

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: FEP+	0.85	[95%: 0.66, 1.02]	kcal/mol	RMSE: FEP+	1.04	[95%: 0.76, 1.28]	kcal/mol	RMSE: FEP+	1.14	[95%: 0.94, 1.32]	kcal/mol	RMSE: FEP+	1.04	[95%: 0.81, 1.25]	kcal/mol	RMSE: FEP+	0.97	[95%: 0.80, 1.14]	kcal/mol	RMSE: FEP+	0.80	[95%: 0.52, 1.08]	kcal/mol	RMSE: FEP+	0.54	[95%: 0.30, 0.76]	kcal/mol	RMSE: FEP+	0.57	[95%: 0.34, 0.78]	kcal/mol
RMSE: AMBER TI	1.32	[95%: 0.97, 1.75]	kcal/mol	RMSE: AMBER TI	1.08	[95%: 0.76, 1.35]	kcal/mol	RMSE: AMBER TI	1.13	[95%: 0.79, 1.42]	kcal/mol	RMSE: AMBER TI	1.48	[95%: 1.20, 1.74]	kcal/mol	RMSE: AMBER TI	1.62	[95%: 1.22, 1.99]	kcal/mol	RMSE: AMBER TI	1.01	[95%: 0.66, 1.31]	kcal/mol	RMSE: AMBER TI	0.51	[95%: 0.25, 0.74]	kcal/mol	RMSE: AMBER TI	1.13	[95%: 0.74, 1.48]	kcal/mol
MUE : FEP+	0.66	[95%: 0.49, 0.83]	kcal/mol	MUE : FEP+	0.88	[95%: 0.62, 1.15]	kcal/mol	MUE : FEP+	1.05	[95%: 0.87, 1.23]	kcal/mol	MUE : FEP+	0.84	[95%: 0.66, 1.04]	kcal/mol	MUE : FEP+	0.86	[95%: 0.71, 1.01]	kcal/mol	MUE : FEP+	0.60	[95%: 0.41, 0.83]	kcal/mol	MUE : FEP+	0.42	[95%: 0.23, 0.63]	kcal/mol	MUE : FEP+	0.44	[95%: 0.28, 0.64]	kcal/mol
MUE : AMBER TI	1.03	[95%: 0.79, 1.33]	kcal/mol	MUE : AMBER TI	0.90	[95%: 0.59, 1.21]	kcal/mol	MUE : AMBER TI	0.90	[95%: 0.61, 1.19]	kcal/mol	MUE : AMBER TI	1.24	[95%: 1.01, 1.49]	kcal/mol	MUE : AMBER TI	1.28	[95%: 0.97, 1.61]	kcal/mol	MUE : AMBER TI	0.76	[95%: 0.49, 1.04]	kcal/mol	MUE : AMBER TI	0.37	[95%: 0.18, 0.58]	kcal/mol	MUE : AMBER TI	0.89	[95%: 0.56, 1.24]	kcal/mol
R2 : FEP+	-0.23	[95%: -1.68, 0.40]	kcal/mol	R2 : FEP+	0.22	[95%: -0.53, 0.51]	kcal/mol	R2 : FEP+	-0.84	[95%: -3.49, -0.03]	kcal/mol	R2 : FEP+	0.02	[95%: -0.69, 0.46]	kcal/mol	R2 : FEP+	0.05	[95%: -0.86, 0.44]	kcal/mol	R2 : FEP+	0.62	[95%: 0.05, 0.80]	kcal/mol	R2 : FEP+	-0.08	[95%: -3.22, 0.67]	kcal/mol	R2 : FEP+	0.79	[95%: 0.50, 0.92]	kcal/mol
R2 : AMBER TI	-1.98	[95%: -5.86, -0.41]	kcal/mol	R2 : AMBER TI	0.16	[95%: -0.48, 0.41]	kcal/mol	R2 : AMBER TI	-0.80	[95%: -2.90, 0.14]	kcal/mol	R2 : AMBER TI	-0.97	[95%: -2.45, -0.17]	kcal/mol	R2 : AMBER TI	-1.66	[95%: -4.71, -0.33]	kcal/mol	R2 : AMBER TI	0.39	[95%: -0.34, 0.72]	kcal/mol	R2 : AMBER TI	0.04	[95%: -1.71, 0.76]	kcal/mol	R2 : AMBER TI	0.19	[95%: -0.91, 0.60]	kcal/mol
rho : FEP+	0.78	[95%: 0.62, 0.89]	kcal/mol	rho : FEP+	0.48	[95%: 0.09, 0.83]	kcal/mol	rho : FEP+	0.84	[95%: 0.68, 0.95]	kcal/mol	rho : FEP+	0.77	[95%: 0.65, 0.85]	kcal/mol	rho : FEP+	0.65	[95%: 0.48, 0.78]	kcal/mol	rho : FEP+	0.80	[95%: 0.62, 0.92]	kcal/mol	rho : FEP+	0.71	[95%: 0.20, 0.94]	kcal/mol	rho : FEP+	0.89	[95%: 0.73, 0.97]	kcal/mol
rho : AMBER TI	0.43	[95%: 0.07, 0.73]	kcal/mol	rho : AMBER TI	0.47	[95%: 0.22, 0.72]	kcal/mol	rho : AMBER TI	0.47	[95%: 0.10, 0.76]	kcal/mol	rho : AMBER TI	0.65	[95%: 0.46, 0.79]	kcal/mol	rho : AMBER TI	0.38	[95%: 0.13, 0.63]	kcal/mol	rho : AMBER TI	0.71	[95%: 0.46, 0.88]	kcal/mol	rho : AMBER TI	0.76	[95%: 0.35, 0.94]	kcal/mol	rho : AMBER TI	0.57	[95%: 0.16, 0.84]	kcal/mol

