Resource Summary Report

Generated by dkNET on May 19, 2025

Assisted Model Building with Energy Refinement (AMBER)

RRID:SCR_014230
Type: Tool

Proper Citation

Assisted Model Building with Energy Refinement (AMBER) (RRID:SCR_014230)

Resource Information

URL: http://ambermd.org/

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Description: Software package of molecular simulation programs. It is distributed into AmberTools15 and Amber14. AmberTools15 is a software package which can carry out complete molecular dynamics simulations with either explicit water or generalized Born solvent models. It is distributed in source code format and must be compiled in order to be used. Amber14 builds on AmberTools15 by adding the pmemd program, which provides better performance on multiple CPUs and dramatic speed improvements on GPUs compared to sander (molecular dynamics). GPU info, manuals, and tutorials are available on the website.

Abbreviations: AMBER

Synonyms: Assisted Model Building with Energy Refinement

Resource Type: software resource, software application, standalone software, simulation software

Keywords: molecular simulation, simulation software, software package, molecular dynamics, pmemed, sander, bio.tools

Funding:

Availability: Acknowledgement requested

Resource Name: Assisted Model Building with Energy Refinement (AMBER)

Resource ID: SCR_014230

Alternate IDs: biotools:amber

Alternate URLs: https://bio.tools/amber

License: Licenses vary depending on the type of user purchasing the AMBER license

Record Creation Time: 20220129T080319+0000

Record Last Update: 20250517T060127+0000

Ratings and Alerts

No rating or validation information has been found for Assisted Model Building with Energy Refinement (AMBER).

No alerts have been found for Assisted Model Building with Energy Refinement (AMBER).

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 3982 mentions in open access literature.

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

Jaumotte JD, et al. (2025) Physiologic and structural characterization of desisobutyryl-ciclesonide, a selective glucocorticoid receptor modulator in newborn rats. PNAS nexus, 4(1), pgae573.

Ned?lníková A, et al. (2025) Atomistic Insights Into Interaction of Doxorubicin With DNA: From Duplex to Nucleosome. Journal of computational chemistry, 46(3), e70035.

Basmenj ER, et al. (2025) Computational epitope-based vaccine design with bioinformatics approach; a review. Heliyon, 11(1), e41714.

Benslama O, et al. (2025) Silymarin as a Therapeutic Agent for Hepatocellular Carcinoma: A Multi-Approach Computational Study. Metabolites, 15(1).

Nguyen A, et al. (2025) Structural and functional characterization of integrin ?5-targeting antibodies for anti-angiogenic therapy. bioRxiv : the preprint server for biology.

Jane?ek M, et al. (2025) Computer Folding of Parallel DNA G-Quadruplex: Hitchhiker's Guide to the Conformational Space. Journal of computational chemistry, 46(1), e27535.

Choutka J, et al. (2025) End-Point Affinity Estimation of Galectin Ligands by Classical and Semiempirical Quantum Mechanical Potentials. Journal of chemical information and modeling, 65(2), 762.

Xie S, et al. (2025) Molecular basis of the CYFIP2 and NCKAP1 autism-linked variants in the WAVE regulatory complex. Protein science : a publication of the Protein Society, 34(1), e5238.

Aponte-Diaz D, et al. (2025) Non-lytic spread of poliovirus requires the nonstructural protein 3CD. mBio, 16(1), e0327624.

Sasa N, et al. (2025) Intratumor heterogeneity of HPV integration in HPV-associated head and neck cancer. Nature communications, 16(1), 1052.

Rivas-Gastélum MF, et al. (2025) Lyophilized and Oven-Dried Manilkara zapota Extracts: Characterization and In Vitro, In Vivo, and In Silico Analyses. Plants (Basel, Switzerland), 14(2).

Wang X, et al. (2025) BioStructNet: Structure-Based Network with Transfer Learning for Predicting Biocatalyst Functions. Journal of chemical theory and computation, 21(1), 474.

Singh S, et al. (2025) Molecular mechanisms underlying allosteric behavior of Escherichia coli DgoR, a GntR/FadR family transcriptional regulator. Nucleic acids research, 53(1).

Bhati AP, et al. (2025) Equilibrium and Nonequilibrium Ensemble Methods for Accurate, Precise and Reproducible Absolute Binding Free Energy Calculations. Journal of chemical theory and computation, 21(1), 440.

Wang J, et al. (2025) Semi-rational design of an aromatic dioxygenase by substrate tunnel redirection. iScience, 28(1), 111570.

Rekhtman N, et al. (2025) Chromothripsis-Mediated Small Cell Lung Carcinoma. Cancer discovery, 15(1), 83.

Zgarbová M, et al. (2025) Refinement of the Sugar Puckering Torsion Potential in the AMBER DNA Force Field. Journal of chemical theory and computation, 21(2), 833.

Kumosani TA, et al. (2025) Investigating Pb2 CAP-binding domain inhibitors from marine bacteria for targeting the influenza A H5N1. PloS one, 20(1), e0310836.

Zhang H, et al. (2025) Machine learning and genetic algorithm-guided directed evolution for the development of antimicrobial peptides. Journal of advanced research, 68, 415.

Naveed M, et al. (2025) Scrutinizing the evidence of anthracene toxicity on adrenergic receptor beta-2 and its bioremediation by fungal manganese peroxidase via in silico approaches. Scientific reports, 15(1), 3795.