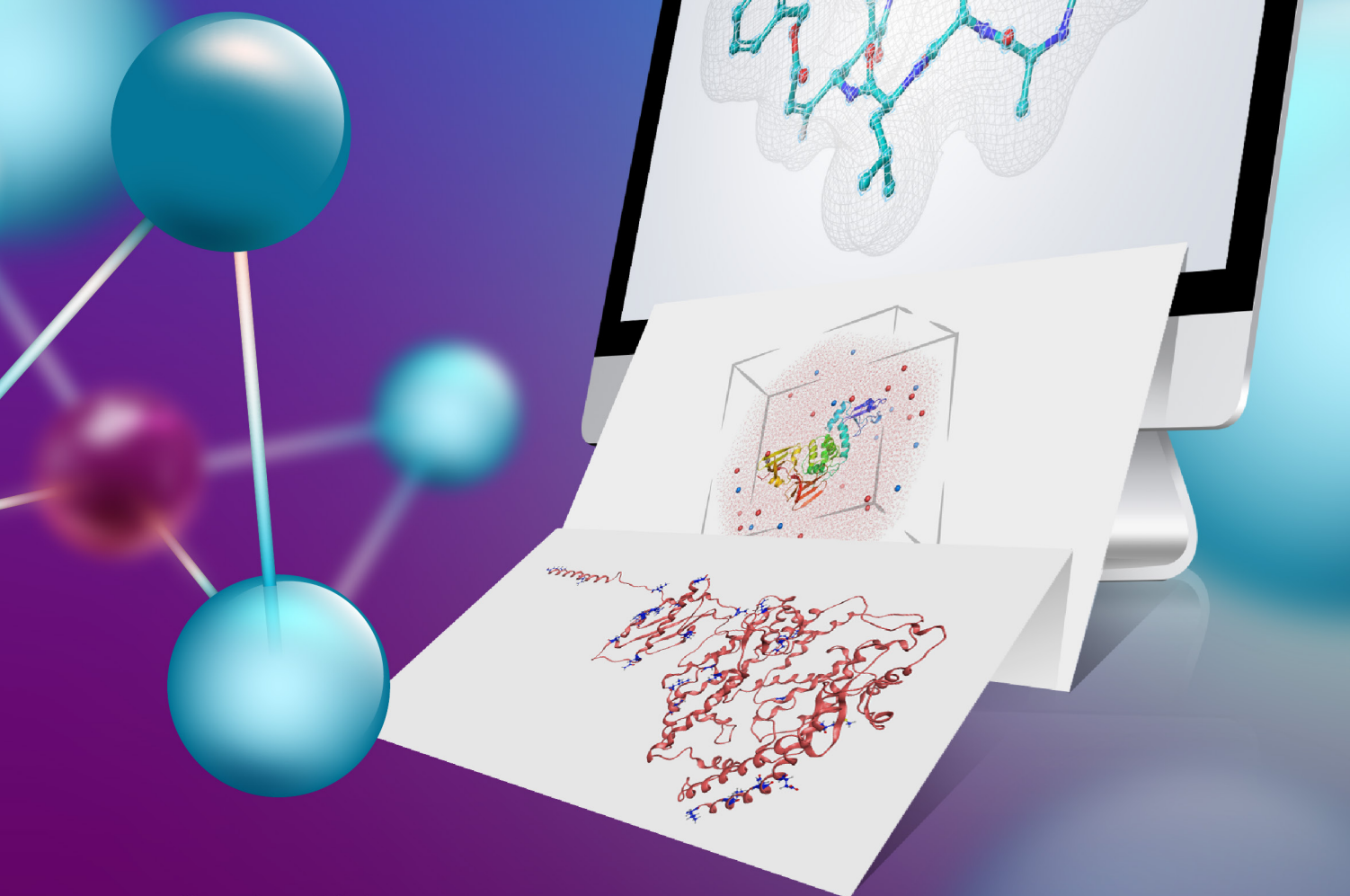


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MolModSim Connect

A Journal Specialized in
Molecular Modeling & Simulations



Editor-in-Chief

Vannajan Sanghiran Lee, PhD



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MolModSim Connect

A Journal Specialized in Molecular Modeling & Simulations

Volume: 1, Issue: 1, 2024

Subject Categories

Chemistry

Molecular Modelling

Drug Discovery

Computational Biology

Target Audience

MolModSim Connect is tailored for researchers, academics, industry professionals, and practitioners immersed in the dynamic realms of molecular modeling and simulation, spanning across disciplines such as chemistry, biochemistry, materials science, drug discovery, and computational biology.



Vannajan Sanghiran Lee

Editor-in-Chief

University of Malaya, Kuala Lumpur Malaysia

Message from EiC

Dear Esteemed Colleagues,

I am thrilled to announce the launch of "MolModSim Connect," a new journal dedicated to advancing molecular sciences through innovative modeling and simulations. As Editor-in-Chief, I am excited to lead this initiative aimed at fostering collaboration and knowledge exchange among experts in our dynamic field. "MolModSim Connect" will provide a platform for driving material discoveries across diverse domains. In addition to research and review articles, we will publish Commentaries, Editorials, and Perspectives, providing a dynamic space for expressing opinions, sparking discussions, and offering unique insights. Join us in shaping the future of molecular modeling and simulation! Let's push the boundaries of possibility together and pave the way for groundbreaking discoveries.

Aims and Scope

MolModSim Connect is a global, peer-reviewed, open-access journal dedicated to pioneering innovation at the forefront of molecular sciences through modeling and simulations. Published biannually in print and online, it serves as the central catalyst for cutting-edge research, driving material discoveries across diverse domains.

Key Topics

The journal encompasses a broad range of topics within molecular modeling and simulation, including but not limited to:

Molecular Dynamics Simulations

Novel techniques and methodologies for simulating the dynamic behavior of molecules and molecular systems.

Protein Structure Prediction and Drug Design

Computational approaches for predicting protein structures, protein-ligand interactions, and rational drug design.

Molecular Docking and Virtual Screening

Computational techniques for predicting the binding affinity and specificity of ligands to target proteins.

Molecular Modeling in Material Science

Applications of molecular modeling and simulation techniques in the design and characterization of materials with tailored properties.

Computational Chemistry Software and Tools

Development and validation of software packages, algorithms, and tools for molecular modeling and simulation.


Molecular Visualization and Data Analysis

Visualization techniques and data analysis methods for interpreting molecular structures and simulation results.



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