Resource Summary Report

Generated by NIF on May 8, 2025

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

Proper Citation: CHARMM (RRID:SCR_014892)

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: software application, simulation software, software resource

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

Funding:

Availability: Commercial

Resource Name: CHARMM

Resource ID: SCR_014892

Record Creation Time: 20220129T080322+0000

Record Last Update: 20250508T065557+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 873 mentions in open access literature.

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

Haas-Neill L, et al. (2025) The structural influence of the oncogenic driver mutation N642H in the STAT5B SH2 domain. Protein science : a publication of the Protein Society, 34(1), e70022.

Islam S, et al. (2025) Analysis of how antigen mutations disrupt antibody binding interactions toward enabling rapid and reliable antibody repurposing. mAbs, 17(1), 2440586.

Brown E, et al. (2024) Inhibitors of the small membrane (M) protein viroporin prevent Zika virus infection. eLife, 13.

Barden M, et al. (2024) Integrating binding affinity and tonic signaling enables a rational CAR design for augmented T cell function. Journal for immunotherapy of cancer, 12(12).

Oladele JO, et al. (2024) Chlorophyll-Amended Organoclays for the Detoxification of Ochratoxin A. Toxins, 16(11).

Wozniak S, et al. (2024) Accurate Predictions of Molecular Properties of Proteins via Graph Neural Networks and Transfer Learning. bioRxiv : the preprint server for biology.

Cojal González JD, et al. (2024) Heavy-boundary mode patterning and dynamics of topological phonons in polymer chains and supramolecular lattices on surfaces. Nature communications, 15(1), 10674.

Yeshaya N, et al. (2024) VWD domain stabilization by autocatalytic Asp-Pro cleavage. Protein science : a publication of the Protein Society, 33(3), e4929.

Hussain A, et al. (2024) Guiding discovery of protein sequence-structure-function modeling. Bioinformatics (Oxford, England), 40(1).

Wu Y, et al. (2024) Identifying Artifacts from Large Library Docking. bioRxiv : the preprint server for biology.

Chatterjee BK, et al. (2024) Small molecule FICD inhibitors suppress endogenous and pathologic FICD-mediated protein AMPylation. bioRxiv : the preprint server for biology.

Nam K, et al. (2024) Magnesium induced structural reorganization in the active site of adenylate kinase. Science advances, 10(32), eado5504.

Kern NR, et al. (2024) CHARMM-GUI Multicomponent Assembler for modeling and simulation of complex multicomponent systems. Nature communications, 15(1), 5459.

Abdullah S, et al. (2024) Anti-enzymatic and DNA docking studies of montelukast: A multifaceted molecular scaffold with in vitro investigations, molecular expression analysis and molecular dynamics simulations. Heliyon, 10(2), e24470.

Villanelo F, et al. (2024) Connexin channels and hemichannels are modulated differently by charge reversal at residues forming the intracellular pocket. Biological research, 57(1), 31.

Vélez N, et al. (2024) Pore-forming peptide C14R exhibits potent antifungal activity against clinical isolates of Candida albicans and Candida auris. Frontiers in cellular and infection microbiology, 14, 1389020.

Freidel MR, et al. (2024) The Dual-Targeted Fusion Inhibitor Clofazimine Binds to the S2 Segment of the SARS-CoV-2 Spike Protein. Viruses, 16(4).

Montgomery JM, et al. (2024) Quantifying Induced Dipole Effects in Small Molecule Permeation in a Model Phospholipid Bilayer. The journal of physical chemistry. B, 128(30), 7385.

Antila HS, et al. (2024) Evaluating Polarizable Biomembrane Simulations against Experiments. Journal of chemical theory and computation, 20(10), 4325.

Dadhwal G, et al. (2024) Substrate promiscuity of Dicer toward precursors of the let-7 family and their 3'-end modifications. Cellular and molecular life sciences : CMLS, 81(1), 53.