

bace ΔG (N = 36)					cdk2 ΔG (N = 16)					jnk1 ΔG (N = 21)					mcl1 ΔG (N = 42)					p38a ΔG (N = 34)					ptplb ΔG (N = 23)					thrombin ΔG (N = 11)					tyk2 ΔG (N = 16)				
RMSE: OPLS2.1	0.85	[95%: 0.66, 1.03]	kcal/mol		RMSE: OPLS2.1	1.04	[95%: 0.76, 1.28]	kcal/mol		RMSE: OPLS2.1	1.14	[95%: 0.96, 1.33]	kcal/mol		RMSE: OPLS2.1	1.04	[95%: 0.82, 1.28]	kcal/mol		RMSE: OPLS2.1	0.97	[95%: 0.79, 1.13]	kcal/mol		RMSE: OPLS2.1	0.80	[95%: 0.52, 1.08]	kcal/mol		RMSE: OPLS2.1	0.54	[95%: 0.30, 0.76]	kcal/mol						
RMSE: GAFF	1.32	[95%: 0.98, 1.74]	kcal/mol		RMSE: GAFF	1.08	[95%: 0.78, 1.35]	kcal/mol		RMSE: GAFF	1.13	[95%: 0.81, 1.43]	kcal/mol		RMSE: GAFF	1.48	[95%: 1.20, 1.74]	kcal/mol		RMSE: GAFF	1.62	[95%: 1.21, 2.01]	kcal/mol		RMSE: GAFF	1.01	[95%: 0.69, 1.32]	kcal/mol		RMSE: GAFF	0.51	[95%: 0.25, 0.74]	kcal/mol						
MUE : OPLS2.1	0.66	[95%: 0.50, 0.84]	kcal/mol		MUE : OPLS2.1	0.88	[95%: 0.64, 1.19]	kcal/mol		MUE : OPLS2.1	1.05	[95%: 0.87, 1.24]	kcal/mol		MUE : OPLS2.1	0.84	[95%: 0.68, 1.04]	kcal/mol		MUE : OPLS2.1	0.86	[95%: 0.72, 1.01]	kcal/mol		MUE : OPLS2.1	0.60	[95%: 0.40, 0.83]	kcal/mol		MUE : OPLS2.1	0.42	[95%: 0.24, 0.65]	kcal/mol						
MUE : GAFF	1.03	[95%: 0.78, 1.32]	kcal/mol		MUE : GAFF	0.90	[95%: 0.62, 1.22]	kcal/mol		MUE : GAFF	0.90	[95%: 0.63, 1.20]	kcal/mol		MUE : GAFF	1.24	[95%: 1.02, 1.50]	kcal/mol		MUE : GAFF	1.28	[95%: 0.98, 1.61]	kcal/mol		MUE : GAFF	0.76	[95%: 0.50, 1.06]	kcal/mol		MUE : GAFF	0.37	[95%: 0.18, 0.60]	kcal/mol						
R2 : OPLS2.1	-0.23	[95%: -1.67, 0.37]	kcal/mol		R2 : OPLS2.1	0.22	[95%: -0.60, 0.51]	kcal/mol		R2 : OPLS2.1	-0.84	[95%: -3.40, -0.03]	kcal/mol		R2 : OPLS2.1	0.02	[95%: -0.69, 0.45]	kcal/mol		R2 : OPLS2.1	0.05	[95%: -0.76, 0.44]	kcal/mol		R2 : OPLS2.1	0.62	[95%: 0.05, 0.80]	kcal/mol		R2 : OPLS2.1	-0.08	[95%: -2.87, 0.65]	kcal/mol						
R2 : GAFF	-1.98	[95%: -5.77, -0.40]	kcal/mol		R2 : GAFF	0.16	[95%: -0.47, 0.43]	kcal/mol		R2 : GAFF	-0.80	[95%: -3.56, 0.07]	kcal/mol		R2 : GAFF	-0.97	[95%: -2.38, -0.18]	kcal/mol		R2 : GAFF	-1.66	[95%: -4.63, -0.24]	kcal/mol		R2 : GAFF	0.39	[95%: -0.37, 0.70]	kcal/mol		R2 : GAFF	0.04	[95%: -1.65, 0.77]	kcal/mol						
rho : OPLS2.1	0.78	[95%: 0.61, 0.89]	kcal/mol		rho : OPLS2.1	0.48	[95%: 0.13, 0.83]	kcal/mol		rho : OPLS2.1	0.84	[95%: 0.65, 0.95]	kcal/mol		rho : OPLS2.1	0.77	[95%: 0.65, 0.86]	kcal/mol		rho : OPLS2.1	0.65	[95%: 0.47, 0.79]	kcal/mol		rho : OPLS2.1	0.80	[95%: 0.62, 0.92]	kcal/mol		rho : OPLS2.1	0.71	[95%: 0.10, 0.93]	kcal/mol						
rho : GAFF	0.43	[95%: 0.08, 0.74]	kcal/mol		rho : GAFF	0.47	[95%: 0.18, 0.72]	kcal/mol		rho : GAFF	0.47	[95%: 0.11, 0.75]	kcal/mol		rho : GAFF	0.65	[95%: 0.48, 0.79]	kcal/mol		rho : GAFF	0.38	[95%: 0.14, 0.61]	kcal/mol		rho : GAFF	0.71	[95%: 0.47, 0.88]	kcal/mol		rho : GAFF	0.76	[95%: 0.32, 0.94]	kcal/mol						

