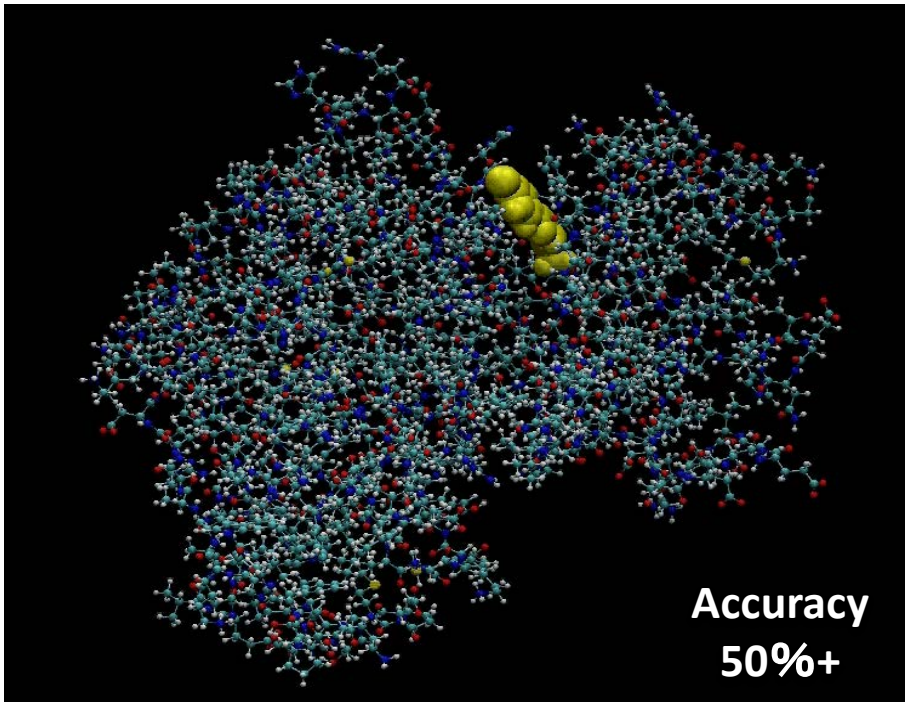
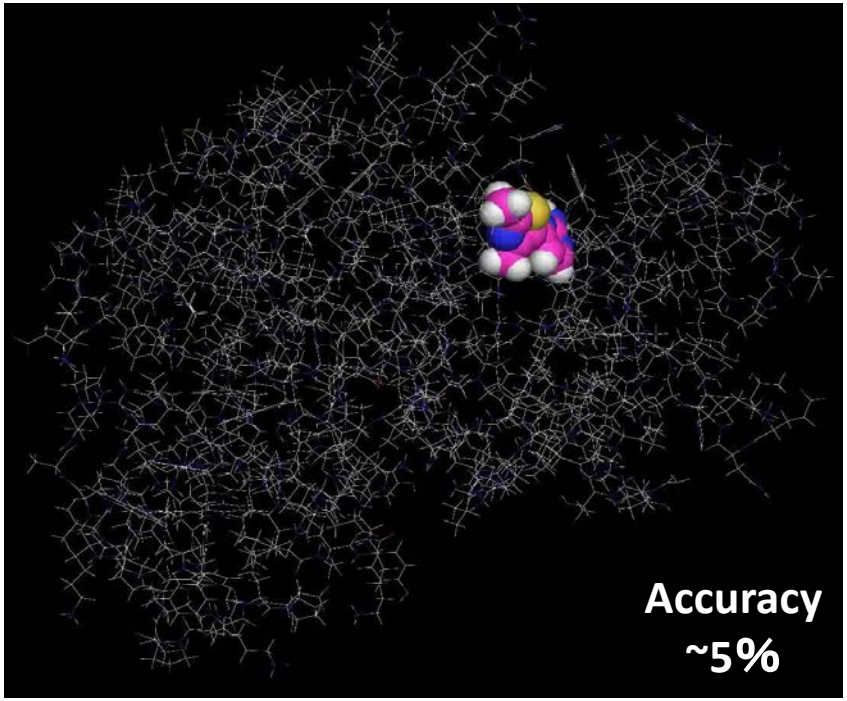
Drug Design

K computer has made molecular dynamics (MD) simulation more easily and reliably useful in MD-based drug design.

simulation with K



simulation before K



Okuno (Kyoto Univ.)

Simulation of molecular behavior including solvent (water molecule) became possible with K. Able to accurately predict binding affinities of several hundred pairs between pharmaceutical candidate compound and protein in a week.