

Transition path sampling and the calculation of free energies: pnp

Schwartz group

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0.1 Choice of reactive trajectory

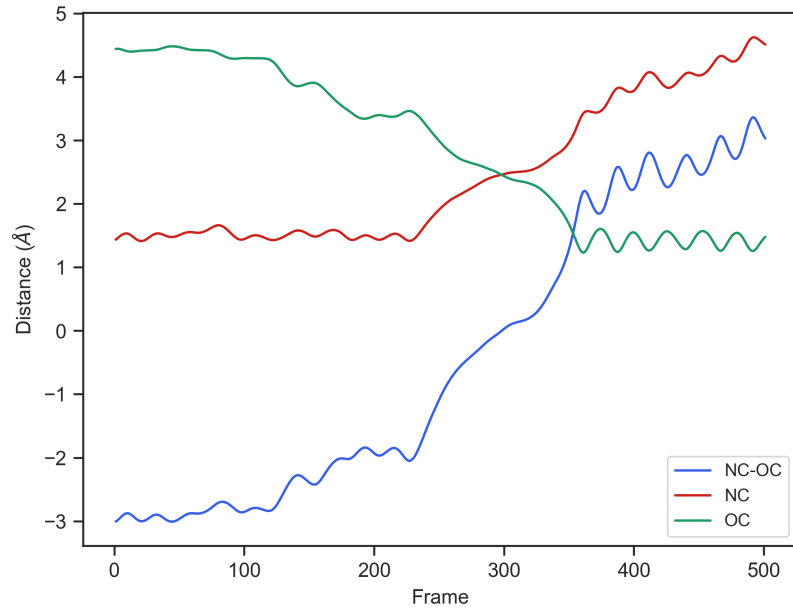


Figure 1: Variation of the order parameters as a function of time for a typical reactive trajectory for the reaction catalyzed by human purine nucleoside phosphorylase

Range	$[-3.04, 3.04]$ Å
Number of windows	30
Window size	0.28 Å
Overlap	0.08 Å

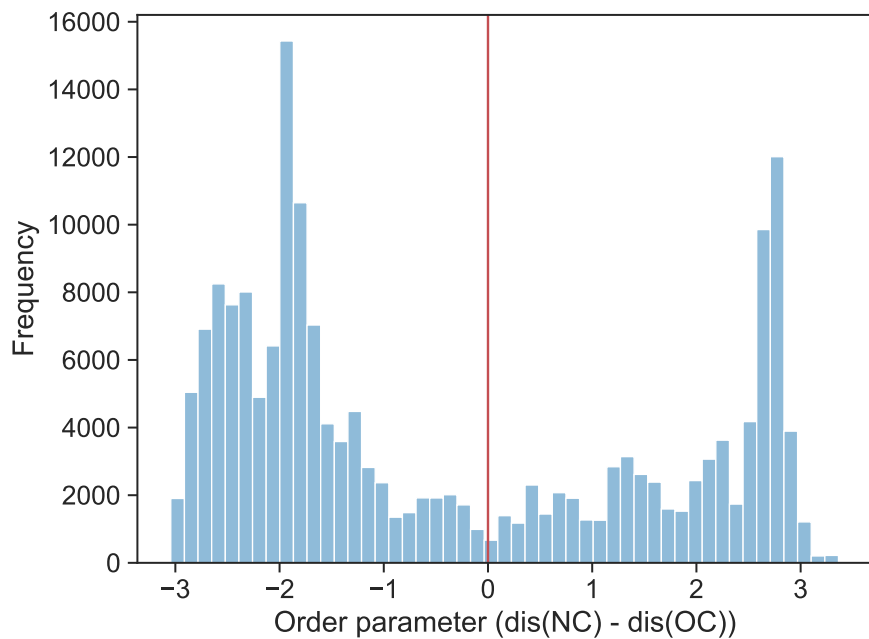


Figure 2: Frequency of the order parameter values observed using short TPS trajectories represented as histograms

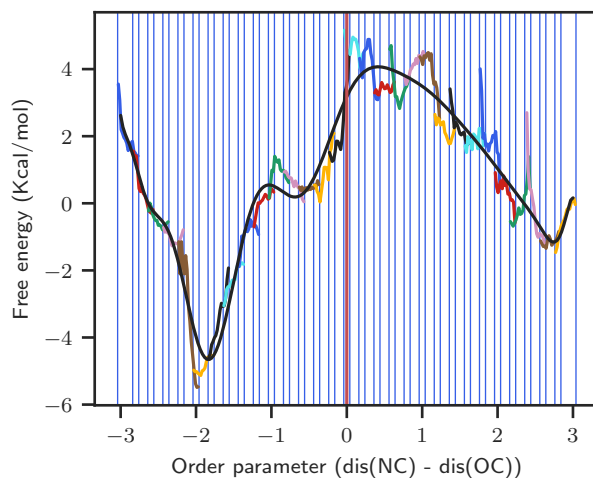


Figure 3: Free energy as a function of the order parameter for the reaction catalyzed by human purine nucleoside phosphorylase