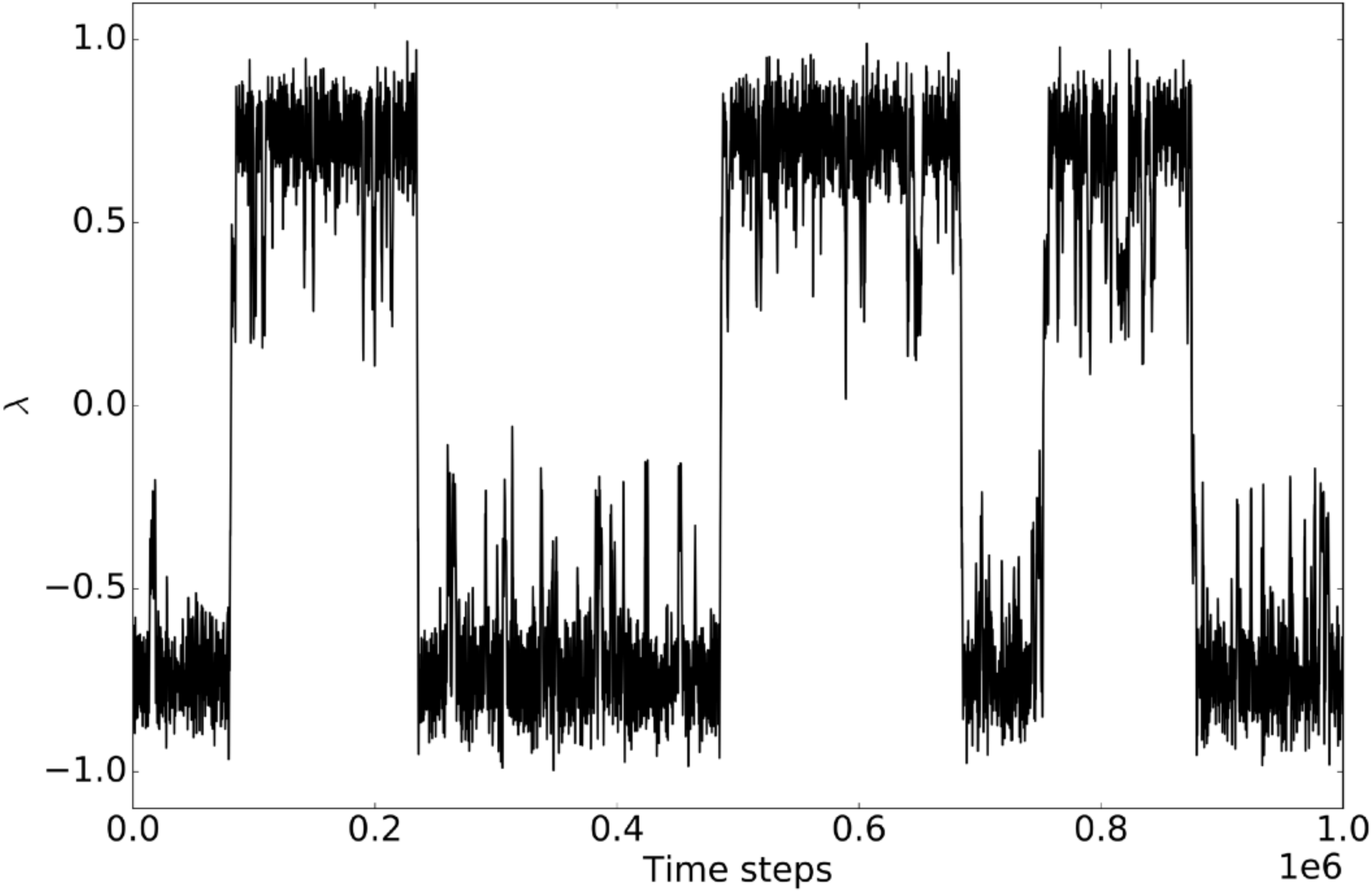
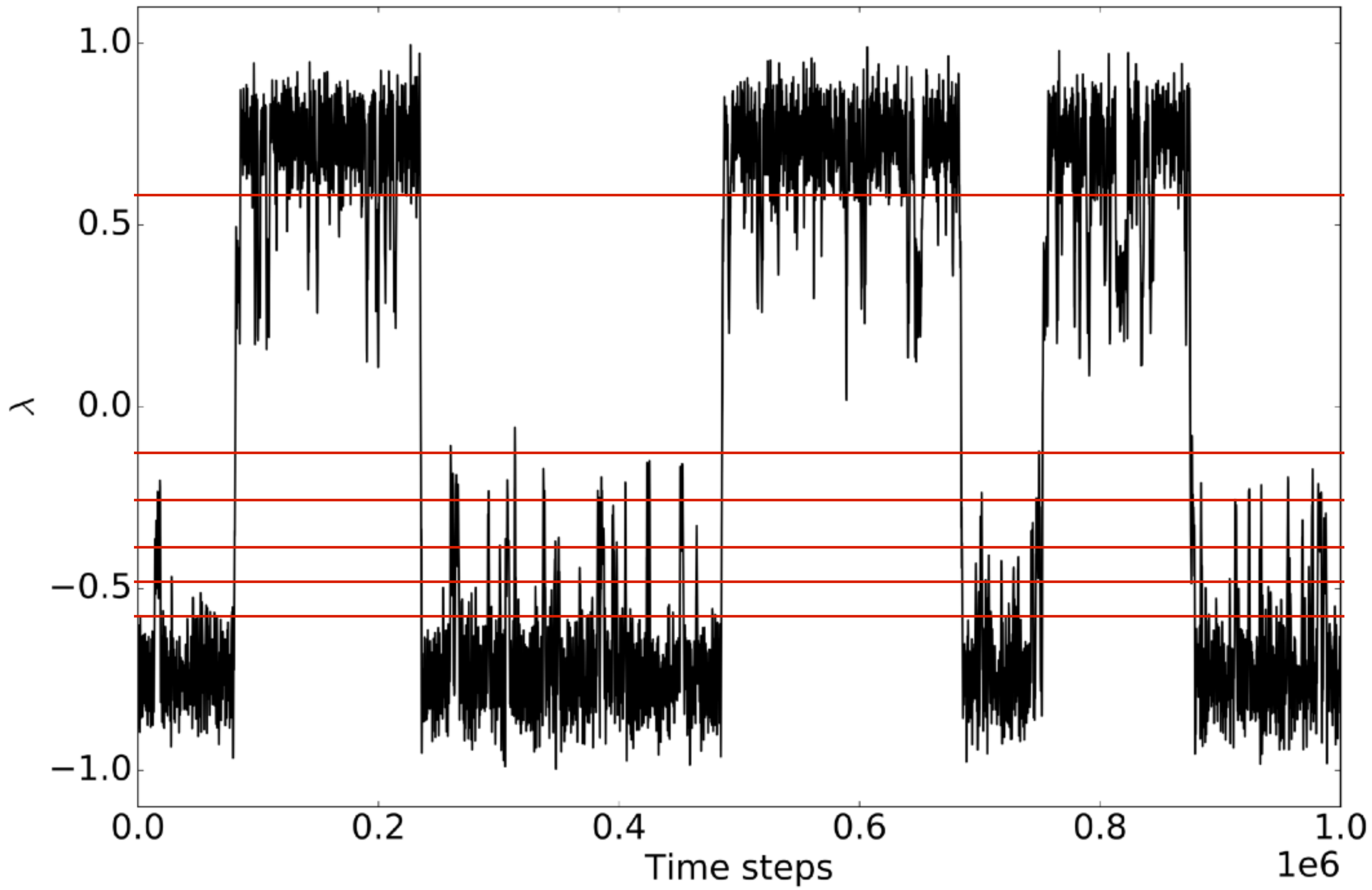

λ
1.0
0.5
0.0
−0.5
−1.0
0.0
0.2
0.4
0.6
0.8
1.0
Time steps
1e6

Calculating the rate with TIS

Successive crossing probabilities: multiply a number ~0.1 a bunch of times to get a very small probability

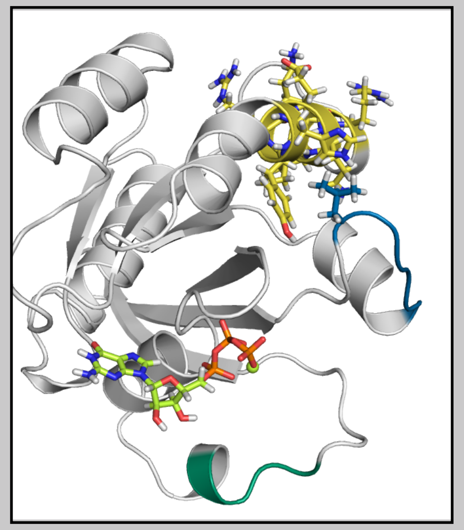
Calculating the rate with TIS



Successive crossing probabilities: multiply a number ~0.1 a bunch of times to get a very small probability

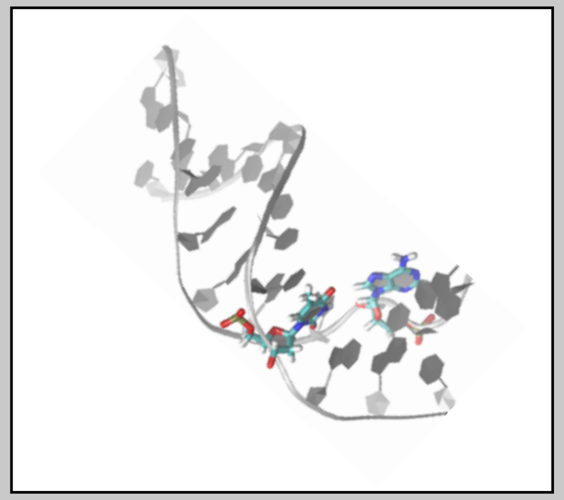
What can we learn?

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

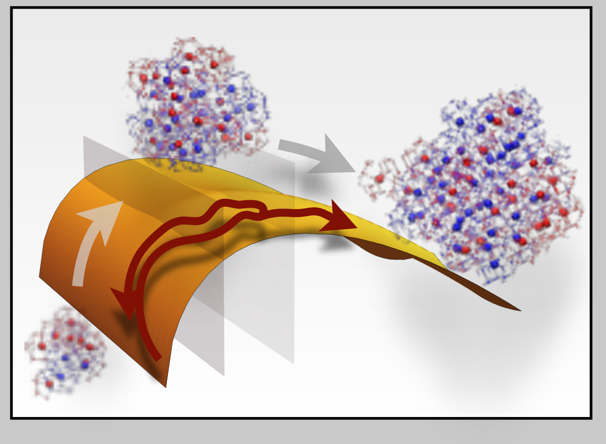


Image © Arjun

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

Arjun, Berendsen, Bolhuis. PNAS 2019