

thrombin mapped edges $\Delta\Delta G$ (N = 16)			tyk2 mapped edges $\Delta\Delta G$ (N = 24)			jnk1 mapped edges $\Delta\Delta G$ (N = 31)			cdk2 mapped edges $\Delta\Delta G$ (N = 25)			ptp1b mapped edges $\Delta\Delta G$ (N = 49)			bace mapped edges $\Delta\Delta G$ (N = 58)			mcl1 mapped edges $\Delta\Delta G$ (N = 71)			p38a mapped edges $\Delta\Delta G$ (N = 56)			all mapped edges $\Delta\Delta G$ (N = 330)		
RMSE: FEP+	0.93	[95%: 0.64, 1.22] kcal/mol	RMSE: FEP+	0.93	[95%: 0.67, 1.17] kcal/mol	RMSE: FEP+	1.00	[95%: 0.74, 1.24] kcal/mol	RMSE: FEP+	1.11	[95%: 0.86, 1.34] kcal/mol	RMSE: FEP+	1.22	[95%: 0.88, 1.58] kcal/mol	RMSE: FEP+	1.03	[95%: 0.86, 1.18] kcal/mol	RMSE: FEP+	1.41	[95%: 1.20, 1.61] kcal/mol	RMSE: FEP+	1.03	[95%: 0.84, 1.22] kcal/mol	RMSE: FEP+	1.14	[95%: 1.05, 1.24] kcal/mol
RMSE: AMBER TI	0.62	[95%: 0.34, 0.87] kcal/mol	RMSE: AMBER TI	1.27	[95%: 0.99, 1.55] kcal/mol	RMSE: AMBER TI	1.45	[95%: 1.00, 1.91] kcal/mol	RMSE: AMBER TI	1.13	[95%: 0.86, 1.37] kcal/mol	RMSE: AMBER TI	1.40	[95%: 1.02, 1.74] kcal/mol	RMSE: AMBER TI	1.47	[95%: 1.24, 1.71] kcal/mol	RMSE: AMBER TI	1.83	[95%: 1.59, 2.09] kcal/mol	RMSE: AMBER TI	1.56	[95%: 1.25, 1.85] kcal/mol	RMSE: AMBER TI	1.50	[95%: 1.37, 1.62] kcal/mol
MUE : FEP+	0.76	[95%: 0.49, 1.03] kcal/mol	MUE : FEP+	0.75	[95%: 0.52, 1.00] kcal/mol	MUE : FEP+	0.78	[95%: 0.59, 1.00] kcal/mol	MUE : FEP+	0.91	[95%: 0.66, 1.16] kcal/mol	MUE : FEP+	0.89	[95%: 0.67, 1.15] kcal/mol	MUE : FEP+	0.84	[95%: 0.69, 0.99] kcal/mol	MUE : FEP+	1.16	[95%: 0.97, 1.34] kcal/mol	MUE : FEP+	0.80	[95%: 0.63, 0.97] kcal/mol	MUE : FEP+	0.90	[95%: 0.82, 0.98] kcal/mol
MUE : AMBER TI	0.46	[95%: 0.27, 0.67] kcal/mol	MUE : AMBER TI	1.07	[95%: 0.81, 1.38] kcal/mol	MUE : AMBER TI	1.07	[95%: 0.73, 1.45] kcal/mol	MUE : AMBER TI	0.97	[95%: 0.76, 1.21] kcal/mol	MUE : AMBER TI	1.06	[95%: 0.82, 1.32] kcal/mol	MUE : AMBER TI	1.20	[95%: 0.97, 1.42] kcal/mol	MUE : AMBER TI	1.52	[95%: 1.28, 1.75] kcal/mol	MUE : AMBER TI	1.20	[95%: 0.96, 1.46] kcal/mol	MUE : AMBER TI	1.17	[95%: 1.07, 1.28] kcal/mol
R2 : FEP+	-3.16	[95%: -7.66, -0.94] kcal/mol	R2 : FEP+	0.33	[95%: -0.34, 0.61] kcal/mol	R2 : FEP+	-1.56	[95%: -3.97, -0.40] kcal/mol	R2 : FEP+	0.07	[95%: -0.58, 0.32] kcal/mol	R2 : FEP+	0.37	[95%: 0.10, 0.54] kcal/mol	R2 : FEP+	-0.53	[95%: -1.82, 0.09] kcal/mol	R2 : FEP+	-0.51	[95%: -1.34, 0.01] kcal/mol	R2 : FEP+	0.29	[95%: -0.19, 0.55] kcal/mol	R2 : FEP+	-0.02	[95%: -0.24, 0.15] kcal/mol
R2 : AMBER TI	-0.89	[95%: -4.38, 0.47] kcal/mol	R2 : AMBER TI	-0.24	[95%: -1.53, 0.23] kcal/mol	R2 : AMBER TI	-4.43	[95%: -9.85, -1.64] kcal/mol	R2 : AMBER TI	0.05	[95%: -1.17, 0.50] kcal/mol	R2 : AMBER TI	0.17	[95%: -0.35, 0.45] kcal/mol	R2 : AMBER TI	-2.16	[95%: -4.32, -0.87] kcal/mol	R2 : AMBER TI	-1.55	[95%: -2.79, -0.74] kcal/mol	R2 : AMBER TI	-0.64	[95%: -1.80, 0.06] kcal/mol	R2 : AMBER TI	-0.74	[95%: -1.19, -0.41] kcal/mol
rho : FEP+	0.42	[95%: -0.18, 0.75] kcal/mol	rho : FEP+	0.70	[95%: 0.49, 0.84] kcal/mol	rho : FEP+	0.59	[95%: 0.25, 0.81] kcal/mol	rho : FEP+	0.39	[95%: 0.16, 0.62] kcal/mol	rho : FEP+	0.66	[95%: 0.53, 0.79] kcal/mol	rho : FEP+	0.61	[95%: 0.43, 0.73] kcal/mol	rho : FEP+	0.51	[95%: 0.34, 0.65] kcal/mol	rho : FEP+	0.79	[95%: 0.67, 0.86] kcal/mol	rho : FEP+	0.60	[95%: 0.53, 0.67] kcal/mol
rho : AMBER TI	0.71	[95%: 0.38, 0.91] kcal/mol	rho : AMBER TI	0.49	[95%: 0.16, 0.77] kcal/mol	rho : AMBER TI	0.22	[95%: -0.19, 0.65] kcal/mol	rho : AMBER TI	0.59	[95%: 0.34, 0.78] kcal/mol	rho : AMBER TI	0.59	[95%: 0.40, 0.75] kcal/mol	rho : AMBER TI	0.52	[95%: 0.30, 0.70] kcal/mol	rho : AMBER TI	0.40	[95%: 0.21, 0.58] kcal/mol	rho : AMBER TI	0.56	[95%: 0.37, 0.72] kcal/mol	rho : AMBER TI	0.48	[95%: 0.40, 0.56] kcal/mol

