OpenPathSampling:

An open, flexible Python framework for rare event simulations

David W.H. Swenson
Dutch MD Day, 27 February 2015
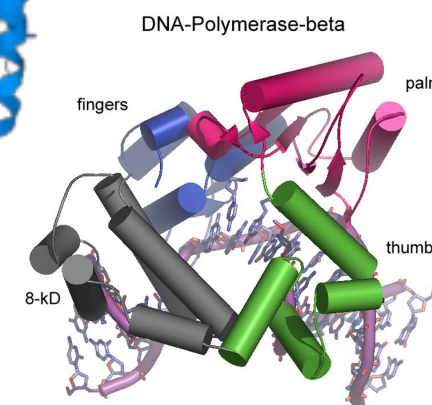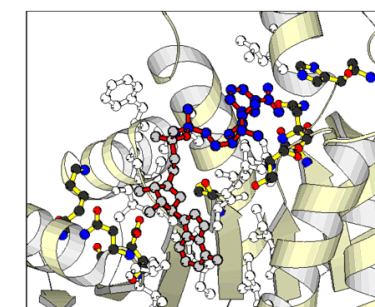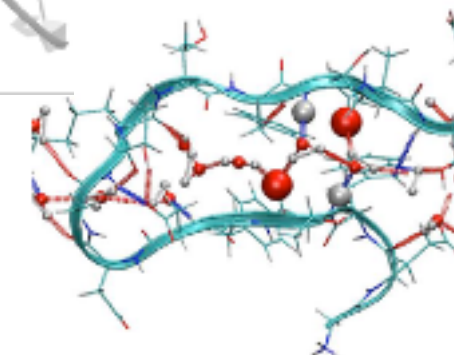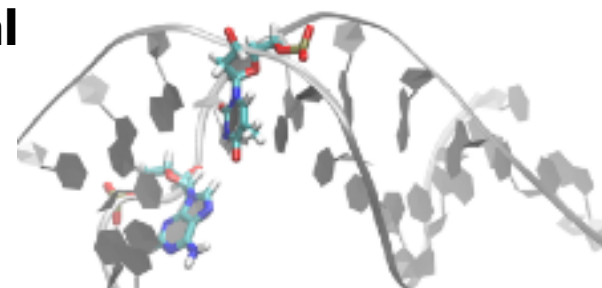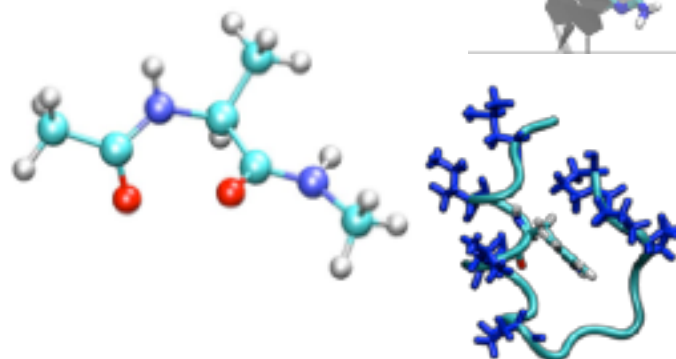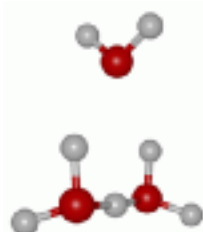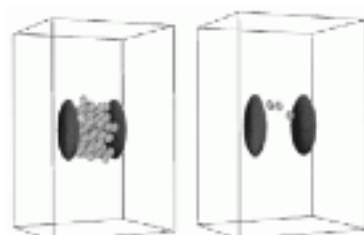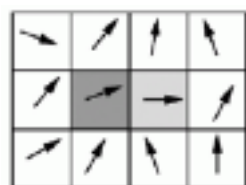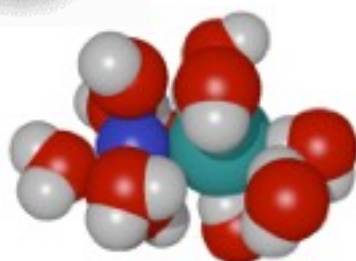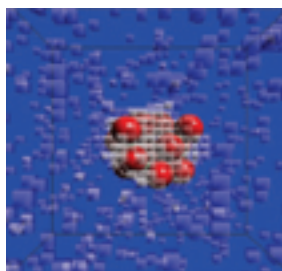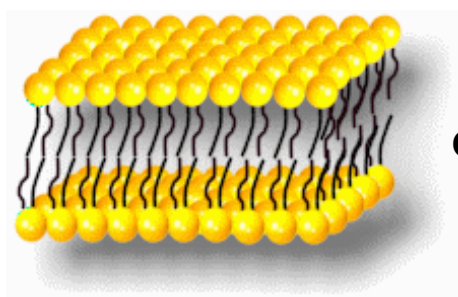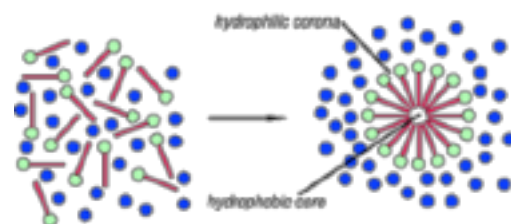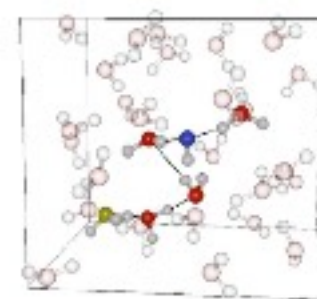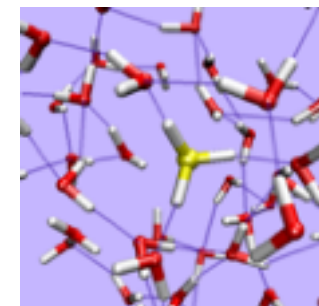
crystallisation

catalysis

reactions

enzyme reactions

complex fluids

RARE EVENTS
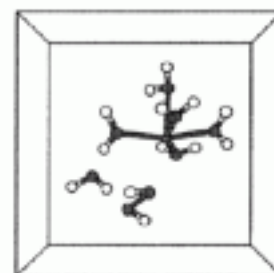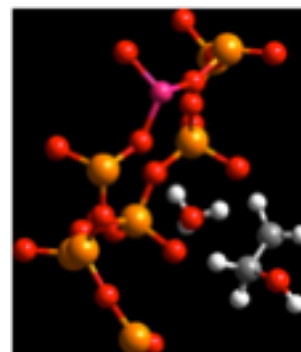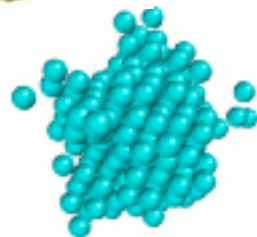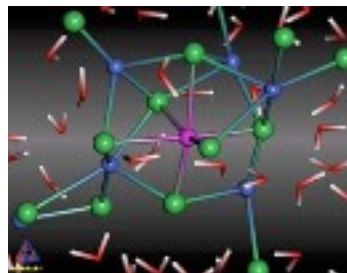
solvent effects

folding & binding

conformational change

DNA-Polymerase-beta

fingers

palm

thumb

8-kD