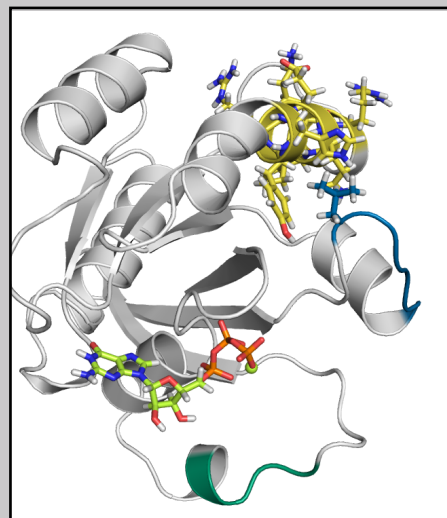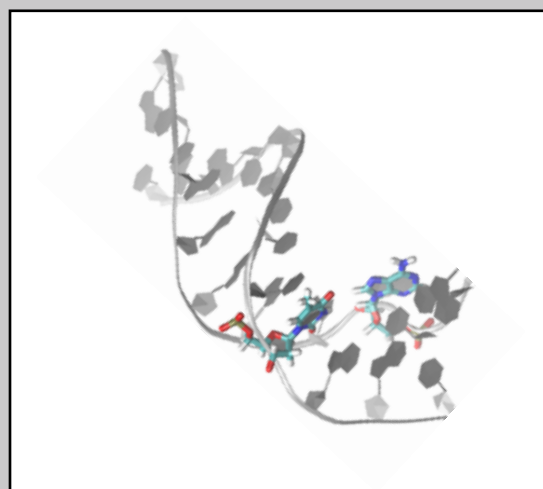# What can we learn?

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 JPCB)

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

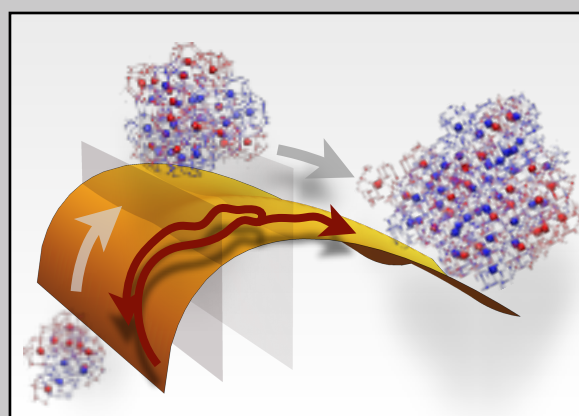Vreede, Perez de Alba Ortíz, Bolhuis, DWHS. Nucl. Acids Res. 2019

Image © Arjun

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

Arjun, Berendsen, Bolhuis. PNAS 2019

OpenPathSampling

http://openpathsampling.org

Twitter: @pathsampling

Development at: http://github.com/openpathsampling/

A Python library for path sampling simulations

✓ **Easy to use**: Beginners can quickly learn to use it

✓ **Easy to extend**: Advanced users can use it to develop new methods

✓ **Independent of dynamics engine**: Useful in many fields and to the broadest audience

Core Python library, plus separate command line interface

DWHS, Prinz, Noé, Chodera, Bolhuis. JCTC 2019