Resource Summary Report

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Allopathfinder

RRID:SCR_002702
Type: Tool

Proper Citation

Allopathfinder (RRID:SCR_002702)

Resource Information

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

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Description: Software application and code base that allows users to compute likely allosteric pathways in proteins. The underlying assumption is that residues participating in allosteric communication should be fairly conserved and that communication happens through residues that are close in space. The initial application for the code provided was to study the allosteric communication in myosin. Myosin is a well-studied molecular motor protein that walks along actin filaments to achieve cellular tasks such as movement of cargo proteins. It couples ATP hydrolysis to highly-coordinated conformational changes that result in a power-stroke motion, or "walking" of myosin. Communication between a set of residues must link the three functional regions of myosin and transduce energy: the catalytic ATP binding region, the lever arm, and the actin-binding domain. They are investigating which residues are likely to participate in allosteric communication pathways. The application is a collection of C++/QT code, suitable for reproducing the computational results of the paper. (PMID 17900617) In addition, they provide input and alignment information to reproduce Figure 3 (a key figure) in the paper. Examples provided will show users how to use AlloPathFinder with other protein families, assumed to exhibit an allosteric communication. To run the application a multiple sequence alignment of representative proteins from the protein family is required along with at least one protein structure.

Abbreviations: AlloPathFinder

Synonyms: Predicting allosteric communication in myosin via a conserved residue pathway

Resource Type: software resource, source code, software application

Defining Citation: PMID:17900617

Keywords: allosteric communication, allostery, allosteric, pathway, protein, residue, prediction, myosin, computational model, protein model, structure-based protein classification, protein classification, myosin allosteric communication

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Availability: MIT License

Resource Name: Allopathfinder

Resource ID: SCR_002702

Alternate IDs: nif-0000-23327

Record Creation Time: 20220129T080214+0000

Record Last Update: 20250425T055302+0000

Ratings and Alerts

No rating or validation information has been found for Allopathfinder.

No alerts have been found for Allopathfinder.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We have not found any literature mentions for this resource.