# Special Issue

## Advances in Molecular Modeling, Docking and Simulations of Protein Structure

**Message from the Guest Editor**

Molecular modeling has been used for decades as a support for or in combination with experimental results. Most in silico experiments in this area have cover the nano-, micro-, and recently meso-scale events/phenomena/mechanisms of interest.

This Special Issue of IJMS aims to compile original research articles or novel communications that address the use of molecular modeling, molecular docking and computer simulations in the context of their predictive power/essential contribution in: (i) identifying novel aspects of molecular mechanisms/structure–activity relationships within protein complexes; (ii) analyses/predictions of protein/peptide structures; (iii) understanding interactions in protein complexes; (iv) designing novel protein-binding ligands/peptides, etc.

Works should utilize computational tools such as molecular dynamics simulations (in all their varieties), molecular docking, Monte Carlo methods, molecular modeling methods, QM/MM, etc.

Systems simulated/analyzed should include amino acid-based proteins or peptides. The study of complexes with DNA/RNA/lipids/ligands, etc., is also encouraged.

**Guest Editor**

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**Deadline for manuscript submissions**

closed (20 June 2024)

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## About the Journal

### 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

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