Molecular Biotechnology
https://doi.org/10.1007/s12033-024-01073-1

EDITORIAL

Special issue: Biomolecular Modelling and Simulation

Yee Siew Choong[1] · Ricardo Mancera[2] · Vannajan Sanghiran Lee[3]

Accepted: 10 January 2024

Computational biomolecular simulation has been demonstrating its value to study the insights of a range of different systems of biotechnological and biomedical interest. The application of molecular modelling methods to address a wide array of topics ranging from viruses to prokaryotes and eukaryotes were collected in this special issue. The use of sequence alignment, phylogenetic analysis, protein structure modelling, virtual drug screening, molecular docking, and molecular dynamics simulation with different algorithms is widely demonstrated. These methods enabled the elucidation and identification of evolutionary relationships, biomolecular conformation/folding, protein–ligand/protein interactions, inhibitor, and vaccine design. The new knowledge generated with the integration of experimental data will be useful to further rapidly increase the development of biomolecular simulation in the future.

The successful publication of this special issue is the outcome of the strong support from all contributing authors and anonymous reviewers from the biomolecular simulation community. We also acknowledge the significant support from the Associate Publisher Ingrid B. Fischer as well as the Editor-in-Chief, Prof Aydin Berenjian. It has been an honour and a wonderful experience to serve Molecular Biotechnology as Guest Editors for this special issue.

✉ Yee Siew Choong
yeesiew@usm.my

Ricardo Mancera
r.mancera@curtin.edu.au

Vannajan Sanghiran Lee
vannajan@um.edu.my

[1] Institute for Research in Molecular Medicine (INFORMM), Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia

[2] Curtin Medical School, Curtin Health Innovation Research Institute, Curtin University, GPO Box U1987, Perth, WA 6845, Australia

[3] Department of Chemistry, Centre for Quantum Information Science and Technology (QIST), Faculty of Science, University of Malaya, 50603 Kuala Lumpur, Malaysia

Published online: 10 February 2024