

# Rosetta / Bench $\Delta\Delta G$ is fast and accurate

	Rosetta <sup>***</sup>	FEP <sup>*</sup>	CC/PBSA <sup>**</sup>	EGAD <sup>**</sup>	Imutant2 <sup>**</sup>	FoldX <sup>**</sup>
R	0.69	0.63	0.56	0.59	0.54	0.50
N	1210	712	478	1065	933	1200

Predictions for the FoldX experimentally stability data set (Guerois, Nielson & Serrano *JMB* **320** 369 (2002))

<sup>\*</sup>From: Steinbrecher, Zhu, Wang, Abel, Negron, Pearlman, Feyfant, Duan & Sherman *JMB* **429** 948 (2017)

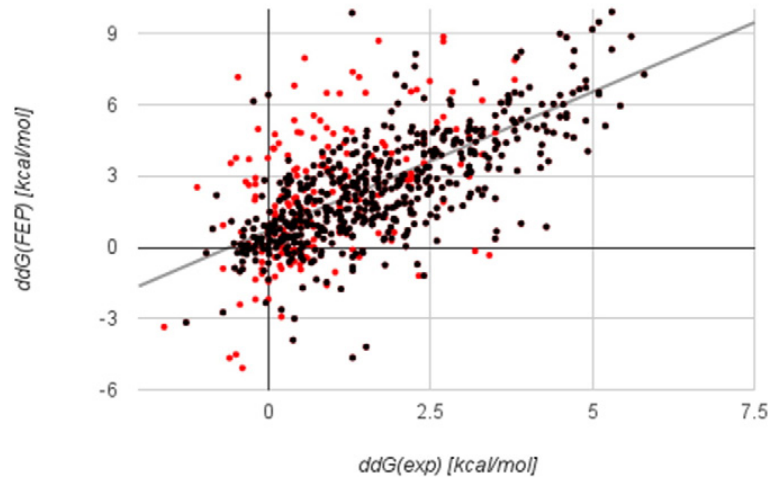
<sup>\*\*</sup>From: Potapov, Cohen & Schreiber *PEDS* **22** 553 (2009)

<sup>\*\*\*</sup>From: Kellogg, Leaver-Fay & Baker *Proteins* **79** 830 (2011)

## Predicted vs experiment:

### FEP<sup>\*</sup>

Throughput: 2-4 mutations/day/GPU card



### Rosetta<sup>\*\*\*</sup>

Bench: Throughput: 5,000-10,000 mutations/day

