Resource Summary Report

Molecular Simulation Trajectories Archive of a Villin Variant

RRID:SCR_002704
Type: Tool

Proper Citation

Molecular Simulation Trajectories Archive of a Villin Variant (RRID:SCR_002704)

Resource Information

URL: https://simtk.org/home/foldvillin

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Description: An archive of hundreds of all-atom, explicit solvent molecular dynamics simulations that were performed on a set of nine unfolded conformations of a variant of the villin headpiece subdomain (HP-35 NleNle). It includes scripts for accessing the archive of villin trajectories as well as a VMD plug-in for viewing the trajectories. In addition, all starting structures used in the trajectories are also provided. The simulations were generated using a distributed computing method utilizing the symmetric multiprocessing paradigm for individual nodes of the Folding_at_home distributed computing network. The villin trajectories in the archive are divided into two projects: PROJ3036 and PROJ3037. PROJ3036 contains trajectories starting from nine non-folded configurations. PROJ3037 contains trajectories starting from the native (folded) state. Runs 0 through 8 (in PROJ3036) correspond to starting configurations 0 through 8 discussed in the paper in J. Mol. Biol. (2007) 374(3):806-816 (see the publications tab for a full reference), whereas RUN9 uses the same starting configuration as RUN8. Each run contains 100 trajectories (named clone 0-99), each with the same starting configuration but different random velocities. Trajectories vary in their length of time and are subdivided into frames, also known as a generation. Each frame contains around 400 configurational snapshots, or timepoints, of the trajectory, with the last configurational snapshot of frame i corresponding to the first configurational snapshot of generation i+1. The goal is to allow researchers to analyze and benefit from the many trajectories produced through the simulations.

Abbreviations: Molecular Simulation Trajectories Archive of a Villin Variant

Resource Type: data or information resource, d spatial image, data set

Defining Citation: PMID:17950314

Keywords: dynamic, atom, headpiece, molecular, simulation, solvent, protein folding, villin, molecule, trajectory, simulation, molecular dynamics trajectory

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NSF MCB-0317072

Availability: Acknowledgement requested, Available in Gromacs and PDB formats.

Resource Name: Molecular Simulation Trajectories Archive of a Villin Variant

Resource ID: SCR_002704

Alternate IDs: nif-0000-23331

License: MIT License

Record Creation Time: 20220129T080214+0000

Record Last Update: 20250516T053641+0000

Ratings and Alerts

No rating or validation information has been found for Molecular Simulation Trajectories Archive of a Villin Variant.

No alerts have been found for Molecular Simulation Trajectories Archive of a Villin Variant.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We have not found any literature mentions for this resource.