

Resource Summary Report

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AmberTools

RRID:SCR_018497

Type: Tool

Proper Citation

AmberTools (RRID:SCR_018497)

Resource Information

URL: <https://ambermd.org/AmberTools.php>

Proper Citation: AmberTools (RRID:SCR_018497)

Description: Software suite that works by themselves, and with Amber20 itself. Can be used to carry out complete molecular dynamics simulations, with either explicit water or generalized Born solvent models.

Synonyms: Amber, AmberTools20, AmberTools MD software packages

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

Defining Citation: [DOI:10.1002/wcms.1121](https://doi.org/10.1002/wcms.1121)

Keywords: Molecular dynamics simulation, water, Born solvent model, molecular dynamics, molecular modeling

Resource Name: AmberTools

Resource ID: SCR_018497

License: GNU GPL

Record Creation Time: 20220129T080340+0000

Record Last Update: 20260905T132837+0000

Ratings and Alerts

No rating or validation information has been found for AmberTools.

No alerts have been found for AmberTools.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 728 mentions in open access literature.

Listed below are recent publications. The full list is available at [dkNET](#) .

Ding XW, et al. (2027) Evolution of alcohol oxidase for improved methanol bioconversion and formaldehyde tolerance. *Synthetic and systems biotechnology*, 15, 22.

Nitsch S, et al. (2026) H4K16 acylations destabilize chromatin architecture and facilitate transcriptional response during metabolic perturbations. *Molecular cell*, 86(1), 24.

Xiong X, et al. (2026) Structure-Guided Engineering of a Promiscuous O-Methyltransferase for a SAM Regeneration Biocatalysis Platform of Methylated Pharmaceuticals. *Advanced science (Weinheim, Baden-Wurttemberg, Germany)*, 13(13), e17794.

Lin C, et al. (2026) An innovative strategy coupling cluster fraction with ultrafiltration UPLC-QTOF-MS/MS for screening α -glucosidase inhibitors from barley seedlings. *Food chemistry: X*, 34, 103685.

Li R, et al. (2026) Multi-omics and network pharmacology identify IGFBP1 as an m6A-Epigenetic target of pueraria in NSCLC therapy. *PLoS computational biology*, 22(3), e1014050.

Song J, et al. (2026) Structural Elucidation and Engineering of the (S)-scoulerine 2-O-Methyltransferase Enabling Regioselective Epiberberine Biosynthesis in *Coptis chinensis*. *Plant biotechnology journal*, 24(7), 4528.

Fan Z, et al. (2026) Glutamine Synthetase 1 Functions in Spermatogenesis in the Silkworm, *Bombyx mori*. *Insects*, 17(2).

Azeez KRA, et al. (2026) Discovery and Development of a Potent LIMK2 Isoform-Specific Degradar. *ACS chemical biology*, 21(5), 1158.

Wang R, et al. (2026) Mg²⁺ Catalyzes Nonenzymatic RNA Primer Extension through a Concerted Outer-Sphere Mechanism. *Journal of the American Chemical Society*, 148(23), 24379.

Zhang J, et al. (2026) In-silico identification and optimization of MMP-9 inhibitors for cerebral ischemia using structure based virtual screening, MD simulation, and binding free energy calculations. *PloS one*, 21(5), e0346627.

Niu T, et al. (2026) Development and Test of Highly Accurate End Point Free Energy Methods. 4. Expanding Solvents Capability and logBB Prediction. *The journal of physical chemistry. B*, 130(19), 4994.

Widerek K, et al. (2026) The pivotal role of γ -lactone stereochemistry in the development of SARS-CoV-2 Mpro inhibitors. *Protein science : a publication of the Protein Society*, 35(7), e70680.

DePaolo-Boisvert JA, et al. (2026) Molecular Dynamics Analysis of Inhibitor Binding Interactions in the *Vibrio cholerae* Respiratory Complex NQR. *Proteins*, 94(2), 649.

Dai W, et al. (2026) Engineered Coiled-Coils Convert Cholera Toxin B-Pentamers into Programmable Membrane Fusogens. *ACS nano*, 20(20), 14645.

Acconcia C, et al. (2026) Structural and Dynamics Insights into Melatonin Binding to MT1 Receptor. *Chembiochem : a European journal of chemical biology*, 27(10), e70376.

Deyawe Kongmeneck A, et al. (2026) Allosteric Mechanisms Underlying Long QT Syndrome Type 2 (LQT2)-Associated Mutations in hERG Channels. *bioRxiv : the preprint server for biology*.

Yusuf A, et al. (2026) Design, synthesis, and experimental evaluation of rupestonic acid derivatives as novel anti-tumor agents guided by network pharmacology and molecular docking. *Scientific reports*, 16(1).

Martino G, et al. (2026) Controlled dynamic remodeling of the spliceosome active site enables the first step of splicing. *Proceedings of the National Academy of Sciences of the United States of America*, 123(1), e2522293123.

Li X, et al. (2026) Dynamic adaptive coassembled sericin protein orchestrating stem cell development for nucleus pulposus regeneration. *Science advances*, 12(1), eadx2768.

AlHussaini KI, et al. (2026) Capsaicin Inhibits Biofilm and Its Related Functions in *Helicobacter pylori*. *Microorganisms*, 14(6).