

# Resource Summary Report

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## 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 or information resource, data repository, database, service resource, storage service 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

**Availability:** Free, Freely available

**Resource Name:** AMBER parameter database

**Resource ID:** SCR\_018815

**Record Creation Time:** 20220129T080342+0000

**Record Last Update:** 20260919T195359+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 17 mentions in open access literature.

**Listed below are recent publications.** The full list is available at [nidm-terms](#) .

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).

Cui G, et al. (2023) Evolutional insights into the interaction between Rab7 and RILP in lysosome motility. *iScience*, 26(7), 107040.

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

Pallara C, et al. (2022) Peptidomimetics designed to bind to RAS effector domain are promising cancer therapeutic compounds. *Scientific reports*, 12(1), 15810.

Tian M, et al. (2022) Application of per-Residue Energy Decomposition to Design Peptide Inhibitors of PSD95 GK Domain. *Frontiers in molecular biosciences*, 9, 848353.

Zhang Y, et al. (2022) Computational Investigation of Structural Basis for Enhanced Binding of Isoflavone Analogues with Mitochondrial Aldehyde Dehydrogenase. *ACS omega*, 7(9), 8115.

Tu G, et al. (2022) In Silico Study of the Acquired Resistance Caused by the Secondary Mutations of KRAS G12C Protein Using Long Time Molecular Dynamics Simulation and Markov State Model Analysis. *International journal of molecular sciences*, 23(22).

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

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.

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.

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

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.