Special Issue

Biophysical Studies of Protein Structure-Function Relationships

Message from the Guest Editors

Traditionally, the structural characterization of proteins has relied on experimental techniques such as X-ray crystallography, nuclear magnetic resonance, cryo-electron microscopy, absorption, and fluorescence. These spectroscopic and imaging methods have contributed significantly to our current understanding of protein architecture at the atomic level. In recent years, computational methods have emerged as powerful complementary tools. Molecular modeling, molecular dynamics simulations, and AI-based structure prediction tools, such as AlphaFold, allow researchers to explore protein structures with increasing accuracy and efficiency. Importantly, new algorithms are being developed to better capture the conformational ensembles of IDPs and predict their interaction networks. When combined with experimental data, these in silico approaches offer a more complete picture of protein behavior. Knowledge of protein structure — including the dynamic and disordered nature of IDPs — allows for the rational design of molecules that can modulate protein function, paving the way for targeted therapies in numerous diseases.

Guest Editors

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Deadline for manuscript submissions

20 February 2026

International
Journal of
Molecular
Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed

mdpi.com/si/253670

International Journal of Molecular Sciences
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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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