Resource Summary Report

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Theoretical and Computational Biophysics Group (TCBG)

RRID:SCR_013598
Type: Tool

Proper Citation

Theoretical and Computational Biophysics Group (TCBG) (RRID:SCR_013598)

Resource Information

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

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Description: The Theoretical and Computational Biophysics Group (TCBG), an NIH Resource for Macromolecular Modeling and Bioinformatics, was founded by Professor Klaus Schulten in 1989 and is located at the Beckman Institute of the University of Illinois at Urbana-Champaign (UIUC). The group is led by Professor Klaus Schulten (Physics, Biophysics, Chemistry) with Professors Laxmikant Kale (Computer Science), Zaida Luthey-Schulten (Chemistry) and Alek Aksimentiev (Physics), and with the Resource"s assistant director Dr. Emad Tajkhorshid (Biophysics). Research and development activities of the TCBG center on the structure and function of supramolecular systems in the living cell, and on the development of new algorithms and efficient computing tools for structural biology. :The TCBG brings the most advanced molecular modeling, bioinformatics, and computational technologies to bear on questions of biomedical relevance. We extend, refine and deliver these technologies in response to experimental progress and emerging needs of the wide biomedical research community. We magnify the impact of our work through direct collaboration with experimental researchers, the distribution of cutting-edge and user-friendly software, and via extensive training, service, and dissemination efforts. :cell, algorithm, simulation software, membrane potential, genome, molecule, ion channel, chromatin, Image Processing software, data Data visualization software, simulation software; Membrane Biophysics, Mechanobiology, Nanoengineering, Bioenergetics, Neurobiology, Molecular Dynamics, cellular membrane, osmotic pressure, proteins (use protein), Gatekeeper Protein, membrane, mechanosensitive channel of small conductance (MscS), Visual Molecular Dynamics (VMD), Quantum Biology, quantum chemistry, Molecular Dynamics Simulator, Nanoscale Imaging, cellular membrane tension, bacterial cell, electron paramagnetic measurements, computer modeling, atomic detail, computational microscope, Lipoproteins [high density lipoproteins (HDL)], Petascale Computing, Macromolecular Modeling, Bioinformatics,

supramolecular systems, living cell, algorithms (use algorithm), computing tools, structural biology, molecular modeling, computational technologies, membrane proteins, structural information, molecular visualization, Molecular modeling tools, structural information, bioinformatics databases, molecular dynamics simulations, interactive modeling, collaborations, theoretical, experimental researchers, light energy, electrical membrane potentials (use membrane potential, add term as syn), synthesis of ATP, photosynthetic systems, storage and control of genetic information, classical and quantum dynamical motion of biopolymers, numerical experiments, non-equilibrium statistical mechanics, elasticity theory, theory of disordered systems, collaborative environment, Software Development, cells (use cell), molecular graphics viewer, static and dynamic structures, DNA sequencing, genomes (use genome), direct manipulation and observation, single molecules (use molecule), bioenergetic proteins, nanotechnology, steered/interactive molecular dynamics, dissemination, coarse-graining methods, residue-based and shape-based coarse graining, CG, polymeric systems, Computational Environment, Training, Workshops, Tutorials, Case Studies, Classes, research, Highly Cited, compute power, visualization equipment, desktop workstations, lipid bilayers, allow passage of ions across the membrane (use ion channel), mechanotransduction, membrane tension, 3-D graphics, built-in scripting, animating, analyzing, ideal DNA interbasepair helical parameters, plugin, nucleosomes, antialiasing, depthcueing, Molecular Representations, analysis and Data visualization software (use Image Processing software, and data Data visualization software, add terms as syn.), computer simulations (use simulation software), photosynthetic systems, computational clusters :

Synonyms: TCBG

Resource Type: database, data or information resource, image processing software, data processing software, software application, software resource

Resource Name: Theoretical and Computational Biophysics Group (TCBG)

Resource ID: SCR_013598

Alternate IDs: nif-0000-00420

Record Creation Time: 20220129T080317+0000

Record Last Update: 20260810T040618+0000

Ratings and Alerts

No rating or validation information has been found for Theoretical and Computational Biophysics Group (TCBG).

No alerts have been found for Theoretical and Computational Biophysics Group (TCBG).

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 19 mentions in open access literature.

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

Shakour N, et al. (2026) Rational Design of Novel Inhibitors: Integrating 3D-QSAR and Molecular Dynamics. BioMed research international, 2026, 4138899.

Agyemang E, et al. (2026) Activation dynamics of a water-soluble human mu-opioid receptor. The Journal of biological chemistry, 302(5), 111393.

Hosseini M, et al. (2025) Computational and experimental design of L-amino acid-based alternatives to ketorolac. Scientific reports, 15(1), 42161.

Nagae F, et al. (2024) Molecular mechanism of parental H3/H4 recycling at a replication fork. Nature communications, 15(1), 9485.

Senanayaka D, et al. (2024) Autoregulatory mechanism of enzyme activity by the nuclear localization signal of lysine-specific demethylase 1. The Journal of biological chemistry, 300(9), 107607.

Barani Pour S, et al. (2023) Investigation the effect of water addition on intermolecular interactions of fatty acids-based deep eutectic solvents by molecular dynamics simulations. Scientific reports, 13(1), 7433.

Omidi-Shahsavandi M, et al. (2023) Effect of silibinin and trans-chalcone in an Alzheimer's disease-like model generated by insulin amyloids. Brazilian journal of medical and biological research = Revista brasileira de pesquisas medicas e biologicas, 56, e12443.

Salimi A, et al. (2022) The use of machine learning modeling, virtual screening, molecular docking, and molecular dynamics simulations to identify potential VEGFR2 kinase inhibitors. Scientific reports, 12(1), 18825.

Tong Y, et al. (2021) SUCLA2-coupled regulation of GLS succinylation and activity counteracts oxidative stress in tumor cells. Molecular cell, 81(11), 2303.

Liu R, et al. (2021) Choline kinase alpha 2 acts as a protein kinase to promote lipolysis of lipid droplets. Molecular cell, 81(13), 2722.

Liu S, et al. (2021) Structure-Function Analysis of Resistance to Bamlanivimab by SARS-CoV-2 Variants Kappa, Delta, and Lambda. Journal of chemical information and modeling, 61(10), 5133.

Hern??ndez-Huerta MT, et al. (2021) Analysis of SARS-CoV-2 mutations in Mexico, Belize, and isolated regions of Guatemala and its implication in the diagnosis. Journal of medical virology, 93(4), 2099.

Barrera EE, et al. (2021) Dissecting the role of glutamine in seeding peptide aggregation. Computational and structural biotechnology journal, 19, 1595.

Maculins T, et al. (2020) Discovery of Protein-Protein Interaction Inhibitors by Integrating Protein Engineering and Chemical Screening Platforms. Cell chemical biology, 27(11), 1441.

Broser M, et al. (2020) NeoR, a near-infrared absorbing rhodopsin. Nature communications, 11(1), 5682.

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.

Fang Z, et al. (2016) Improved catalytic efficiency, thermophilicity, anti-salt and detergent tolerance of keratinase KerSMD by partially truncation of PPC domain. Scientific reports, 6, 27953.

D??az-Franulic I, et al. (2015) Pore dimensions and the role of occupancy in unitary conductance of Shaker K channels. The Journal of general physiology, 146(2), 133.

Panja AS, et al. (2015) Protein Thermostability Is Owing to Their Preferences to Non-Polar Smaller Volume Amino Acids, Variations in Residual Physico-Chemical Properties and More Salt-Bridges. PloS one, 10(7), e0131495.