

Resource Summary Report

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NAMD

RRID:SCR_014894

Type: Tool

Proper Citation

NAMD (RRID:SCR_014894)

Resource Information

URL: <http://www.ks.uiuc.edu/Research/namd/>

Proper Citation: NAMD (RRID:SCR_014894)

Description: Parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. NAMD uses the popular molecular graphics program VMD for simulation setup and trajectory analysis, but is also file-compatible with AMBER, CHARMM, and X-PLOR.

Resource Type: source code, software application, software resource, simulation software

Defining Citation: [PMID:16222654](#)

Keywords: simulation, molecules, biomolecular systems, visualization

Availability: Open source

Resource Name: NAMD

Resource ID: SCR_014894

Record Creation Time: 20220129T080322+0000

Record Last Update: 20260801T191210+0000

Ratings and Alerts

No rating or validation information has been found for NAMD.

No alerts have been found for NAMD.

Data and Source Information

Usage and Citation Metrics

We found 2632 mentions in open access literature.

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

de Araujo Neto MF, et al. (2026) Development of a Novel Aedes aegypti Repellent: An Integrated Approach Combining In Silico and Bioassays. Chemistry & biodiversity, 23(1), e01251.

Xu L, et al. (2026) The structural heterogeneity of AKT autoinhibition. Protein science : a publication of the Protein Society, 35(1), e70420.

Santos D, et al. (2025) The molecular mechanisms of visual chromophore release from cellular retinaldehyde-binding protein. Structure (London, England : 1993), 33(8), 1436.

Roze LV, et al. (2025) Increasing thermostability of the key photorespiratory enzyme glycerate 3-kinase by structure-based recombination. Plant biotechnology journal, 23(2), 454.

Mlýnský V, et al. (2025) Can We Ever Develop an Ideal RNA Force Field? Lessons Learned from Simulations of the UUCG RNA Tetraloop and Other Systems. Journal of chemical theory and computation, 21(8), 4183.

Saha P, et al. (2025) Exploring force-driven stochastic folding dynamics in mechano-responsive proteins and implications in phenotypic variation. Nature communications, 16(1), 1018.

Bararia A, et al. (2025) Identification of KCNJ5 gene an adverse prognosis associated novel onco-ionchannel in Indian pancreatic cancer cohort. Discover oncology, 16(1), 236.

Han Y, et al. (2025) Molecular simulations reveal intricate coupling between agonist-bound β -adrenergic receptors and G protein. iScience, 28(2), 111741.

Castellote-Borrell M, et al. (2025) Lymph-Node Inspired Hydrogels Enhance CAR Expression and Proliferation of CAR T Cells. ACS applied materials & interfaces, 17(11), 16548.

Juarez-Contreras I, et al. (2025) Structural dissection of ergosterol metabolism reveals a pathway optimized for membrane phase separation. Science advances, 11(17), eadu7190.

Cetin E, et al. (2025) A Thermodynamic Cycle to Predict the Competitive Inhibition Outcomes of an Evolving Enzyme. Journal of chemical theory and computation, 21(9), 4910.

Xu Y, et al. (2025) TCMD: A High-Throughput and Rapid Method for Screening Antimicrobial Ingredients from Renewable Bio-Based Resources. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 12(27), e2502156.

Liu Z, et al. (2025) Uridine, a Therapeutic Nucleoside, Exacerbates Alcoholic Liver Disease via SRC Kinase Activation: A Network Toxicology and Molecular Dynamics Perspective. *International journal of molecular sciences*, 26(12).

Romero AM, et al. (2025) Mechanisms of Ion Permeation in the AMPA Receptor Ion Channel. *bioRxiv : the preprint server for biology*.

Lee H, et al. (2025) TMC1 and TMC2 are cholesterol-dependent scramblases that regulate membrane homeostasis in auditory hair cells. *bioRxiv : the preprint server for biology*.

Ishikawa-Fukuda M, et al. (2025) The Na⁺-pumping mechanism driven by redox reactions in the NADH-quinone oxidoreductase from *Vibrio cholerae* relies on dynamic conformational changes. *bioRxiv : the preprint server for biology*.

Benjamin PL, et al. (2025) Magnetosensitivity of Model Flavin-Tryptophan Radical Pairs in a Dynamic Protein Environment. *The journal of physical chemistry. B*, 129(24), 5937.

Corliss L, et al. (2025) Subcellular determinants of orthoflavivirus protease activity. *The Journal of biological chemistry*, 301(8), 110451.

Ferreira PS, et al. (2025) Influence of Cholesterol on the Insertion and Interaction of SARS-CoV-2 Proteins with Lipid Membranes. *ACS applied bio materials*, 8(6), 5380.

Lestari B, et al. (2025) Discovery of pyroptosis-inducing natural products in neuroblastomas: computational studies with experimental validation. *BMC complementary medicine and therapies*, 25(1), 279.