Resource Summary Report

Generated by PRECISE-TBI on Jul 30, 2026

sietraj

RRID:SCR_018021
Type: Tool

Proper Citation

sietraj (RRID:SCR_018021)

Resource Information

URL: https://www2.bri.nrc.ca/ccb/pub/sietraj_main.php

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Description: Software tool for binding free energies from Amber-generated MD trajectories. Alternative to MM-PBSA software provided by AMBER distribution. Virtual alanine mutations are also possible. Solvated interaction energies are calculated using parameters that have been fitted to reproduce binding free energies of data set of 99 protein-ligand complexes.

Resource Type: software application, simulation software, software resource

Keywords: Binding free energy, Amber, MD trajctory, MM-PBSA, virtual alanine mutation, solvated interaction energy, calculation, parameter, protein-ligand complex

Availability: Restricted

Resource Name: sietraj

Resource ID: SCR_018021

Record Creation Time: 20220129T080338+0000

Record Last Update: 20260728T043540+0000

Ratings and Alerts

No rating or validation information has been found for sietraj.

No alerts have been found for sietraj.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 2 mentions in open access literature.

Listed below are recent publications. The full list is available at PRECISE-TBI .

Yan FF, et al. (2021) Comparison of the binding characteristics of SARS-CoV and SARS-CoV-2 RBDs to ACE2 at different temperatures by MD simulations. Briefings in bioinformatics, 22(2), 1122.

Martin ER, et al. (2020) In vivo crystals reveal critical features of the interaction between cystic fibrosis transmembrane conductance regulator (CFTR) and the PDZ2 domain of Na+/H+ exchange cofactor NHERF1. The Journal of biological chemistry, 295(14), 4464.