal/mol	R2 : GAFF	-1.66	[95%: -4.59, -0.32]	kcal/mol	R2 : GAFF	0.39	[95%: -0.39, 0.72]	kcal/mol	R2 : GAFF	0.04	[95%: -1.66, 0.78]	kcal/mol	R2 : GAFF	0.19	[95%: -1.04, 0.60]	kcal/mol
rho : OPLS3	0.78	[95%: 0.61, 0.89]	kcal/mol	rho : OPLS3	0.48	[95%: 0.11, 0.82]	kcal/mol	rho : OPLS3	0.84	[95%: 0.70, 0.95]	kcal/mol	rho : OPLS3	0.77	[95%: 0.67, 0.86]	kcal/mol	rho : OPLS3	0.65	[95%: 0.45, 0.79]	kcal/mol	rho : OPLS3	0.80	[95%: 0.64, 0.92]	kcal/mol	rho : OPLS3	0.71	[95%: 0.07, 0.94]	kcal/mol	rho : OPLS3	0.89	[95%: 0.74, 0.98]	kcal/mol
rho : GAFF	0.43	[95%: 0.07, 0.71]	kcal/mol	rho : GAFF	0.47	[95%: 0.24, 0.71]	kcal/mol	rho : GAFF	0.47	[95%: 0.07, 0.77]	kcal/mol	rho : GAFF	0.65	[95%: 0.44, 0.78]	kcal/mol	rho : GAFF	0.38	[95%: 0.14, 0.60]	kcal/mol	rho : GAFF	0.71	[95%: 0.41, 0.89]	kcal/mol	rho : GAFF	0.76	[95%: 0.32, 0.94]	kcal/mol	rho : GAFF	0.57	[95%: 0.13, 0.84]	kcal/mol

