Resource Summary Report

Generated by dkNET on Sep 8, 2026

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

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: 20260905T133400+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

Source: SciCrunch Registry

Usage and Citation Metrics

We found 2754 mentions in open access literature.

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

Bhattacharya S, et al. (2026) Development of a highly active engineered PETase enzyme for polyester degradation. The FEBS journal, 293(2), 443.

Ralph D, et al. (2026) Molecular Interactions of Fluoroquinolone Antibiotics with Lipid Membranes. Langmuir : the ACS journal of surfaces and colloids, 42(6), 4386.

Rossi Sebastiano M, et al. (2026) MK4 Repositioning for IAHSP: Overcoming In Vivo Data Gaps through In Silico Refinement and In Vitro Validation. ACS chemical neuroscience, 17(6), 1115.

Ajmera P, et al. (2026) Molecular Mechanism of Mitochondrial Complex I Disruption by m.14484T>C Underlying Leber Hereditary Optic Neuropathy. bioRxiv : the preprint server for biology.

Roth R, et al. (2026) PUFA modulation of ASIC3 involves both specific and lipid solvent-like interactions. bioRxiv : the preprint server for biology.

Wiley B, et al. (2026) Atomistic Insights into Anomeric and Stereochemical Effects on Glucose Transport by GLUTs. Journal of the American Chemical Society, 148(5), 5189.

Biswas KH, et al. (2026) E50A Mutation Increases the Bioluminescence Activity of picALuc. Biosensors, 16(3).

Peña-Vilches N, et al. (2026) Identification of 14-3-3 Proteins as Binding Partners of TRP Channels. Journal of chemical information and modeling, 66(7), 3987.

Brownd M, et al. (2026) An Investigation of the Conformational Dynamics of ABC Exporter PCAT1 using Microsecond-Level MD Simulations. bioRxiv : the preprint server for biology.

Ricaña CL, et al. (2026) Lenacapavir prevents production of infectious HIV-1 by abrogating immature virus assembly. bioRxiv : the preprint server for biology.

de Oliveira Filho JA, et al. (2026) Virtual screening of compounds for the development of thyroid hormone analogues for potential application in cardiac regeneration. Journal of computer-aided molecular design, 40(1).

Pan L, et al. (2026) Dual ubiquitin signalling by SLOMO controls AUX1 activity and turnover during root gravitropism. The EMBO journal, 45(8), 2739.

Zdorevskyi O, et al. (2026) Catalytic relevance of a quinol anion in biological energy conversion by respiratory complex I. Chemical science, 17(13), 6688.

Callahan TJ, et al. (2026) Interpretable machine learning uncovers structural determinants of Wnt-Wntless binding specificity from atomistic simulations. Communications chemistry, 9(1).

Penfield J, et al. (2026) Molecular Behavior of Human ? Defensin Type 3 Embedded in Different Model Lipid Membranes. Journal of chemical information and modeling, 66(9), 5357.

Haspel N, et al. (2026) How Functional Variants Reconfigure the Rac2 Conformational Landscape. bioRxiv : the preprint server for biology.

Trujillo-González F, et al. (2026) RNase A is inhibited by the cysteine-rich protein thionein but not by the metal-containing form metallothionein. Molecular and cellular biochemistry, 481(5), 1989.

Pang YT, et al. (2026) DeepPath: overcoming data scarcity for protein transition pathway prediction using physics-based deep learning. Chemical science, 17(24), 12055.

Tellería F, et al. (2026) PSG6: A mitochondrially-targeted gentisic acid derivative exerts antiplatelet action via mitochondrial complex I inhibition. Redox biology, 94, 104200.

Wang S, et al. (2026) Identifying potential binding sites for complex formation between Tyrosyl-DNA phosphodiesterase 1 and poly [ADP-ribose] polymerase 1. Physical chemistry chemical physics : PCCP, 28(23), 14017.