Resource Summary Report

Generated by NIF on Apr 19, 2025

AMBER parameter database

RRID:SCR_018815
Type: Tool

Proper Citation

AMBER parameter database (RRID:SCR_018815)

Resource Information

URL: http://research.bmh.manchester.ac.uk/bryce/amber

Proper Citation: AMBER parameter database (RRID:SCR_018815)

Description: Assisted model building with energy refinement parameter database. Family of force fields for molecular dynamics of biomolecules. Collection of equations and associated constants designed to reproduce molecular geometry and selected properties of tested structures.

Synonyms: Assisted Model Building with Energy Refinement parameter database

Resource Type: data repository, storage service resource, database, service resource, data or information resource

Keywords: Model building, energy refinement, parameter, force field, molecular dynamics, biomolecule, equation collection, constants collection, molecular geometry reproduction, tested structure property reproduction, computational biophysics, drug design

Funding:

Availability: Free, Freely available

Resource Name: AMBER parameter database

Resource ID: SCR_018815

Record Creation Time: 20220129T080342+0000

Record Last Update: 20250419T055646+0000

Ratings and Alerts

No rating or validation information has been found for AMBER parameter database.

No alerts have been found for AMBER parameter database.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 12 mentions in open access literature.

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

Jiang W, et al. (2023) Repurposing Drugs for Inhibition against ALDH2 via a 2D/3D Ligand-Based Similarity Search and Molecular Simulation. Molecules (Basel, Switzerland), 28(21).

Zhou B, et al. (2022) Virtual Screening of FDA-Approved Drugs for Enhanced Binding with Mitochondrial Aldehyde Dehydrogenase. Molecules (Basel, Switzerland), 27(24).

Gomila AMJ, et al. (2022) Phosphorylation disrupts long-distance electron transport in cytochrome c. Nature communications, 13(1), 7100.

Wang J, et al. (2021) Boosted activity by engineering the enzyme microenvironment in cascade reaction: A molecular understanding. Synthetic and systems biotechnology, 6(3), 163.

Lin Y, et al. (2021) Structure of an inactive conformation of GTP-bound RhoA GTPase. Structure (London, England : 1993), 29(6), 553.

Zhan J, et al. (2021) Definition of the immune evasion-replication interface of rabies virus P protein. PLoS pathogens, 17(7), e1009729.

Gheyouche E, et al. (2021) Structural Design and Analysis of the RHOA-ARHGEF1 Binding Mode: Challenges and Applications for Protein-Protein Interface Prediction. Frontiers in molecular biosciences, 8, 643728.

Calzadiaz-Ramirez L, et al. (2020) In Vivo Selection for Formate Dehydrogenases with High Efficiency and Specificity toward NADP. ACS catalysis, 10(14), 7512.

Cui G, et al. (2020) Design, synthesis and biological evaluation of indole-2-carboxylic acid derivatives as IDO1/TDO dual inhibitors. European journal of medicinal chemistry, 188, 111985.

Jepsen L, et al. (2020) Effects of Nucleotide and End-Dependent Actin Conformations on

Polymerization. Biophysical journal, 119(9), 1800.

Arrington ME, et al. (2020) The molecular basis for immune dysregulation by the hyperactivated E62K mutant of the GTPase RAC2. The Journal of biological chemistry, 295(34), 12130.

Campagne S, et al. (2019) Structural basis of a small molecule targeting RNA for a specific splicing correction. Nature chemical biology, 15(12), 1191.