

Resource Summary Report

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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: software resource, web application

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: 20260806T054811+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

Usage and Citation Metrics

We found 86 mentions in open access literature.

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

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

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.

Saadabadi A, et al. (2025) Insights into Molecular Interactions and Biological Effect of Natural Stilbenoids at the TRPA1 Ion Channel. *ChemMedChem*, 20(3), e202400501.

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.

Rashwan ME, et al. (2025) In silico prediction of GRP78-CRIPTO binding sites to improve therapeutic targeting in glioblastoma. *Scientific reports*, 15(1), 16660.

Irham LM, et al. (2025) Deciphering anti-colorectal cancer potential of *Avicennia alba* bioactives via network pharmacology and in vitro validation. *Scientific reports*, 15(1), 27976.

Vasconcelos M, et al. (2025) Photodynamic Inactivation as a New Weapon Against Plant Fire Blight Disease: Proof of a New Dawn of Environmentally Friendly Crop Protection. *Journal of agricultural and food chemistry*, 73(32), 19958.

Al-Theyab NS, et al. (2025) In Silico and in vitro evaluation of the anticancer effect of a 1,5-Benzodiazepin-2-One derivative (3b) revealing potent dual inhibition of HER2 and HDAC1. *Scientific reports*, 15(1), 13424.

Al-Rasheed LS, et al. (2025) Design, synthesis, biological evaluation and in silico studies of 2-anilino- 4-(benzimidazol- 1-yl)pyrimidine scaffold as antitumor agents. *Saudi pharmaceutical journal : SPJ : the official publication of the Saudi Pharmaceutical Society*, 33(3), 12.

Hung SC, et al. (2025) Structural and molecular dynamics insights into the competitive inhibition of the platelet-activating factor receptor by acyl-PAF. *The Journal of biological chemistry*, 301(12), 110831.

Cui X, et al. (2025) Pharmacological Dissection Identifies Retatrutide Overcomes the Therapeutic Barrier of Obese TNBC Treatments through Suppressing the Interplay between Glycosylation and Ubiquitylation of YAP. *Advanced science (Weinheim, Baden-Wurttemberg, Germany)*, 12(11), e2407494.

García-García M, et al. (2025) Electrospun Membranes Loaded with Melanin Derived from Pecan Nutshell (*Carya illinoensis*) Residues for Skin-Care Applications. *Membranes*, 15(2).

Millan-Casarrubias EJ, et al. (2025) Molecular Docking and Pharmacological In Silico Evaluation of Camptothecin and Related Ligands as Promising HER2-Targeted Therapies for Breast Cancer. *Current issues in molecular biology*, 47(3).

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

Ruiz-Castelan JE, et al. (2025) The β/β_3 complex of human voltage-gated sodium channel hNav1.7 to study mechanistic differences in presence and absence of auxiliary subunit β_3 . *Journal of molecular modeling*, 31(6), 168.

De Coninck T, et al. (2025) OsAPSE modulates non-covalent interactions between arabinogalactan protein O-glycans and pectin in rice cell walls. *Frontiers in plant science*, 16, 1588802.

Sinthopweha W, et al. (2025) Methyl itaconate-anthracene adducts (MIAs) facilitate the enantiomeric separation of 1,1'-bi-2-naphthols via thin-layer chromatography (TLC) with trends predicted by molecular dynamics simulations. *RSC advances*, 15(34), 28063.

Kuang Z, et al. (2025) Identifying resonant frequencies of viruses for microwave-based detection and inactivation of pathogenic viruses. *Scientific reports*, 15(1), 43920.

Nagasato Y, et al. (2025) In silico analysis of sodium ion permeation mechanisms in transient receptor potential vanilloid 1. *Scientific reports*, 15(1), 44955.

Afshari SG, et al. (2025) Discovery of hyde C1 a broad spectrum antimicrobial peptide derived from chicory. *Scientific reports*, 15(1), 33449.