

Special Issue

Computational Molecular Biology of Metabolic Pathways and Signal Transduction Pathways

Message from the Guest Editor

The regulation of metabolic pathways and the associated signal transduction has received immense therapeutic importance due to their key role in major neural disorders and tumor regulations and onco-metabolism. Furthermore, the metabolic pathways and signal transduction are entirely regulated through interactions of small bio-ligands, signaling molecules, neurotransmitters with receptors, proteins, and membrane bilayer proteins. The complete understanding of these interactions, their binding mode, and their associated biological function are dependent on how good we establish or understand the structure–activity relationship that actually helps in comprehension of these biological functions. Computational structural and molecular biology has emerged as an interdisciplinary discipline in combination with theoretical and computational chemistry and biophysics to explore the biological functions at molecular and atomistic levels. Since I have been working in the quoted areas with my colleague Dr. Khair Bux, thus, it would be a great pleasure to work as the Guest editor for this Special Issue of *IJMS*.

Guest Editor

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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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