Resource Summary Report

Generated by NIF on May 8, 2025

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, simulation software, software resource

Defining Citation: PMID:16222654

Keywords: simulation, molecules, biomolecular systems, visualization

Funding:

Availability: Open source

Resource Name: NAMD

Resource ID: SCR_014894

Record Creation Time: 20220129T080322+0000

Record Last Update: 20250508T065557+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 2446 mentions in open access literature.

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

Finke F, et al. (2025) Different receptor models show differences in ligand binding strength and location: a computational drug screening for the tick-borne encephalitis virus. Molecular diversity, 29(1), 281.

Visitsatthawong S, et al. (2025) Mechanistic insights into allosteric regulation of the reductase component of p-hydroxyphenylacetate 3-hydroxylase by p-hydroxyphenylacetate: a model for effector-controlled activity of redox enzymes. RSC chemical biology, 6(1), 81.

Su L, et al. (2025) Inhibition of HMGA2 binding to AT-rich DNA by its negatively charged C-terminus. Nucleic acids research, 53(3).

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.

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.

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

Sesti V, et al. (2025) Membrane-targeted push-pull azobenzenes for the optical modulation of membrane potential. Light, science & applications, 14(1), 8.

Hernández ÁP, et al. (2025) Insights into podophyllotoxin lactone features: New cyclolignans as potential dual tubulin-topoisomerase II inhibitors. Archiv der Pharmazie, 358(1),

e2400600.

Ryan B, et al. (2025) Hospital to community in Wales: What is the value of optometrists playing a greater role in managing neovascular AMD and glaucoma in primary care? Ophthalmic & physiological optics : the journal of the British College of Ophthalmic Opticians (Optometrists), 45(1), 280.

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.

Berksoz M, et al. (2025) Ranking Single Fluorescent Protein-Based Calcium Biosensor Performance by Molecular Dynamics Simulations. Journal of chemical information and modeling, 65(1), 338.

Giese APJ, et al. (2025) Complexes of vertebrate TMC1/2 and CIB2/3 proteins form hair-cell mechanotransduction cation channels. eLife, 12.

Joshi R, et al. (2025) Exploring pyrazolines as potential inhibitors of NSP3-macrodomain of SARS-CoV-2: synthesis and in silico analysis. Scientific reports, 15(1), 767.

Ortega JT, et al. (2025) Discovery of non-retinoid compounds that suppress the pathogenic effects of misfolded rhodopsin in a mouse model of retinitis pigmentosa. PLoS biology, 23(1), e3002932.

Zhegalova IV, et al. (2025) Convergent pairs of highly transcribed genes restrict chromatin looping in Dictyostelium discoideum. Nucleic acids research, 53(2).

Shin Y, et al. (2025) Mycobacterium tuberculosis CrgA Forms a Dimeric Structure with Its Transmembrane Domain Sandwiched between Cytoplasmic and Periplasmic ?-Sheets, Enabling Multiple Interactions with Other Divisome Proteins. bioRxiv : the preprint server for biology.

Rachuri S, et al. (2025) Mutational analysis of an antimalarial drug target, PfATP4. Proceedings of the National Academy of Sciences of the United States of America, 122(2), e2403689122.

Zhang B, et al. (2025) London dispersion forces and steric effects within nanocomposites tune interaction energies and chain conformation. Communications chemistry, 8(1), 21.