

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/>

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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: 20260801T042743+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 [kravitz2](#) .

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

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.

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

Montenegro I, et al. (2025) Anticandidal activity of Clinopodium chilense essential oil. Frontiers in pharmacology, 16, 1634250.

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.

Wang Y, et al. (2025) Living plastics from plasticizer-assisted thermal molding of silk protein. Nature communications, 16(1), 52.

Ashcroft FJ, et al. (2025) Next generation thiazolyl ketone inhibitors of cytosolic phospholipase A2 ? for targeted cancer therapy. Nature communications, 16(1), 164.

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.

AsthaGiri DN, et al. (2025) Consequences of the failure of equipartition for the p-V behavior of liquid water and the hydration free energy components of a small protein. Chemical science, 16(17), 7503.

Han Y, et al. (2025) Molecular simulations reveal intricate coupling between agonist-bound ?-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.

Karimullina E, et al. (2025) Structural architecture of TolQ-TolR inner membrane protein complex from opportunistic pathogen *Acinetobacter baumannii*. *Science advances*, 11(14), eadq9845.

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).

Tüting C, et al. (2025) Conserved hydrophilic checkpoints tune FocA-mediated formate:H⁺ symport. *Nature communications*, 16(1), 9476.

Hernández-Torres L, et al. (2025) HERPUD1 mediates palmitic acid-induced UPR sustaining TNBC aggressiveness and is destabilized by CK2 pharmacological inhibition. *Cell death & disease*, 16(1), 793.

Raza S, et al. (2025) Molecular Modeling and Molecular Dynamics Simulation of a Packed and Intact Bacterial Microcompartment. *The journal of physical chemistry. B*, 129(50), 12811.

Gargano S, et al. (2025) Comparison among Amber-ff14SB, Amber-ff19SB, and CHARMM36 Force Fields for Ionic and Electroosmotic Flows in Biological Nanopores. *Journal of chemical theory and computation*, 21(22), 11772.

Kuang Z, et al. (2025) Identifying resonant frequencies of viruses for microwave-based detection and inactivation of pathogenic viruses. *Scientific reports*, 15(1), 43920.

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