

## Special Issue

# Computational Intelligence in Structure and Function Prediction and Modeling of Proteins—2nd Edition

### Message from the Guest Editors

Exploring the functions and structures of proteins is paramount for understanding the molecular mechanisms of life. The analyses and predictions of protein functional residues contribute to the research of protein function. The traditional approaches used to extract information regarding protein structures and functions all rely on biophysical or biochemical-associated technologies. These technologies need expensive experimental instruments, complex experimental procedures, and elaborate human resources. They benefit from the development of bioinformatics, which uses intelligent computing methods to accurately predict protein structure information and functional residues.

This Special Issue of *Biomolecules* is dedicated to computational methods and analyses focusing on the identification, elucidation, and analysis of protein function-related factors. We welcome both original articles and surveys that cover state-of-the-art advances in this rapidly developing area. We also encourage the submission of experimental studies that are coupled with computational analysis.

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### Guest Editors

Dr. Jian Zhang

Dr. Bi Zhao

Dr. Haiting Chai

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### Deadline for manuscript submissions

15 June 2026



## Biomolecules

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### Message from the Editorial Board

*Biomolecules* is a multidisciplinary open-access journal that reports on all aspects of research related to biogenic substances, from small molecules to complex polymers. We invite manuscripts of high scientific quality that pertain to the diverse aspects relevant to organic molecules, irrespective of the biological question or methodology. We aim for a competent, fair peer review and rapid publication. Please look at some of the exciting work that has been published in *Biomolecules* so far. We would be delighted to welcome you as one of our authors.

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