Topical Collection

Computational Studies of Biomolecules

Message from the Collection Editors

The current Topical Collection aims to attract high-quality contributions of modeling biomolecular structures, dynamics, functions, and interactions with the potential of interpretation of experimental data and applications 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;
- Modeling of protein and nucleic acid dynamics;
- Protein docking;
- Protein–ligand interactions;
- Nucleic acid–ligand interactions;
- Protein design;
- Computational enzymology–enzymatic reaction mechanisms;
- Protein homology modeling.

Collection Editors

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The *International Journal of Molecular Sciences* (*IJMS*) 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, and molecular biophysics. *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

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