



## Computational Studies of Biomolecules

Guest Editors:

**Assoc. Prof. Tatyana  
Karabancheva-Christova**

Department of Chemistry,  
Michigan Technological  
University, Houghton, MI 49931,  
USA

tatyanak@mtu.edu

**Assoc. Prof. Christo Z.  
Christov**

Department of Chemistry,  
Michigan Technological  
University, Houghton, MI 49931,  
USA

christov@mtu.edu

Deadline for manuscript  
submissions:  
**closed (20 January 2020)**

### Message from the Guest Editors

Dear Colleagues,

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





an Open Access Journal by MDPI

## Editors-in-Chief

**Prof. Dr. Charles Brennan**

**Prof. Dr. Andreas Taubert**

**Prof. Dr. Kurt A. Jellinger**

**Prof. Dr. Ian A. Nicholls**

**Dr. Stephen A. Bustin**

**Prof. Dr. Xiaofeng Jia**

**Prof. Dr. Maurizio Battino**

**Prof. Dr. Guido R.M.M. Haenen**

**Prof. Dr. Setsuko Komatsu**

**Prof. Dr. Claudiu T. Supuran**

**Prof. Dr. Irmgard Tegeder**

## Message from the Editorial Board

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.

## Author Benefits

**Open Access:** free for readers, with article processing charges (APC) paid by authors or their institutions.

**High Visibility:** indexed by the **Science Citation Index Expanded** (Web of Science), MEDLINE (PubMed), Scopus and other databases.

**Rapid Publication:** manuscripts are peer-reviewed and a first decision provided to authors approximately 16.2 days after submission; acceptance to publication is undertaken in 2.5 days (median values for papers published in this journal in the second half of 2019).

## Contact Us

*International Journal of Molecular  
Sciences*  
MDPI, St. Alban-Anlage 66  
4052 Basel, Switzerland

Tel: +41 61 683 77 34  
Fax: +41 61 302 89 18  
www.mdpi.com

mdpi.com/journal/ijms  
ijms@mdpi.com  
@IJMS\_MDPI