Resource Summary Report

Generated by T1D on Aug 9, 2026

CHARMM-GUI

RRID:SCR_025037
Type: Tool

Proper Citation

CHARMM-GUI (RRID:SCR_025037)

Resource Information

URL: https://www.charmm-gui.org/

Proper Citation: CHARMM-GUI (RRID:SCR_025037)

Description: Web-based platform to interactively build complex systems and prepare their inputs with well established and reproducible simulation protocols for molecular simulations.

Resource Type: web application, software resource

Defining Citation: PMID:18351591

Keywords: Web-based platform, molecular simulations,

Funding: University of Kansas

Availability: Free, Freely available

Resource Name: CHARMM-GUI

Resource ID: SCR_025037

Record Creation Time: 20240305T200904+0000

Record Last Update: 20260808T190709+0000

Ratings and Alerts

No rating or validation information has been found for CHARMM-GUI.

No alerts have been found for CHARMM-GUI.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 207 mentions in open access literature.

Listed below are recent publications. The full list is available at T1D .

Parnandi VA, et al. (2026) A small Candida glabrata protein promotes hyphal growth in C. albicans during mixed-species invasive candidiasis. Current biology : CB, 36(1), 1.

Pinto CS, et al. (2026) Actin arginylation alters myosin engagement and F-actin patterning despite structural conservation. The Journal of cell biology, 225(1).

Li M, et al. (2026) ELMO2 is a therapeutic vulnerability in mesenchymal-like and drug-resistant non-small cell lung cancer. Nature communications, 17(1).

Abdalla MS, et al. (2026) Synergistic Potential of Repurposing non-?-lactam Compounds as Class A serine ?-lactamases Inhibitor: Insights from MolecularDocking, Molecular Dynamics Simulations and Antimicrobial Potentiation. Scientific reports, 16(1).

Páez-León SY, et al. (2026) Molecular Interaction and Biological Activity of Fatty Acids and Sterols: An In Silico and In Vitro Approach Against Haemonchus contortus. Pharmaceuticals (Basel, Switzerland), 19(1).

Rebouças Borges EL, et al. (2026) Europium Metal Complex [Eu(dbm)3.LAP] Promotes Antinociceptive Behavior via TRPA1 Neuromodulation and an Anti-Inflammatory Effect in Adult Zebrafish. Chemistry & biodiversity, 23(3), e71141.

Gutiérrez-Flores J, et al. (2026) Residue-Level Affinity Decomposition via Quantum Electron Density: A Multivariable Framework Applied to HIV-1 Protease Inhibitors. The journal of physical chemistry. B, 130(15), 4080.

Méndez-Reséndiz A, et al. (2026) Molecular mechanism of menthol-induced TRPV5 channel inhibition. Nature communications, 17(1).

de Sousa GF, et al. (2026) Comparative Analysis of Banana Lectins rBanLec-Like and H84T-BanLec: An In Silico and In Vitro Approach. The protein journal, 45(2), 318.

Costa F, et al. (2026) An inter-subunit path is required for entropically-driven and negatively cooperative binding of cyclic nucleotides in the HCN2 channel. Communications biology, 9(1).

Wang R, et al. (2026) Dimeric Polyphenol Effect on Liquid-Ordered and Liquid-Disordered Membranes: Combined Insights from Molecular Dynamics Simulation and Langmuir Balance Measurements. Langmuir : the ACS journal of surfaces and colloids, 42(13), 9021.

Liu H, et al. (2026) Target-Centric Multiplexed Screening of an Herbal Extract Identifies a Novel Dual A2A/A2B Receptor Antagonist for Cancer Immunotherapy. ACS central science, 12(3), 358.

Murathan Z, et al. (2026) Probing the Interaction Between Thioacetamide Fungicide and Bovine Serum Albumin Through Fluorescence, Electrochemical, and Docking Analyses. Luminescence : the journal of biological and chemical luminescence, 41(4), e70477.

Montaño GH, et al. (2026) In Silico Comparative Analysis of the Plant Growth Regulators Forchlorfenuron (CPPU) and Strigol (STG) Interacting with the Gibberellin Biosynthetic Enzyme GA3Ox2 and the Auxin Signaling Protein Receptor IAA7. International journal of molecular sciences, 27(7).

Yin Z, et al. (2026) Development of Membrane-Targeting Cannabigerol Derivatives as Potent Broad-Spectrum Antibacterial Agents. Drug design, development and therapy, 20, 558606.

Luo G, et al. (2026) Breaking disulfide bonds in a weakly bactericidal ?-defensin unleashes a potent antimicrobial peptide with an altered conformation. PLoS pathogens, 22(2), e1013954.

Dabiri M, et al. (2026) Computational optimization of DEK1 calpain domain solubility through integrated structural modelling and data-driven targeted mutagenesis. Scientific reports, 16(1).

Lira AL, et al. (2026) Molecular basis for inhibition of ?-thrombin activity by bacterial lipopolysaccharides. Scientific reports, 16(1).

Starnovskaya SS, et al. (2026) Isolation, Bromination, and Antimicrobial Activity of 3-Ethyl-4-hydroxy-6-methyl-2H-pyran-2-one from Sea Cucumber-Associated Fungus Trichoderma koningii KMM 4751. Antibiotics (Basel, Switzerland), 15(6).

Aguilera Morales ME, et al. (2026) Study of In Silico Binding Interactions and In Vitro Biosorption of Type A Trichothecenes Using Devil Fish Chitosan. Toxins, 18(6).