Special Issue

Molecular Simulation of Protein Structure and Interactions

Message from the Guest Editors

Molecular simulation methods allow the study of biomolecules in exquisite atomistic detail, enabling the characterisation of molecular mechanisms and their associated thermodynamics and kinetics properties. Developments in force fields and enhanced sampling methods, alongside the wider availability of exascale computing resources, are facilitating the investigation of much more complex systems at substantially larger time and length scales. The interface of biology and materials in molecular sciences are also being increasingly characterised by various molecular simulation and artificial intelligence approaches. This special issue is aimed at recent research using molecular simulation approaches to study complex biomolecular systems such as intrinsically disordered proteins, protein aggregation, liquid-liquid phase separation, membrane receptor activation, peptide- and protein-membrane interactions, macrobiomolecular complex formation and interactions, protein-surface interactions, and proteins in biomaterials. New methods and force fields developed for these systems, including the use of artificial intelligence, are also of particular interest.

Guest Editors

Prof. Dr. Ricardo L. Mancera
Curtin Medical School, Curtin University, Perth, WA 6845, Australia

Dr. Nevena Todorova
School of Engineering, RMIT University, GPO Box 2476, Melbourne, VIC 3001, Australia

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Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
ijms@mdpi.com

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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

Editor-in-Chief

Prof. Dr. Maurizio Battino
Department of Odontostomatologic and Specialized Clinical Sciences, Sez-Biochimica, Faculty of Medicine, Università Politecnica delle Marche, Via Ranieri 65, 60100 Ancona, Italy

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