

STRUCTURE-BASED ESTIMATION

Physics-based
simulations:



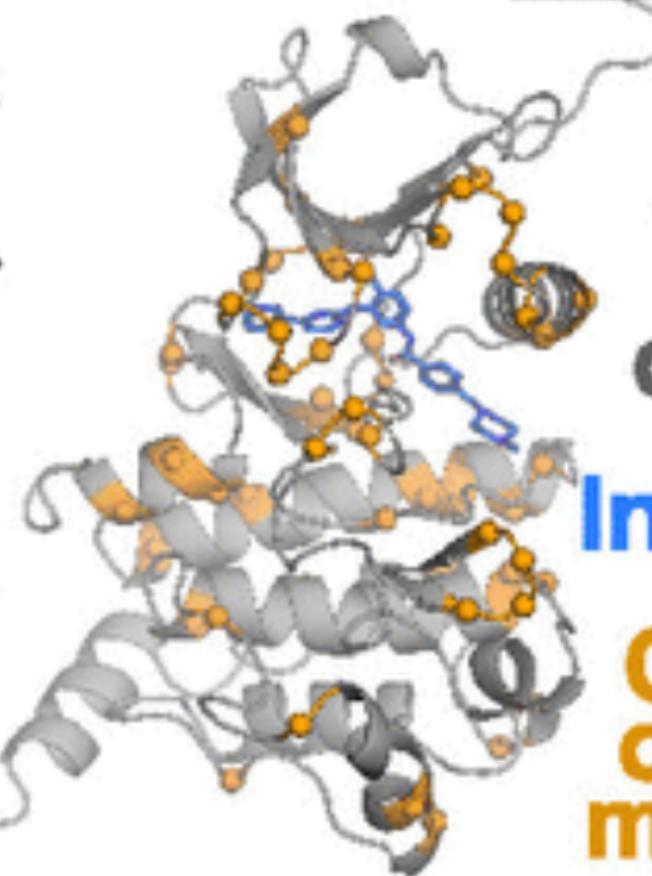
**MUTATIONS &
INHIBITOR**



Data-driven
methods:



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



THE BENCHMARK SYSTEM:

**ABL1A
kinase
domain**

Inhibitor

**Clinically
observed
mutations**