

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 building tools.

Resource Type: software resource, software application, simulation software

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: 20260801T042740+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 936 mentions in open access literature.

Listed below are recent publications. The full list is available at [T1D](#).

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

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.

Berselli A, et al. (2026) The effect of ionic strength on PETase enzymes: An experimental and computational study. Protein science : a publication of the Protein Society, 35(1), e70386.

Borar P, et al. (2025) Dual-specific autophosphorylation of kinase IKK2 enables phosphorylation of substrate I?B? through a phosphoenzyme intermediate. eLife, 13.

Shaikh M, et al. (2025) Multimodal evaluation of nitazoxanide as an antidepressant: behavioral, biochemical, and molecular docking insights. Metabolic brain disease, 40(7), 262.

Tefft NM, et al. (2025) Controlled Enzyme Cargo Loading in Engineered Bacterial Microcompartment Shells. Biochemistry, 64(6), 1285.

Princiotta S, et al. (2025) Chromenone Derivatives as CRM1 Inhibitors for Targeting Glioblastoma. Chembiochem : a European journal of chemical biology, 26(15), e202500195.

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

Barron MP, et al. (2025) Quantifying the Structural and Energetic Consequences of EXOSC3 S1 Domain Variants from a Comparative Assessment of ?-Dynamics with Two Charge-Changing Perturbation Strategies. bioRxiv : the preprint server for biology.

Recktenwald M, et al. (2025) Extracellular Peptide-Ligand Dimerization Actuator Receptor Design for Reversible and Spatially Dosed 3D Cell-Material Communication. ACS synthetic biology, 14(7), 2494.

Noji T, et al. (2025) How the Electron-Transfer Cascade is Maintained in Chlorophyll-d Containing Photosystem I. Biochemistry, 64(1), 203.

Yu X, et al. (2025) Investigating the binding mechanism of AML inhibitors based on panobinostat with HDAC3 proteins using Gaussian accelerated molecular dynamics. RSC advances, 15(32), 26240.

Hushpulian DM, et al. (2025) Functional analysis of bipartite NRF2 activators that overcome feedback regulation for age-related chronic diseases. *Redox biology*, 86, 103794.

Oladele JO, et al. (2025) Green-Engineered Montmorillonite Clays for the Adsorption, Detoxification, and Mitigation of Aflatoxin B1 Toxicity. *Toxins*, 17(3).

Kugawa M, et al. (2025) Structural insights into lipid chain-length selectivity and allosteric regulation of FFA2. *Nature communications*, 16(1), 2809.

Toth D, et al. (2025) Allosteric Mechanisms Triggering Substrate and Cofactor Binding in the SULT1A1 Dimer as Revealed by Molecular Dynamics Simulations. *Journal of chemical information and modeling*, 65(19), 10503.

Kagelmacher M, et al. (2025) HMGB1 B-Box Domain Associates Promote Protein-Polyelectrolyte Interactions. *The journal of physical chemistry. B*, 129(37), 9293.

Vargas-Rosales PA, et al. (2025) Disrupting Amyloid Filaments of Tau by Means of Electric Fields. *The journal of physical chemistry. B*, 129(36), 9124.

Lawrenz J, et al. (2025) Trypstatin as a Novel TMPRSS2 Inhibitor with Broad-Spectrum Efficacy against Corona and Influenza Viruses. *Advanced science (Weinheim, Baden-Wurttemberg, Germany)*, 12(25), e2506430.

Gistelinck K, et al. (2025) Expression and characterization of an endo- β -1,6-galactanase from *Arabidopsis thaliana*. *The Biochemical journal*, 482(24), 1935.