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Molecular Modeling Connect

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Open Access Peer-Reviewed Journal Specialized in
Molecular Modeling and Simulation

Editor-in-Chief
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Molecular Modeling Connect

A Journal Specialized in Molecular Modeling and Simulations

Volume: 3, 2026

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

As Molecular Modeling Connect enters its 2026 volume, I am pleased to reflect on the strong foundation established during our inaugural years and to look ahead to the opportunities that lie before us. The journal continues to grow as a dynamic forum for high-quality research in molecular modeling, simulation, and computational science that bridges theory, experiment, and real-world applications. We are proud to offer a visible and accessible platform, driven by an engaged international editorial board and a rigorous peer-review process designed to support authors and accelerate the dissemination of cutting-edge results. In 2026, we remain committed to upholding the highest standards of scholarly excellence while fostering innovation, transparency, and cross-disciplinary collaboration. We particularly welcome emerging approaches, including data-driven and AI-enhanced modeling. I warmly invite researchers from around the world to contribute their best work and to join Molecular Modeling Connect in shaping the future of molecular-level understanding across chemistry, biology, and materials science.

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. The journal 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.