

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

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