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Editorial

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Preface

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Welcome to the inaugural volume of *MolMod Connect*—a dynamic, peer-reviewed, open-access journal dedicated to advancing the frontiers of molecular modeling and simulation. Published biannually in print and online, *MolMod Connect* offers an inclusive and thoughtfully curated platform for high-quality research that pushes the boundaries of knowledge and innovation in this rapidly evolving field.

Molecular modeling has sparked what can be described as a predictive revolution in science, enabling researchers worldwide to simulate and understand molecular systems with unprecedented precision. This revolution not only accelerates discovery and optimizes resource use but also expands opportunities by creating new pathways for researchers across disciplines and geographies to contribute meaningfully.

To highlight this vision, we begin with a Short Communication from the Editorial Board, titled "*The Predictive Revolution: Rethinking Science Through Molecular Modeling*," outlining the latest trends and the vital importance of nurturing growth and excellence in the field.

Following this foundational perspective, the research articles in this issue illustrate the wide-ranging applications and methodological innovations of molecular modeling:

- **Fundamental Molecular Simulations and Spectroscopic Characterization**

  Effect of Acyl Chain Variation and Cholesterol on Structural and Dynamic Properties of Lipid Bilayer Probed by Simulation
  Investigates the fundamental behavior of lipid membranes in cell biology and drug delivery. https://doi.org/10.69709/MolModC.2025.165214
  Study of the 3-(3,3-Dimethylbutanoyl)-4-hydroxy-6-neopentyl-2H-pyran-2-one by IR, Raman Spectroscopy, and DFT
  Combines experimental vibrational spectroscopy with density functional theory to elucidate molecular structure. https://doi.org/10.69709/MolModC.2024.118203

- **Molecular Interactions and Enzyme Dynamics**

  Unusual Arrangement of Catalytic Loops of the Alcohol Dehydrogenase Enzyme During the Adsorption Process on a Graphitic Carbon Surface
  Explores enzyme behavior at interfaces relevant to biotechnology and biosensors. https://doi.org/10.69709/MolModC.2025.101003

- **Biomedical Applications: Drug Mechanism and Therapeutics**

  Exploring Artesunate and Dihydroartemisinin for Mechanism on MMP-3 and MMP-13 via Molecular Docking and Molecular Dynamics
  Provides insight into anti-inflammatory and anti-cancer drug mechanisms through computational docking and dynamics. https://doi.org/10.69709/MolModC.2025.142325
  Food and Medicine Homology Substance in Cancer Treatment: Mechanism of Astragalus against Pancreatic Cancer
  Examines bioactive compounds from traditional medicine with implications for cancer therapy. https://doi.org/10.69709/MolModC.2025.131915
  In Silico Investigation of the Constituents of Aroeira Honey (Astronium urundeuva) and the Binding Affinity with Important Proteins of M. leprae and M. tuberculosis

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Investigates natural product interactions with pathogen proteins, advancing infectious disease research. https://doi.org/10.69709/MolModC.2024.113103

- **Environmental and Material Science Applications**

  Smart Gas Sensing by (Al/C/Si)-Doped Boron Nitride Nanomaterial Towards Grabbing Nitric Oxide: A Novel Applied Technique for Air Pollution Reduction by DFT Analysis
  Demonstrates novel nanomaterial design for environmental sensing and pollution control. https://doi.org/10.69709/MolModC.2025.339955

These contributions embody *MolMod Connect*'s dedication to fostering interdisciplinary collaboration and maintaining the highest standards of scientific quality and care. We aim to foster a global community where researchers, whether emerging or established, can share their discoveries, challenge prevailing conventions, and collectively advance the field of molecular modeling.

I extend my heartfelt gratitude to our editorial board, peer reviewers, and the devoted team at Scifiniti for their invaluable efforts in launching this journal. Together, we look forward to *MolMod Connect* becoming a catalyst for innovation, providing equitable opportunities for researchers everywhere to thrive and shape the future of molecular science.

I invite you to explore this issue with curiosity and enthusiasm, confident that the work presented here will inspire new ideas and accelerate progress across diverse disciplines.

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