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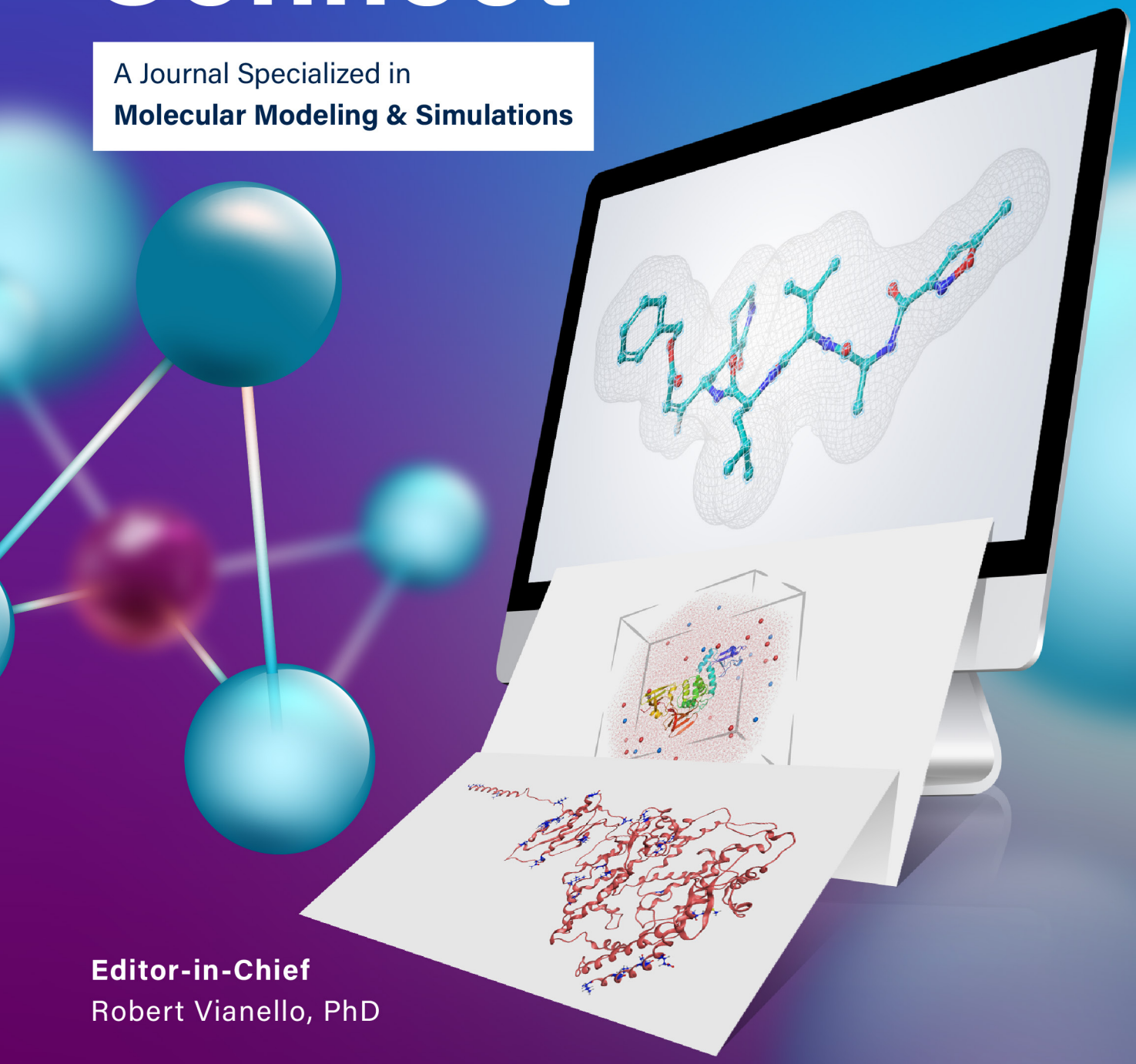
Molecular Modeling Connect

A Journal Specialized in
Molecular Modeling & Simulations



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Subject Categories

Chemistry | Molecular Modelling | Drug Discovery | Computational Biology

Target Audience

Molecular Modeling 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.

Robert Vianello

Editor-in-Chief

Rudjer Boskovic Institute, Croatia

Message from EiC

Dear Colleagues,

It is with great enthusiasm that I welcome you to Molecular Modeling Connect, a premier platform dedicated to advancing the frontiers of interdisciplinary insights in computational simulation. As Editor-in-Chief, I am honoured to lead this vibrant journal, committed to fostering innovative research and facilitating global collaboration.

Our mission is to provide a rigorous and accessible venue for sharing groundbreaking discoveries that shape the future of science. With a commitment to quality, ethical publishing, and open access, we aim to amplify your research's impact and reach. I invite you to submit your work, engage with our community, and contribute to the exciting advancements in molecular modeling and beyond.

Together, let us connect ideas and drive scientific progress!

Aims and Scope

Molecular Modeling 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.