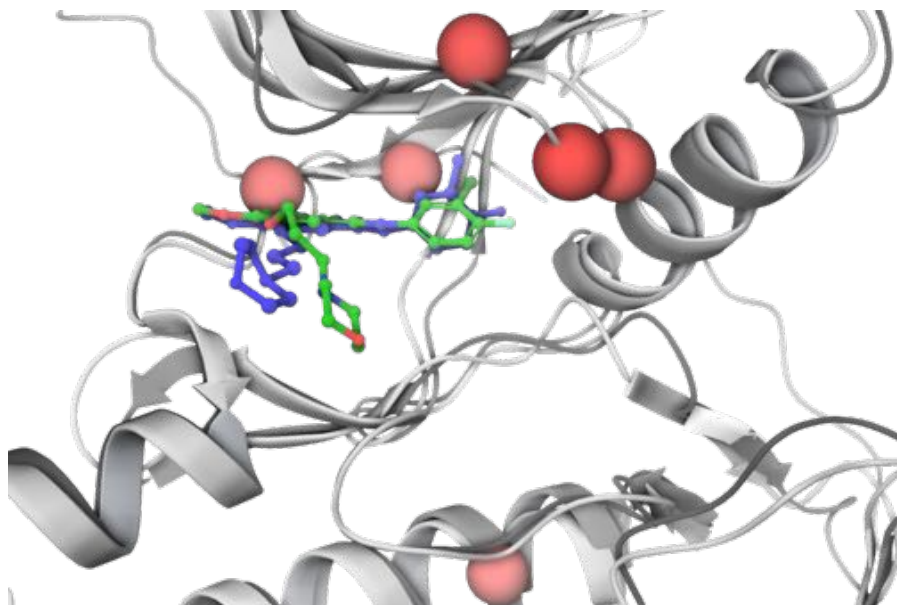


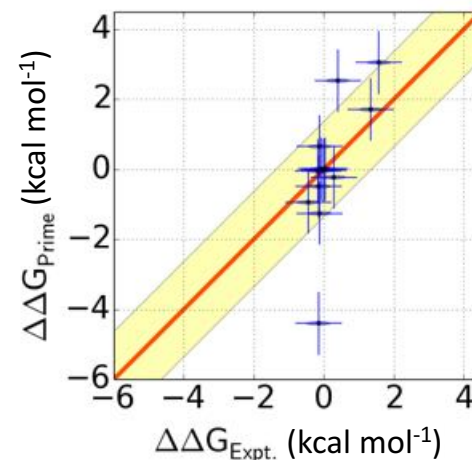
gefitinib

Glide docking



EGFR:gefitinib (PDB: 4WKQ) Abl:gefitinib (Glide)

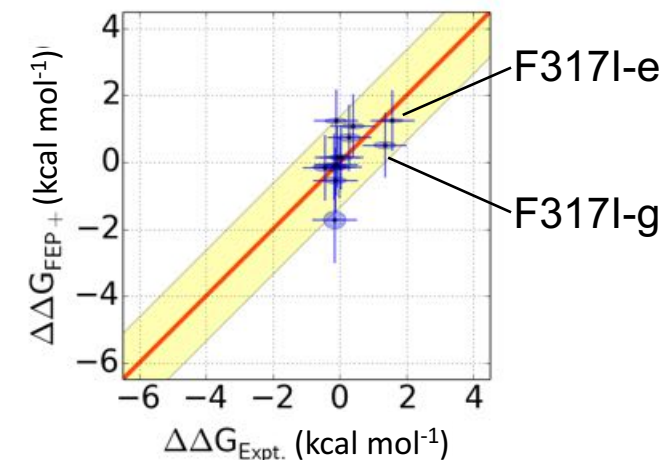
Prime



MUE (kcal mol⁻¹) **0.91**

RMSE (kcal mol⁻¹) **1.45**

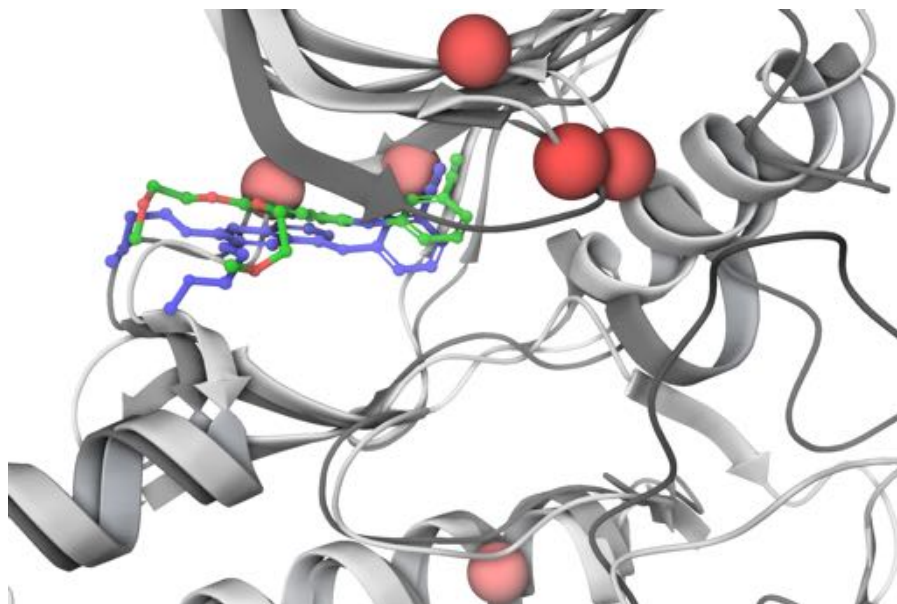
FEP+



MUE (kcal mol⁻¹) **0.50**

RMSE (kcal mol⁻¹) **0.69**

erlotinib



EGFR:erlotinib (PDB: 4HJO) Abl:erlotinib (Glide)

Prediction

Experiment	Prediction	
	n	r
N	10	2
R	0	1

Accuracy **0.85**

Specificity **0.83**

Sensitivity **1.00**

Prediction

Experiment	Prediction	
	n	r
N	12	0
R	1	0

Accuracy **0.92**

Specificity **1.00**

Sensitivity **NA**