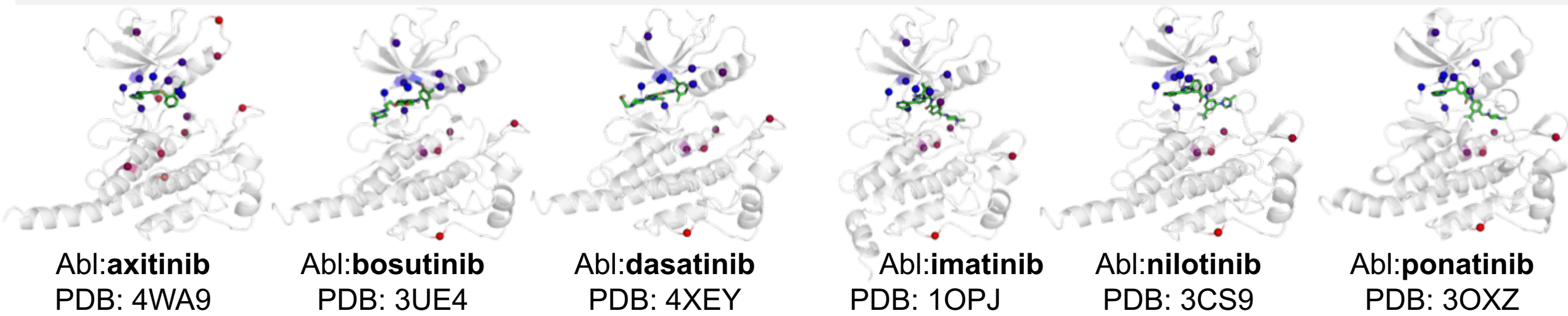
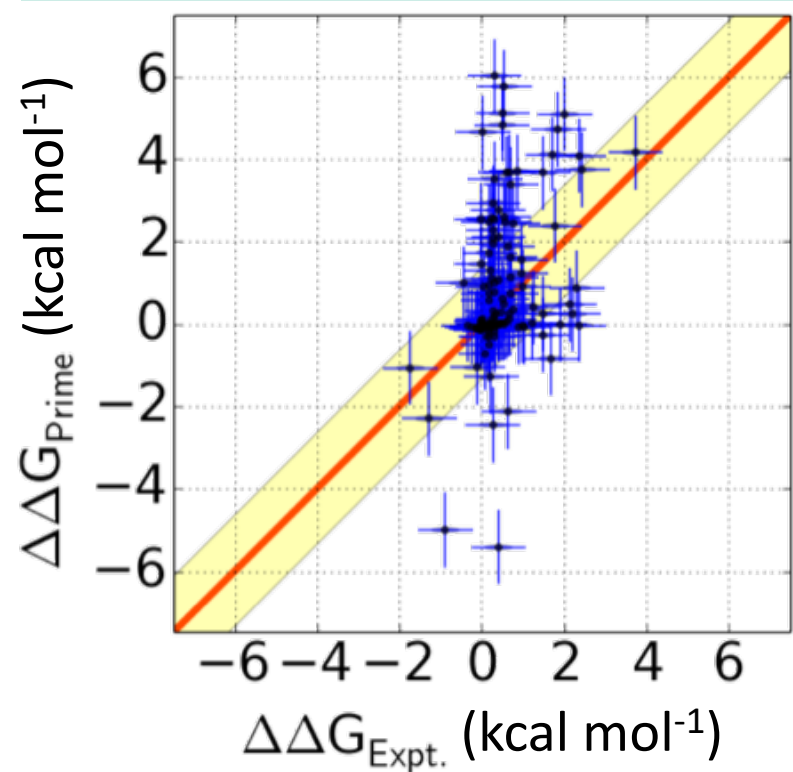


Abl:TKI Co-Crystal Structures

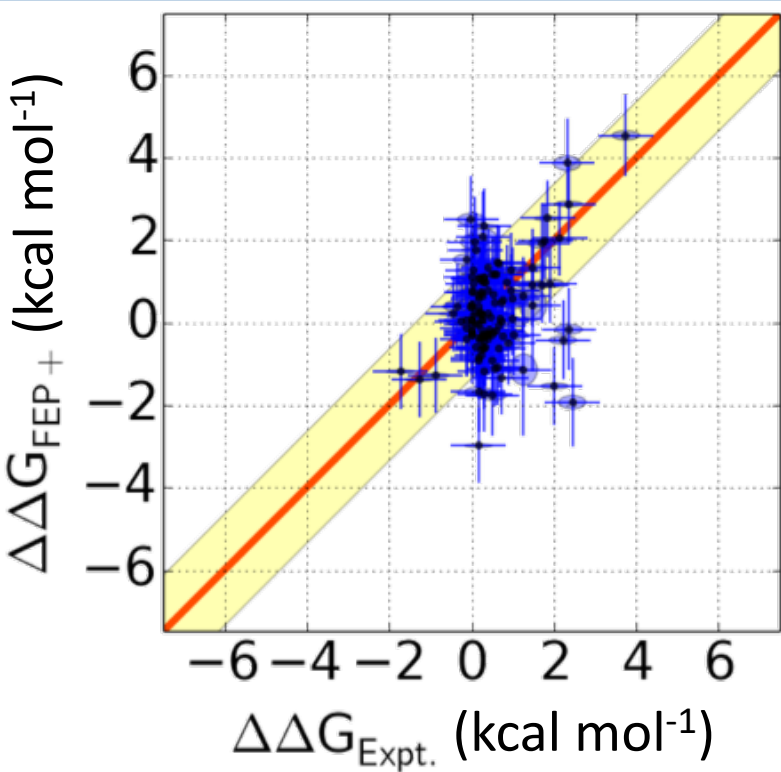


Prime

FEP+



Bootstrap		
MUE (kcal mol ⁻¹)	1.16 ^{1.37} _{0.96}	0.82 ^{0.95} _{0.69}
RMSE (kcal mol ⁻¹)	1.72 ^{2.00} _{1.41}	1.11 ^{1.30} _{0.91}
Bayesian Analysis		
MUE (kcal mol ⁻¹)	*1.40 ^{1.60} _{1.24}	0.79 ^{0.92} _{0.68}
RMSE (kcal mol ⁻¹)	1.76 ^{2.01} _{1.55}	0.99 ^{1.15} _{0.85}



Prime

FEP+

		Prediction	
		s	r
Experiment	S	85	28
	R	9	9

Bootstrap		
Accuracy	0.72 ^{0.79} _{0.64}	0.87 ^{0.92} _{0.81}
Specificity	0.75 ^{0.83} _{0.67}	0.93 ^{0.97} _{0.88}
Sensitivity	0.50 ^{0.73} _{0.25}	0.50 ^{0.74} _{0.29}
Bayesian Analysis		
Accuracy	0.73 ^{0.76} _{0.70}	0.89 ^{0.92} _{0.86}
Specificity	0.74 ^{0.77} _{0.72}	0.91 ^{0.94} _{0.89}
Sensitivity	0.57 ^{0.77} _{0.36}	0.69 ^{1.00} _{0.46}

		Prediction	
		s	r
Experiment	S	105	8
	R	9	9