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Computational Studies in Analysis and Prediction of Protein Properties

Guest Editor:

Dr. Mehdi D. Davari
RWTH Aachen Univeristy

Deadline for manuscript submissions:
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Message from the Guest Editor

Proteins are macromolecules essential for biological life. They play many critical roles in countless biological processes, for instance, they are involved in DNA replication, catalysis and regulation of biochemical reactions and networks, and so on. Protein function and properties can be understood in terms of its three-dimensional structure. Establishing a protein structure–function relationship is crucial for understanding its biological function. Experimental techniques (e.g., X-Ray, NMR, SAXS, and Cryo-EM) have been employed for protein structure prediction in solution and crystal state and to understand the mechanisms defining the function of proteins; however, the determination of the structure and dynamics of large protein complexes and other biomolecular assemblies remains a major challenge in structural biology and biochemistry. Computational structural biology has made enormous progress over the last three decades. These methods include molecular modeling and refinement of 3D structures, de novo design of proteins, protein folding and stability, macromolecular function and protein design and prediction of macromolecular interactions and so on.

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Editor-in-Chief

Prof. Dr. Alessandra Toncelli
Department of Physics, University of Pisa, 56126 Pisa, Italy

Message from the Editor-in-Chief

Welcome to *Crystals*, the journal dedicated to the fascinating world of crystallographic research! Crystals are more than mere decorative elements; they hold the key to understanding the fundamental structure of matter. Our mission is to explore the crucial significance of this research across various fields. From medicine to technology, chemistry to geology, crystals play a vital role. Their structure provides insights into new advanced materials, innovative drugs, and groundbreaking technologies. Through *Crystals*, we delve into the microscopic world to discover solutions that will shape the future. Join us on a journey through the *Crystals*, where science merges with beauty and innovation.

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Contact Us

Crystals Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/crystals
crystals@mdpi.com
𝕏@Crystals_MDPI