Resource Summary Report

Generated by NIF on May 13, 2025

TraDES

RRID:SCR_006142
Type: Tool

Proper Citation

TraDES (RRID:SCR_006142)

Resource Information

URL: https://sites.google.com/a/blueprint.org/trades/

Proper Citation: TraDES (RRID:SCR_006142)

Description: With Trajectory Directed Ensemble Sampling (TraDES) create large ensembles of high-quality protein structures quickly, ranging from near-native to partially unfolded to intrinsically unfolded. TraDES is a system for directly controlling and sampling protein conformational space. TraDES has been previously used for measuring the vastness of protein conformational space and testing the hypothesis of a brute force solution to the protein folding problem. Over 10 Billion protein structures have been produced by TraDES software in previous distributed computing experiments. The package is comprised of binary executable programs and accessory programs and scripts as well as protein structure data files that map out protein conformational space in a probabilistic way. The main programs are: * trades - generates protein structures following the Trajectory Distribution (see below) * seq2trj - makes Trajectory Distributions from sequences for sampling * str2tr - makes Trajectory Distributions from 3D structures for sampling Trajectory Distributions - Controlling the Sampling of Conformational Space The concept of the trajectory distribution may be new to many protein scientists. A trajectory distribution is simply a map of available conformational space at an amino acid residue. NMR scientists are the primary users of the TraDES package.

Abbreviations: TraDES

Synonyms: Trajectory Directed Ensemble Sampling, TraDES - Trajectory Directed Ensemble Sampling

Resource Type: software resource, software application

Defining Citation: PMID:11746699, PMID:10737933

Keywords: protein, protein structure, structure, trajectory, sequence, protein folding

Funding:

Availability: Open-source

Resource Name: TraDES

Resource ID: SCR_006142

Alternate IDs: nlx_151632

Record Creation Time: 20220129T080234+0000

Record Last Update: 20250513T060757+0000

Ratings and Alerts

No rating or validation information has been found for TraDES.

No alerts have been found for TraDES.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 6 mentions in open access literature.

Listed below are recent publications. The full list is available at NIF.

Ni GS, et al. (2024) Tardigrade Dsup: Interactions with DNA and protection of cells from oxidative stress. bioRxiv : the preprint server for biology.

Jagannathan NS, et al. (2021) Computational modeling suggests binding-induced expansion of Epsin disordered regions upon association with AP2. PLoS computational biology, 17(1), e1008474.

Zhao C, et al. (2014) A cooperative jack model of random coil-to-elongation transition of the FH1 domain by profilin binding explains formin motor behavior in actin polymerization. FEBS letters, 588(14), 2288.

Hotta K, et al. (2014) Biophysical properties of intrinsically disordered p130Cas substrate

domain--implication in mechanosensing. PLoS computational biology, 10(4), e1003532.

Ángyán AF, et al. (2013) Ensemble-based interpretations of NMR structural data to describe protein internal dynamics. Molecules (Basel, Switzerland), 18(9), 10548.

Liu C, et al. (2011) Near-membrane ensemble elongation in the proline-rich LRP6 intracellular domain may explain the mysterious initiation of the Wnt signaling pathway. BMC bioinformatics, 12 Suppl 13(Suppl 13), S13.