Ion Simulator Interface

RRID:SCR_008267
Type: Tool

Proper Citation

Ion Simulator Interface (RRID:SCR_008267)

Resource Information

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

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Description: A simple Java graphical user interface for running the program ISIM. ISIM is a package that simulates the thermodynamic ensemble of ions around a macromolecule using a grand canonical Monte Carlo scheme and simple hard sphere ion models. It is meant to provide an alternative mechanism to mean field approaches to allow the calculation of ion distributions around a highly charged molecule using a simple model that takes into account ion-ion correlations and steric interactions. The original source was created in the McCammon group at UCSD but is no longer available. The version of ISIM used is available in the ISIM project on simtk.org.

Abbreviations: ISIM

Synonyms: SimTK ISIM, SimTK Ion Simulator Interface

Resource Type: software application, software resource, simulation software

Keywords: grand canonical ensemble, monte carlo, Java, calculation, ion distribution

Funding:

Resource Name: Ion Simulator Interface

Resource ID: SCR_008267

Alternate IDs: nif-0000-23306

Record Creation Time: 20220129T080246+0000

Record Last Update: 20250410T065713+0000

Ratings and Alerts

No rating or validation information has been found for Ion Simulator Interface.

No alerts have been found for Ion Simulator Interface.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We have not found any literature mentions for this resource.