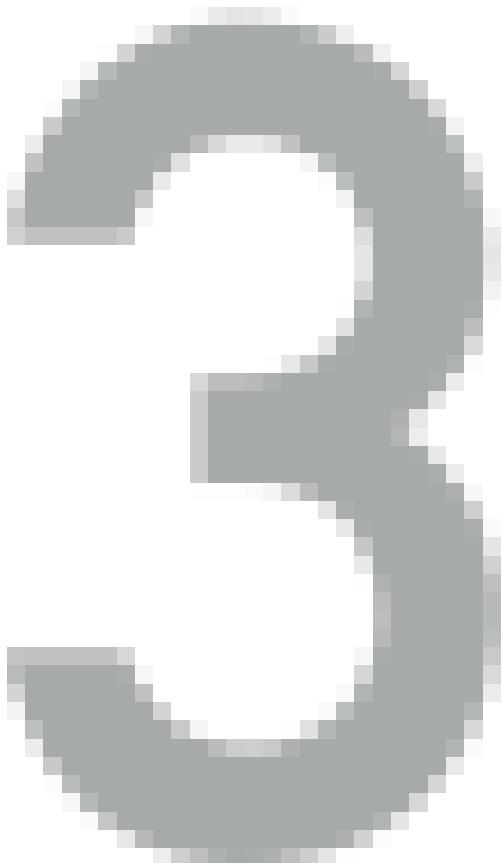
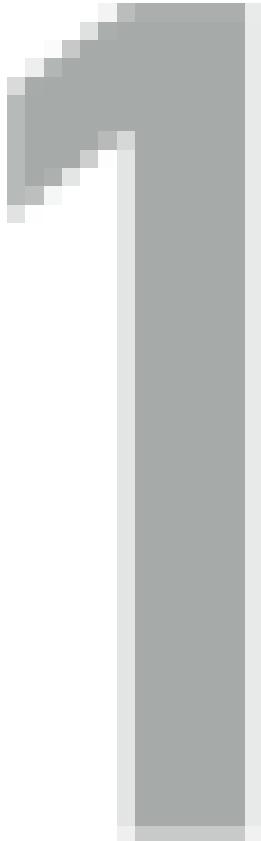


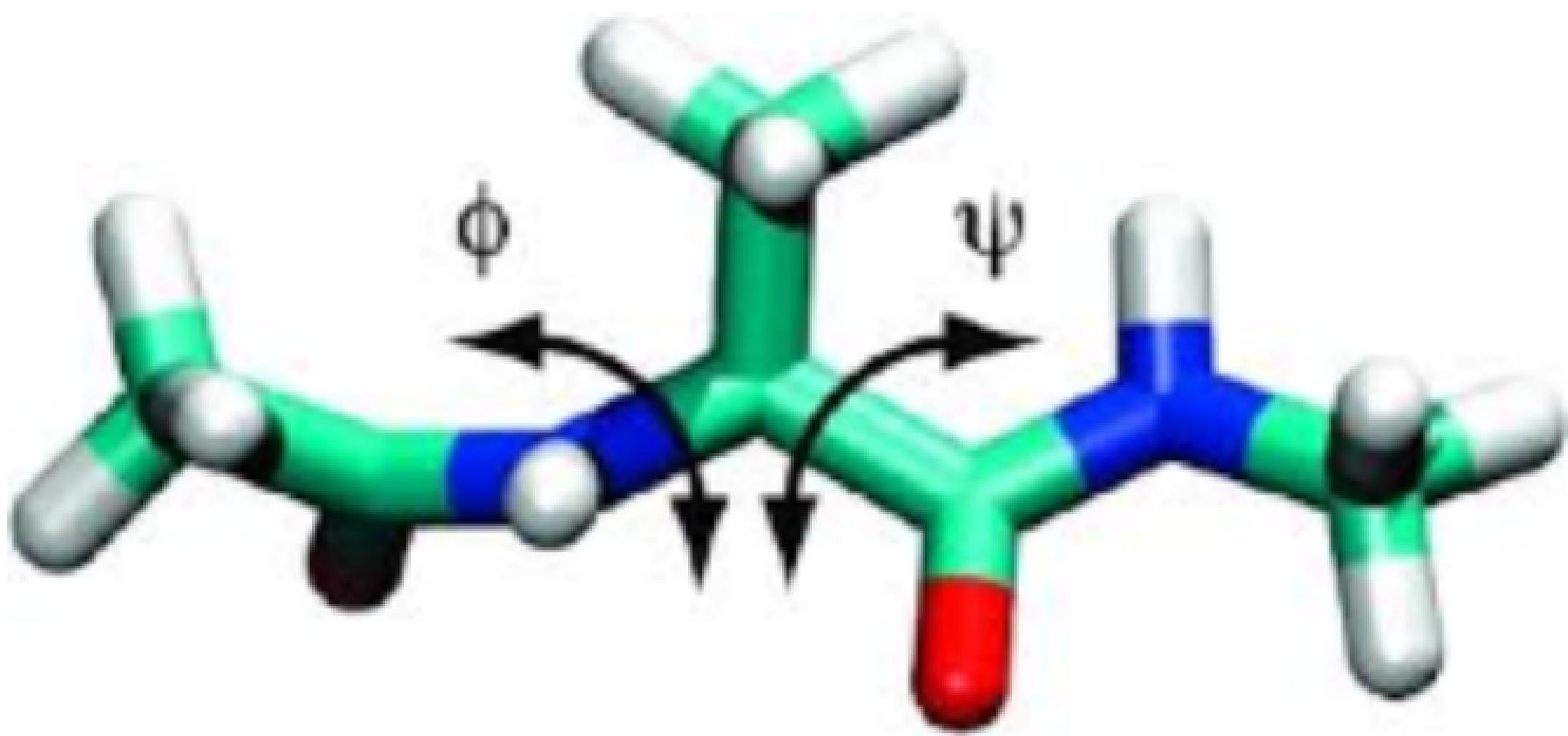


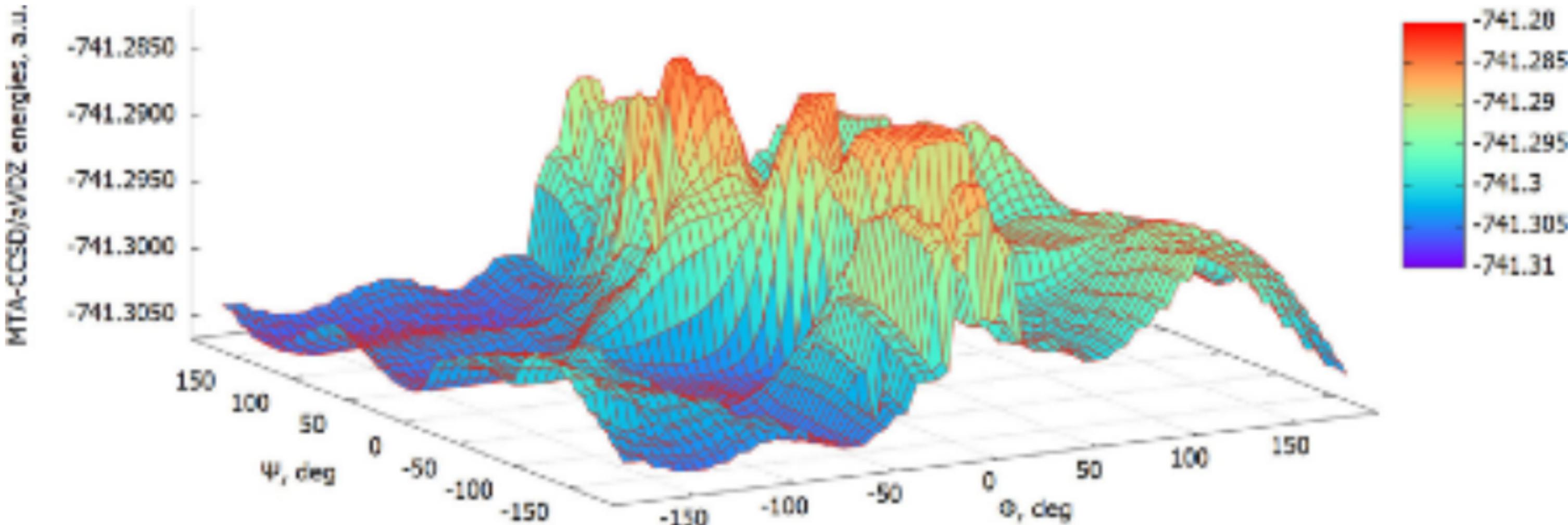
**EXAMPEL** **COLAR** **DYNA** **MOLICOS**



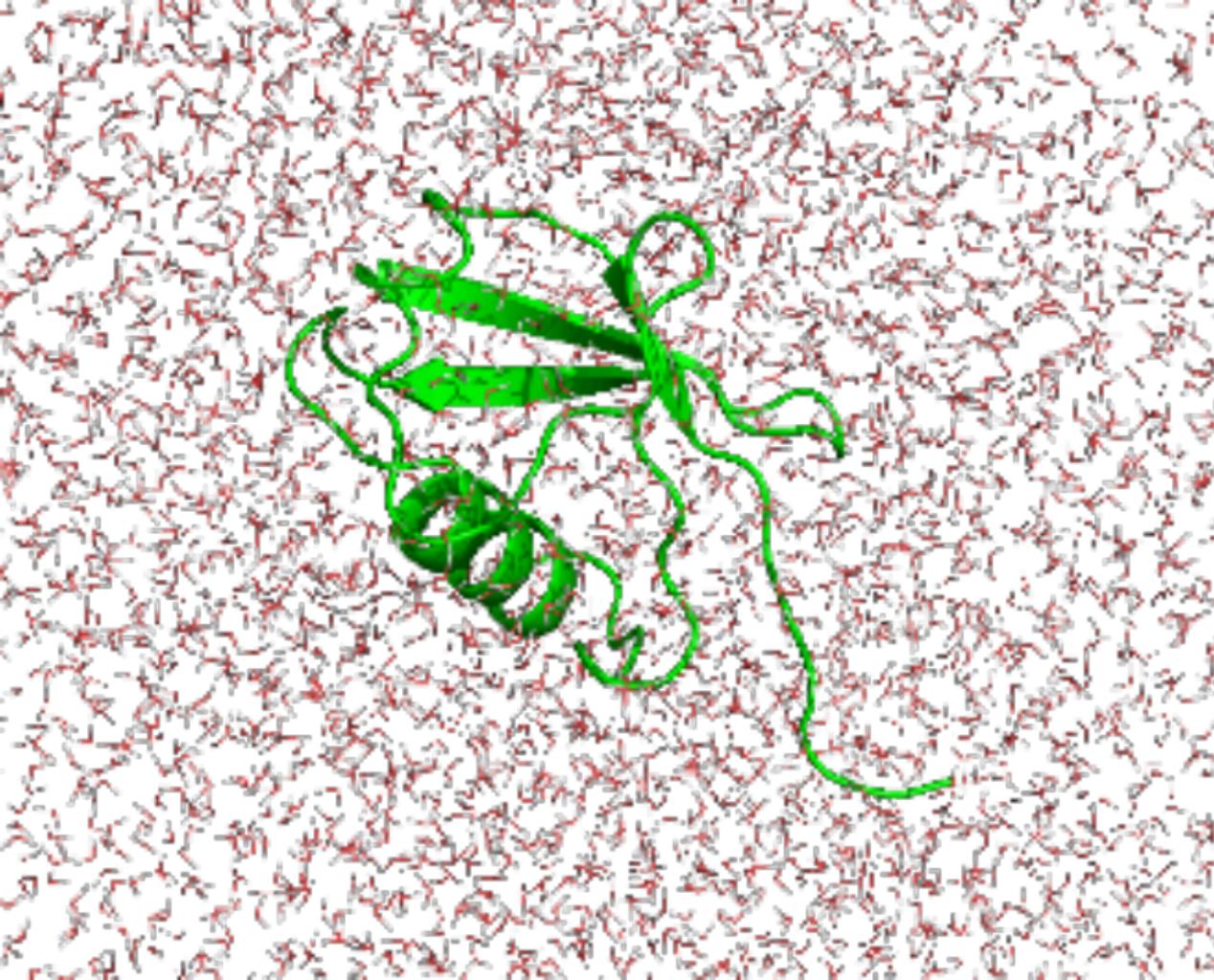
 Molecular dynamics simulates these systems to infer physical properties

Ecological forces between species, and interactions between species, may be mediated by other factors such as predation or competition.

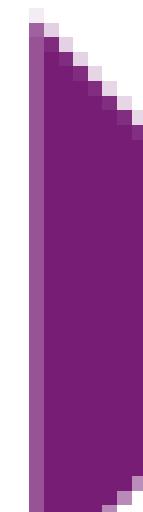


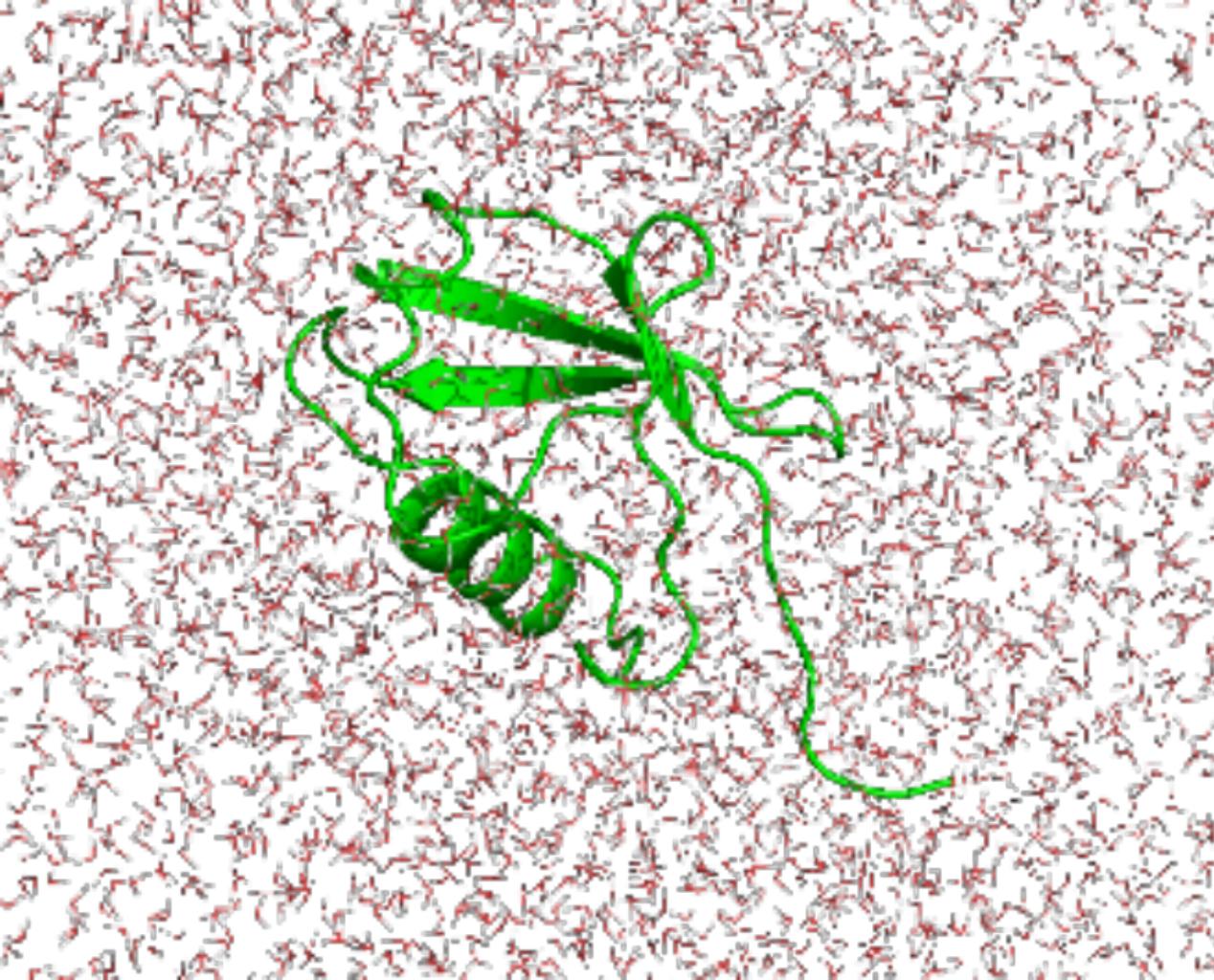


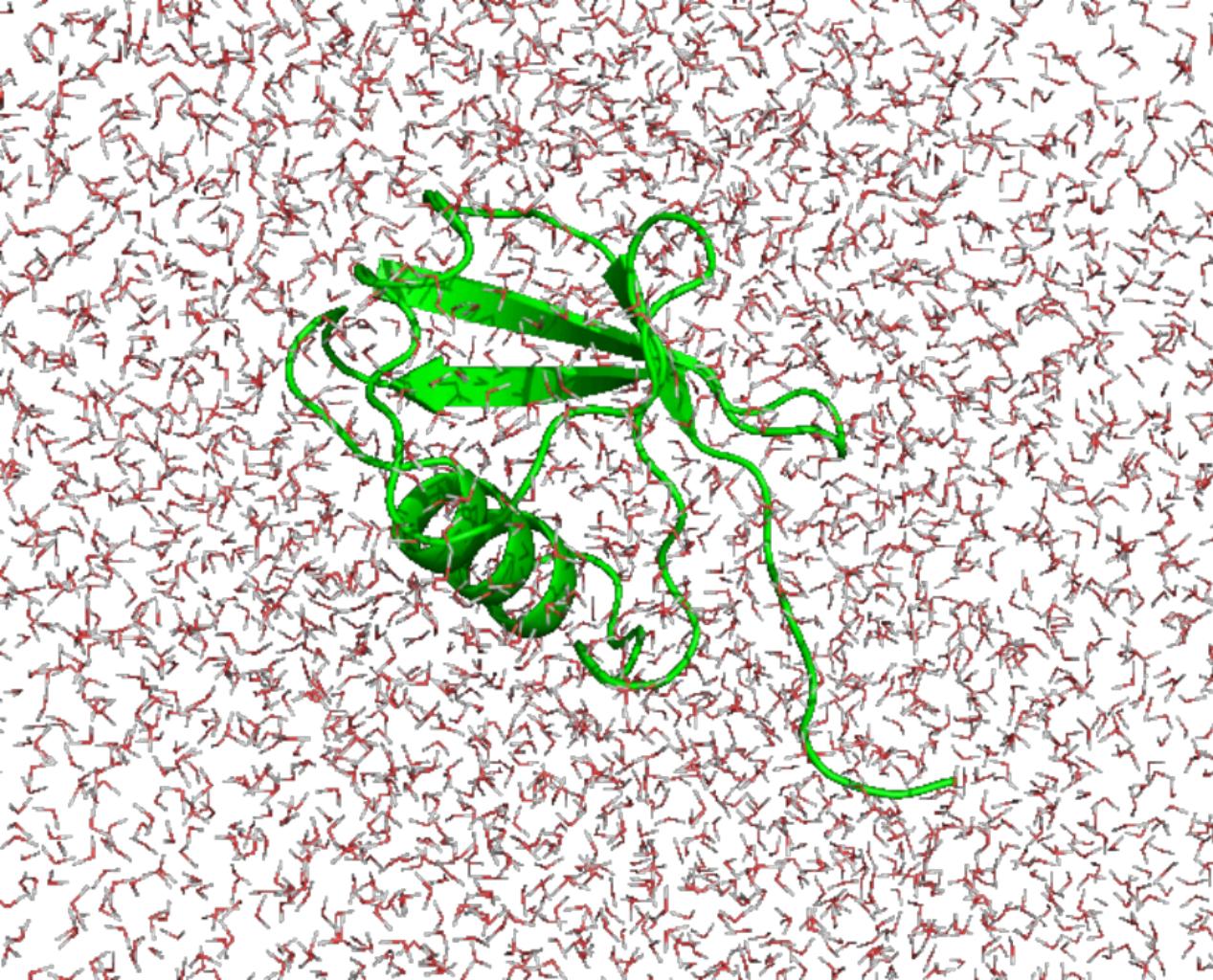
► Statespace configurations represent states of a system



Estimate reactions rates, binding affinity, material properties, etc

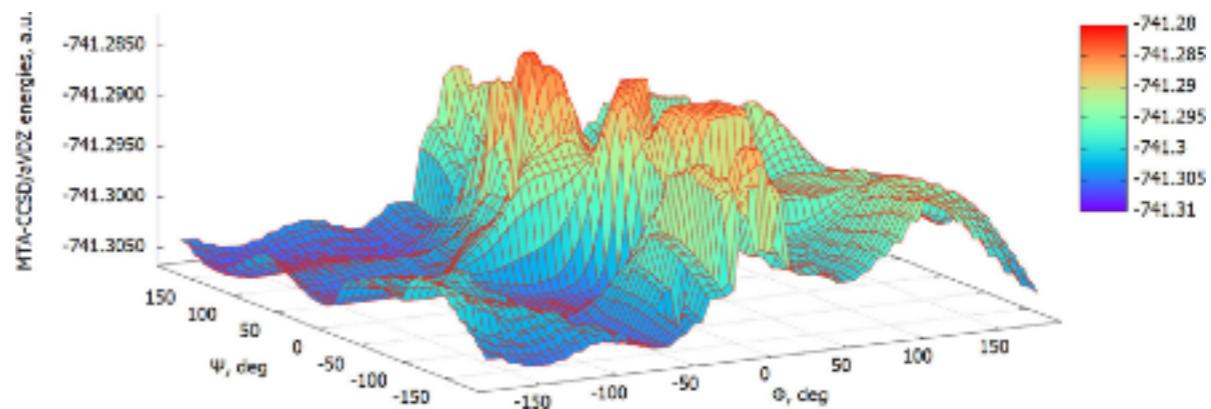
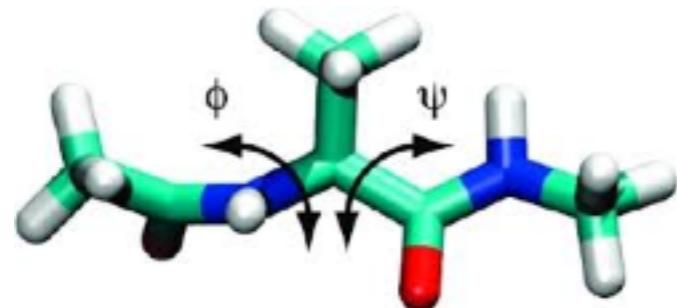
 ➤ **Verifying important discovery**



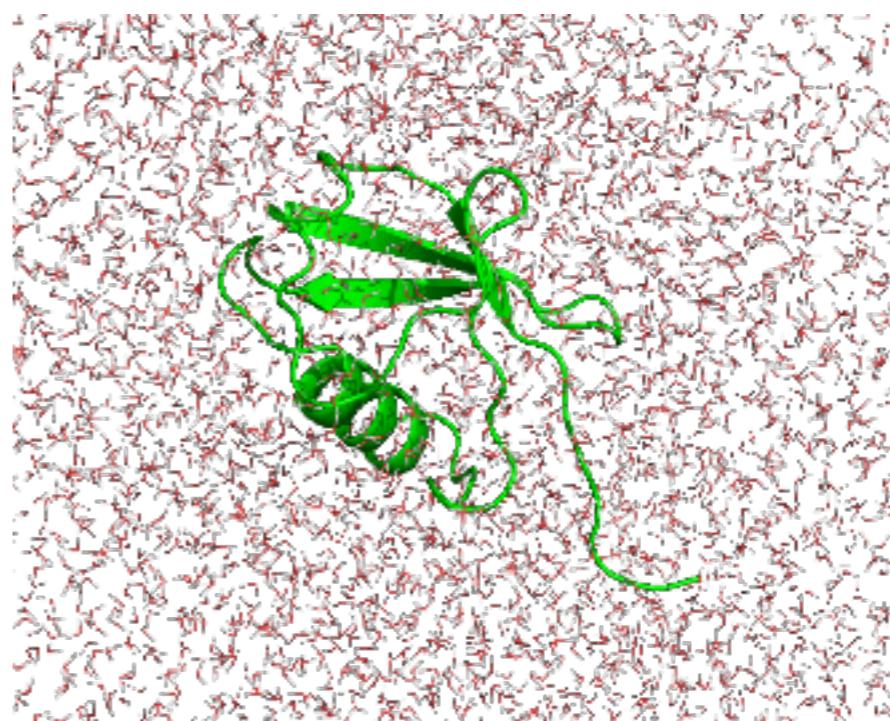


# EXAMPLE: MOLECULAR DYNAMICS

- ▶ Statespace represents different configurations of a system of particles
- ▶ Potential encodes the molecular forces between atoms, molecules, proteins etc



- ▶ Molecular dynamics simulates these systems to infer physical properties
- ▶ Estimate reactions rates, binding affinity, material properties, etc
- ▶ Very important for drug discovery



# EXAMPLE: QUANTUM CHROMODYNAMICS