Resource Summary Report

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NIH Center for Macromolecular Modeling and Bioinformatics

RRID:SCR_001435
Type: Tool

Proper Citation

NIH Center for Macromolecular Modeling and Bioinformatics (RRID:SCR_001435)

Resource Information

URL: http://www.ks.uiuc.edu/

Proper Citation: NIH Center for Macromolecular Modeling and Bioinformatics (RRID:SCR_001435)

Description: Biomedical technology research center focusing on the structure and function of supramolecular systems in the living cell as well as on the development of new algorithms and efficient computing tools for physical biology. They bring the most advanced molecular modeling, bioinformatics, and computational technologies to bear on questions of biomedical relevance. They extend, refine and deliver these technologies in response to experimental progress and emerging needs of the wide biomedical research community. They magnify the impact of their work through direct collaboration with experimental researchers, the distribution of cutting-edge and user-friendly software, and via extensive training, service, and dissemination efforts. The multidisciplinary team is engaged in the modeling of large macromolecular systems in realistic environments, and has produced ground-breaking insights into biomolecular processes coupled with mechanical force, bioelectronic processes in metabolism and vision, and with the function and mechanism of membrane proteins. They are committed and work towards further advancement of * Molecular modeling tools which can integrate structural information with bioinformatics databases and molecular dynamics simulations, and which can be used by a wide audience; * High performance molecular visualization and simulation software, capable of modeling biomolecules in realistic environments of 100,000,000 atoms or more; * Conceptual and methodological foundations of molecular modeling in the fields of quantum biology, mechanobiology, and interactive modeling; * Biomedical science through collaborations between theoretical and experimental researchers; * Support of the entire research process and training through a web-enabled collaborative environment; and * Service, training, and dissemination by leveraging web-based molecular graphics and integrated modeling technologies.

Abbreviations: Center for Macromolecular Modeling and Bioinformatics, TCBG

Synonyms: Resource for Macromolecular Modeling and Bioinformatics, Theoretical and Computational Biophysics Group, NIH Center for Macromolecular Modeling & Bioinformatics

Resource Type: biomedical technology research center, training resource

Keywords: supramolecular system, living cell, cell, algorithm, computing, physical biology, software, molecular dynamics, simulation, molecule, visualization, biomolecule, molecular modeling, bioinformatics, computational technology, computing and informatics technology center, model, macromolecule

Funding: NIGMS P41GM104601

Availability: Free, Freely Available

Resource Name: NIH Center for Macromolecular Modeling and Bioinformatics

Resource ID: SCR_001435

Alternate IDs: nlx_152659

Record Creation Time: 20220129T080207+0000

Record Last Update: 20260905T133321+0000

Ratings and Alerts

No rating or validation information has been found for NIH Center for Macromolecular Modeling and Bioinformatics.

No alerts have been found for NIH Center for Macromolecular Modeling and Bioinformatics.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 39 mentions in open access literature.

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

Ge C, et al. (2026) A deep learning framework (CreoPep) for target-specific design and optimization of conotoxin peptides. Communications chemistry, 9(1), 82.

Su J, et al. (2025) Molecular insights into the ?6?4 nicotinic acetylcholine receptor function and ligand recognition. Nature communications, 16(1), 3153.

Yuan X, et al. (2025) Genome-Wide Identification of the BREVIS RADIX Gene Family in Foxtail Millet: Function, Evolution, and Expression. Genes, 16(4).

Miao RR, et al. (2025) Conjugated bile acids promote metabolic dysfunction-associated steatotic liver disease through inducing nuclear translocation of sphingosine-1-phosphate receptor 2 to disrupt peroxisome proliferator-activated receptor alpha. Cell communication and signaling : CCS, 23(1), 240.

Kramarska E, et al. (2024) A rationally designed antigen elicits protective antibodies against multiple nosocomial Gram-positive pathogens. NPJ vaccines, 9(1), 151.

Shih YC, et al. (2024) The phosphatase DUSP22 inhibits UBR2-mediated K63-ubiquitination and activation of Lck downstream of TCR signalling. Nature communications, 15(1), 532.

Fan S, et al. (2024) Non-transcriptional IRF7 interacts with NF-?B to inhibit viral inflammation. The Journal of biological chemistry, 300(4), 107200.

Petry R, et al. (2024) Interaction of graphene oxide with tannic acid: computational modeling and toxicity mitigation in C. elegans. Beilstein journal of nanotechnology, 15, 1297.

Murray JS, et al. (2022) CDR3 binding chemistry controls TCR V-domain rotational probability and germline CDR2 scanning of polymorphic MHC. Molecular immunology, 144, 138.

Henning-Knechtel A, et al. (2022) Differences in ion-RNA binding modes due to charge density variations explain the stability of RNA in monovalent salts. Science advances, 8(29), eabo1190.

Pastorio C, et al. (2022) Determinants of Spike infectivity, processing, and neutralization in SARS-CoV-2 Omicron subvariants BA.1 and BA.2. Cell host & microbe, 30(9), 1255.

Zhao S, et al. (2022) Computational and functional studies of the PI(4,5)P2 binding site of the TRPM3 ion channel reveal interactions with other regulators. The Journal of biological chemistry, 298(11), 102547.

Zheng M, et al. (2022) Mechanism of interactions between ?-conotoxin RegIIA and carbohydrates at the human ?3?4 nicotinic acetylcholine receptor. Marine life science & technology, 4(1), 98.

Ma Y, et al. (2022) Single-Disulfide Conopeptide Czon1107, an Allosteric Antagonist of the Human ?3?4 Nicotinic Acetylcholine Receptor. Marine drugs, 20(8).

Rossi F, et al. (2021) Extraction and high-throughput sequencing of oak heartwood DNA: Assessing the feasibility of genome-wide DNA methylation profiling. PloS one, 16(11), e0254971.

Eskandarzadeh M, et al. (2021) Inhibition of GSK_3? by Iridoid Glycosides of Snowberry (Symphoricarpos albus) Effective in the Treatment of Alzheimer's Disease Using Computational Drug Design Methods. Frontiers in chemistry, 9, 709932.

Wani TA, et al. (2021) Binding and drug displacement study of colchicine and bovine serum albumin in presence of azithromycin using multispectroscopic techniques and molecular dynamic simulation. Journal of molecular liquids, 333, 115934.

Alsaif NA, et al. (2020) Multi-spectroscopic investigation, molecular docking and molecular dynamic simulation of competitive interactions between flavonoids (quercetin and rutin) and sorafenib for binding to human serum albumin. International journal of biological macromolecules, 165(Pt B), 2451.

Zhang Y, et al. (2020) Self-assembling nanoparticles of dually hydrophobic prodrugs constructed from camptothecin analogue for cancer therapy. European journal of medicinal chemistry, 200, 112365.

Gupta AM, et al. (2020) Non-synonymous mutations of SARS-CoV-2 leads epitope loss and segregates its variants. Microbes and infection, 22(10), 598.