International Journal of
Molecular Sciences

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Computational Studies of Biomolecules

Guest Editor:

Deadline for manuscript submissions:
closed (1 October 2020)

Message from the Guest Editor

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

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Editor-in-Chief

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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.

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