

STRUCTURE-BASED ESTIMATION

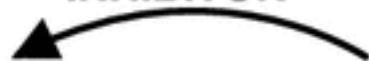
Physics-based
simulations:



Data-driven
methods:



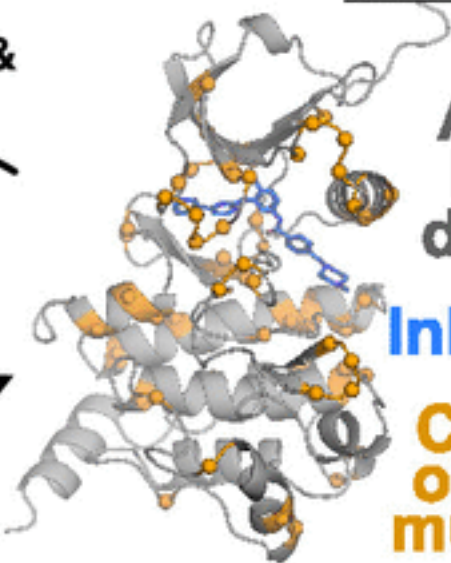
**MUTATIONS &
INHIBITOR**



**PROSPECTIVE
 $\Delta\Delta G$
PREDICTIONS**



THE BENCHMARK SYSTEM:



**ABL1A
kinase
domain**

Inhibitor

**Clinically
observed
mutations**