

Special Issue

Computational Studies of Biomolecules

Message from the Guest Editor

This Special Issue is the continuation of our previous special issue "[Computational Studies of Structure-Dynamics-Function Relationships in Biomolecules](#)". The current Special Issue aims to attract high quality contributions of modeling biomolecular structure, dynamics, function and interactions with potential of interpretation of experimental data and application in drug design and protein design. Topics of interest:

- Development and validation of new Computational Modeling Methods
- Computational Studies of proteins structure-function relationships
- Computational investigations of nucleic acids structure-function relationships
- Modelling of protein and nucleic acids dynamics
- Protein Docking
- Protein-ligand interactions
- Nucleic acid ligand interactions
- Protein design
- Computational enzymology-enzymatic reaction mechanisms
- Proteins homology modeling

Deadline for manuscript submissions

closed (1 October 2020)



International Journal of Molecular Sciences

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Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



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*International Journal of
Molecular Sciences*
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
ijms@mdpi.com

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Message from the Editor-in-Chief

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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