Resource Summary Report

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CHARMM

RRID:SCR_014892
Type: Tool

Proper Citation

CHARMM (RRID:SCR_014892)

Resource Information

URL: https://www.charmm.org/charmm/?CFID=66837e22-4ee5-47ba-bcbf-b4b385c2397e&CFTOKEN=0

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Description: Software program that simulates molecular interactions. It has features that allow broad application to many-particle systems with a comprehensive set of energy functions, a variety of enhanced sampling methods, and support for multi-scale techniques, and a range of implicit solvent models. It also primarily targets biological systems including peptides, proteins, prosthetic groups, small molecule ligands, nucleic acids, lipids, and carbohydrates, as they occur in solution, crystals, and membrane environments. CHARMM can also be applied to inorganic materials with applications in materials design and has a comprehensive set of analysis and model builiding tools.

Resource Type: simulation software, software application, software resource

Keywords: visualization, modeling, molecular simulation, materials design, model building tools, analysis, biological systems, peptides, proteins

Resource Name: CHARMM

Resource ID: SCR_014892

Record Creation Time: 20220129T080322+0000

Record Last Update: 20260905T133259+0000

Ratings and Alerts

No rating or validation information has been found for CHARMM.

No alerts have been found for CHARMM.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 970 mentions in open access literature.

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

Bower JB, et al. (2026) Stabilization versus flexibility: Detergent-dependent trade-offs in neurotensin receptor 1 GPCR ensembles. Protein science : a publication of the Protein Society, 35(2), e70475.

Muthachikavil AV, et al. (2026) Computational Characterization of the Role of LEM2/LaminA Interactions on the Stability of BAF-Dimer Using Molecular Simulations. Proteins, 94(5), 1104.

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.

Dewan D, et al. (2026) Energy Landscape Analysis of Membrane Proteins Using NMR-Based Hybrid Restraint Potentials. Journal of chemical theory and computation, 22(11), 5827.

Nashed A, et al. (2026) An in vitro approach for simulating divergent Golgi O-glycosylation of tumor-associated MUC1 from normal MUC1. Nature communications, 17(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.

Park R, et al. (2026) RBM45 Preferential Binding to m6A: Simulations Suggest Synergy of RRM3 and Other Domains. The journal of physical chemistry. B, 130(21), 5310.

Utichi M, et al. (2026) Role of N-glycosylation as a determinant of ATG9A conformations and activity. Protein science : a publication of the Protein Society, 35(1), e70390.

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

Gharehgozlo S, et al. (2026) Harnessing Bacterial Lipid Coatings on Gold Nanoparticles for Enhanced Cell Adhesion Applications. Small science, 6(2), e202500584.

Liu Q, et al. (2026) Molecular basis for the inhibition of de novo DNA methylation by TCL1A. Nature communications, 17(1).

Hintzen JCJ, et al. (2026) Histidine Ethylation by Histidine Methyltransferases SETD3 and METTL9. Chembiochem : a European journal of chemical biology, 27(12), e70403.

Tyagi M, et al. (2026) Arc mediates intercellular tau transmission via extracellular vesicles. Cell, 189(15), 4706.

Mansour GH, et al. (2026) Computational Discovery of Novel Monkeypox Virus DNA Polymerase Inhibitors from the Zinc20 Database. Current issues in molecular biology, 48(4).

Severiche-Castro J, et al. (2026) Structure-Guided Design of an Interface-Derived Inhibitor Peptide Against Spodoptera frugiperda Digestive Trypsins. Archives of insect biochemistry and physiology, 122(1), e70164.

Regev C, et al. (2026) ERK autoinhibition mechanism informs a drug combination strategy. Protein science : a publication of the Protein Society, 35(6), e70650.

Li J, et al. (2026) Alkyltriphenylphosphonium Binding to Cardiolipin Triggers Oncosis in Cancer Cells. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 13(18), e10237.

Lee YS, et al. (2026) Proton Transfer Mechanisms in the MmpL3 Transporter of Mycobacterium tuberculosis Studied by Computer Simulations. ACS bio & med chem Au, 6(3), 263.

Lima DCA, et al. (2026) The many dimeric faces of Lys49 PLA2-like proteins: Conformational plasticity and membrane binding drive functional dimer states. Protein science : a publication of the Protein Society, 35(2), e70449.

Jang H, et al. (2026) Oncogenic PI3K? variants reveal graded conformational spectrum with mutation-specific cryptic pockets. Communications chemistry, 9(1).