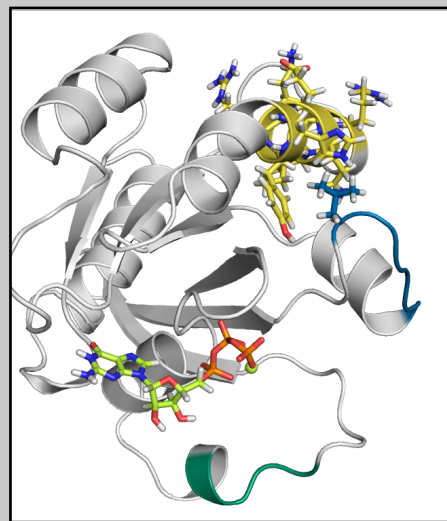


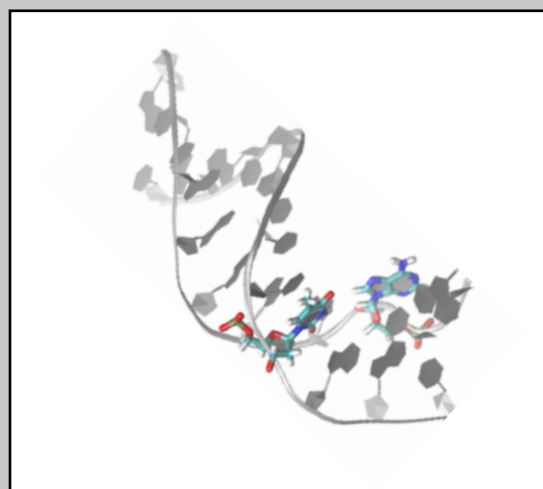
What can we learn?

Mechanisms, rates, free energy landscapes/differences



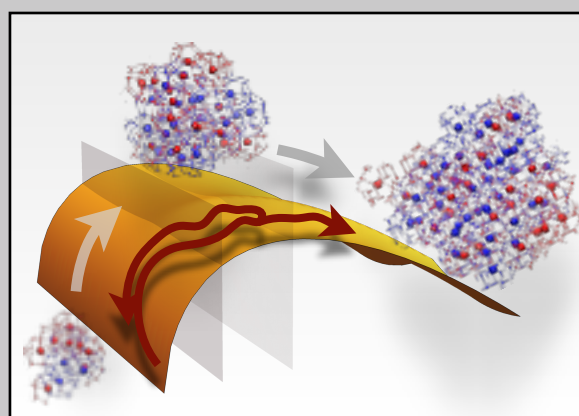
What are the differences in the dynamics of a healthy protein compared to a cancer-causing mutant?

Roet, Hooft, Bolhuis, DWHS, Vreede. ArXiv (submitted JCTC)



Which mechanism is preferred in a DNA conformational change, and what are the associated rates/free energies?

Vreede, Perez de Alba Ortíz, Bolhuis, DWHS. Nucl. Acids Res. 2019



How does the mechanism of methane hydrate formation change with temperature?

Arjun, Berendsen, Bolhuis. PNAS 2019

The Shooting Algorithm

What Monte Carlo move can we use to generate new paths?

