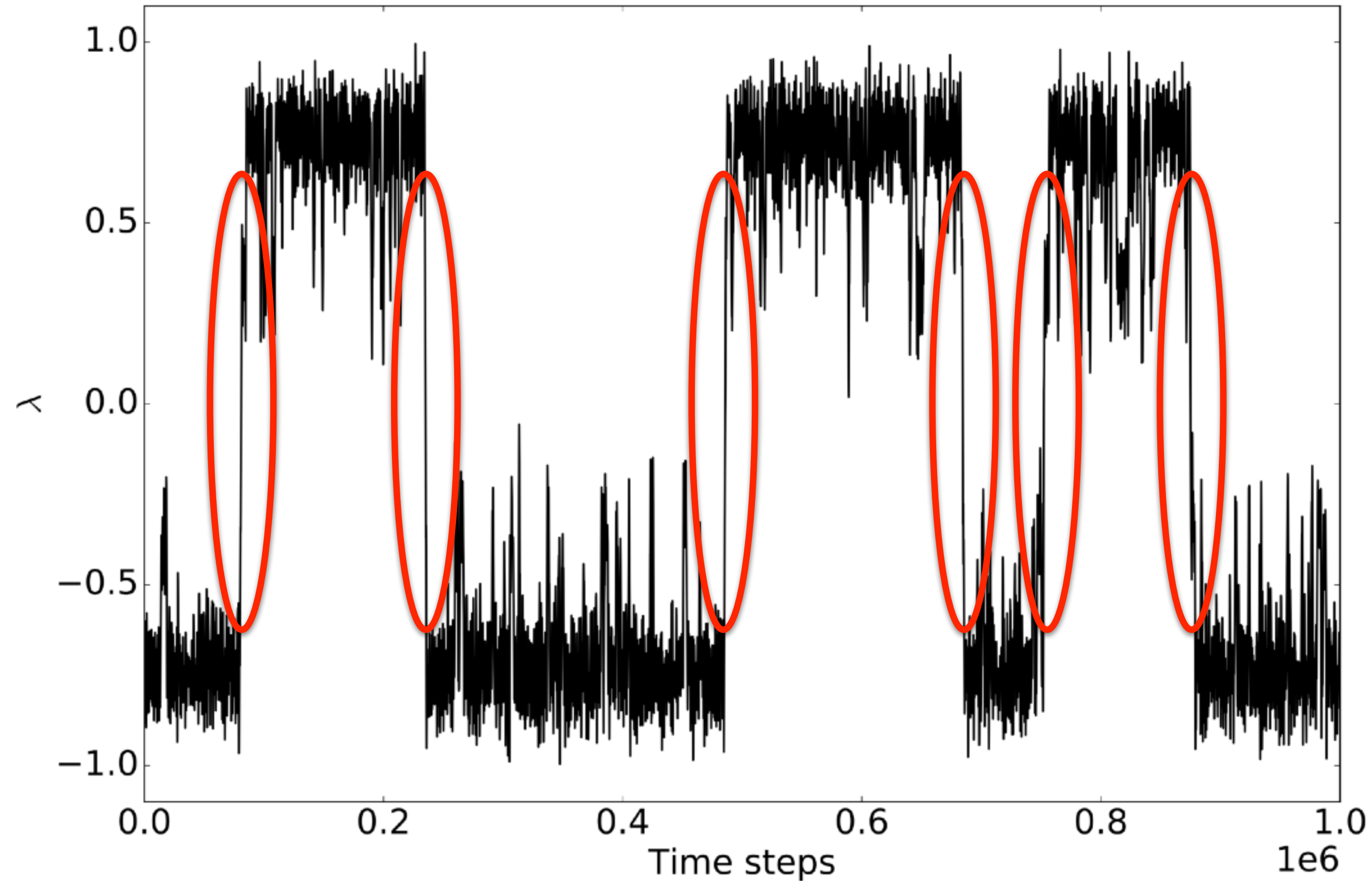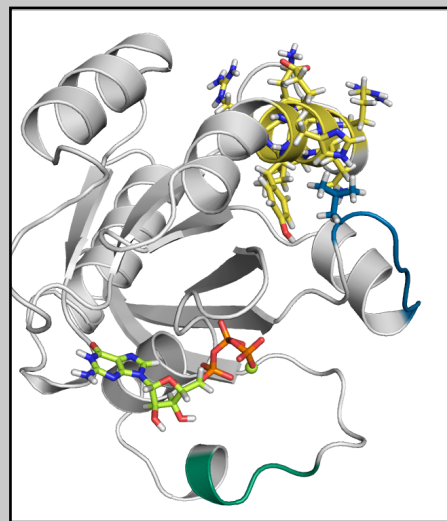# Path sampling

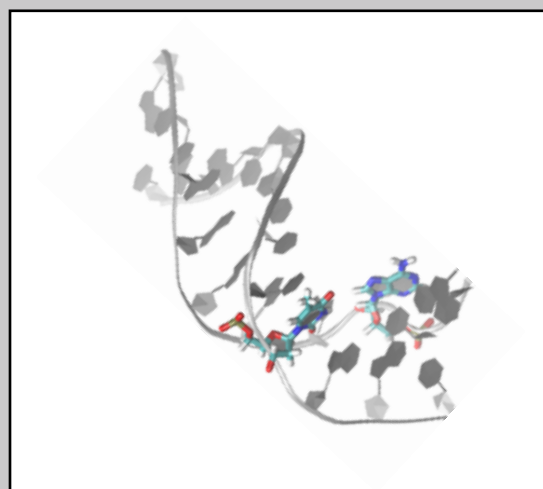Focus on the transition regions

Monte Carlo in path space

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?

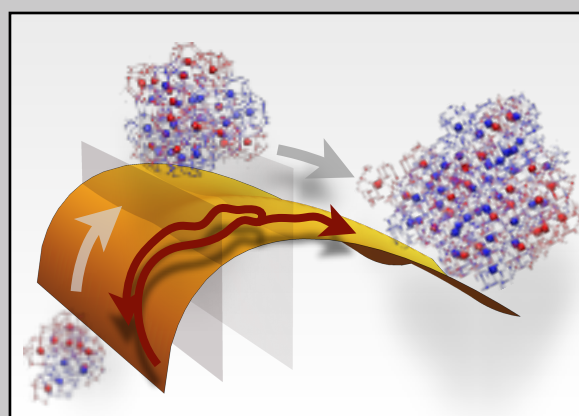Vreede, Perez de Alba Ortíz, Bolhuis, DWHS. Nucl. Acids Res. 2019

Image © Arjun

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

Arjun, Berendsen, Bolhuis. PNAS 2019