

Resource Summary Report

Generated by [NIF](#) on May 8, 2025

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: 20250508T070252+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 35 mentions in open access literature.

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

Lira AL, et al. (2025) The physicochemical properties of lipopolysaccharide chemotypes regulate activation of the contact pathway of blood coagulation. *The Journal of biological chemistry*, 301(1), 108110.

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

Crnčević D, et al. (2025) A dual antibacterial action of soft quaternary ammonium compounds: bacteriostatic effects, membrane integrity, and reduced in vitro and in vivo toxicity. *RSC advances*, 15(2), 1490.

Goyzueta-Mamani LD, et al. (2024) Targeting *Leishmania infantum* Mannosyl-oligosaccharide glucosidase with natural products: potential pH-dependent inhibition explored through computer-aided drug design. *Frontiers in pharmacology*, 15, 1403203.

Nieto-Fabregat F, et al. (2024) Computational toolbox for the analysis of protein-glycan interactions. *Beilstein journal of organic chemistry*, 20, 2084.

Ulmschneider JP, et al. (2024) Melittin can permeabilize membranes via large transient pores. *Nature communications*, 15(1), 7281.

Ferreira JC, et al. (2024) Boosting immunity: synergistic antiviral effects of luteolin, vitamin C, magnesium and zinc against SARS-CoV-2 3CLpro. *Bioscience reports*, 44(8).

Chakraborty MP, et al. (2024) Molecular basis of VEGFR1 autoinhibition at the plasma membrane. *Nature communications*, 15(1), 1346.

Azevedo PHRA, et al. (2024) Statine-based peptidomimetic compounds as inhibitors for SARS-CoV-2 main protease (SARS-CoV-2 Mpro). *Scientific reports*, 14(1), 8991.

de Santiago-Silva KM, et al. (2024) Molecular modelling studies and in vitro enzymatic assays identified A 4-(nitrobenzyl)guanidine derivative as inhibitor of SARS-CoV-2 Mpro. *Scientific reports*, 14(1), 8620.

Chakraborty S, et al. (2024) Structure and function of the human apoptotic scramblase Xkr4. *bioRxiv* : the preprint server for biology.

Chi LA, et al. (2024) Molecular Mechanisms Underlying the Spectral Shift in Zebrafish Cone

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Owolabi AO, et al. (2024) Antimicrobial potential of Hippocratea Indica Willd. Acetone Leaf fractions against Salmonella Typhi: an in vitro and in silico study. Scientific reports, 14(1), 25222.

Alpízar-Pedraza D, et al. (2024) Insights into the Adsorption Mechanisms of the Antimicrobial Peptide CIDEM-501 on Membrane Models. Antibiotics (Basel, Switzerland), 13(2).

Cubisino SAM, et al. (2024) Electrophysiological properties and structural prediction of the SARS-CoV-2 viroprotein E. Frontiers in molecular biosciences, 11, 1334819.

Yu X, et al. (2024) Heparan sulfate-dependent phase separation of CCL5 and its chemotactic activity. eLife, 13.

Piao Y, et al. (2024) Alkylated EDTA potentiates antibacterial photodynamic activity of protoporphyrin. Journal of nanobiotechnology, 22(1), 161.

Lou T, et al. (2024) Effect of Surface-Immobilized States of Antimicrobial Peptides on Their Ability to Disrupt Bacterial Cell Membrane Structure. Journal of functional biomaterials, 15(11).

Villalaín J, et al. (2024) Bisphenol F and Bisphenol S in a Complex Biomembrane: Comparison with Bisphenol A. Journal of xenobiotics, 14(3), 1201.

Rooney J, et al. (2024) Structural and functional analyses of nematode-derived antimicrobial peptides support the occurrence of direct mechanisms of worm-microbiota interactions. Computational and structural biotechnology journal, 23, 1522.