

Bias-Exchange Analyzer

analysis tool for

BIAS-EXCHANGE METADYNAMICS SIMULATIONS

Settings:

Trajectories:

topology (.gro file) Selected Atoms Representation Coloring Name Material Read trajs every frames

COLVAR XTC trajectory

Number of Trajectories

trajectory 0:	<input type="text" value="colvar0"/>	<input type="text" value="traj0.xtc"/>
trajectory 1:	<input type="text" value="colvar1"/>	<input type="text" value="traj1.xtc"/>
trajectory 2:	<input type="text" value="colvar2"/>	<input type="text" value="traj2.xtc"/>
trajectory 3:	<input type="text" value="colvar3"/>	<input type="text" value="traj3.xtc"/>

Hills:

HILLFILE use

Number of HILLS files

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

Cluster analysis:

Equil. time for cluster analysis:

	min	max	NG	use	plot
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CV1: ☒ ☐CV2: ☒ ☐CV3: ☒ ☐CV4: ☒ ☐Number of CVs structures of cluster structures of cluster on pdb file

Compute free energies

Delta KT Equil. time for VG G_CORR N_MIN

Kinetic basins

Number of basins: KT range: