

analysis tool for

BIAS-EXCHANGE METADYNAMICS SIMULATIONS

Settings:

Trajectories:

topology (.gro file) start_gro

Selected Atoms all Representation Licorice

Coloring Name Material Opaque

Load trajs and COLVARS Read trajs every 1 frames

COLVAR XTC trajectory

Number of Trajectories 4 show hide

trajectory 0:	colvar0	traj0.xtc
trajectory 1:	colvar1	traj1.xtc
trajectory 2:	colvar2	traj2.xtc
trajectory 3:	colvar3	traj3.xtc

Hills:

HILLFILE use

Number of HILLS files 4 show hide

hills0	<input checked="" type="checkbox"/>
hills1	<input checked="" type="checkbox"/>
hills2	<input checked="" type="checkbox"/>
hills3	<input checked="" type="checkbox"/>

Cluster analysis:

Equil. time for cluster analysis: 200

min max NG use plot

CV1: -3.141 3.141E10 CV2: -3.141 3.141E10 CV3: -3.141 3.141E10 CV4: -3.141 3.141E10

Number of CVs 4 show

COMPUTE CLUSTERS

show structures of cluster + -

dump structures of cluster on pdb file

Compute free energies

Delta 4

KT 2.4943

Equil. time for VG 200

G_CORR 1

N_MIN 1

RUN WHAM

show profile of HILLFILE

Kinetic basins

Show Diffusion matrix

RUN BASINS

build basins

Number of basins: KT range: