

Special Issue

Protein Domains: Structures and Molecular Functions

Message from the Guest Editors

After the completion of human genome projects, it was shown that more than 70% of the genes are encoding multidomain proteins with two or more domains. Understanding of structure–function relationships of the individual domains should lead to interpretations of new physiological functions of unknown genes. We are motivated by this idea to develop methods for high-throughput structure determination, structure prediction, accurate modeling, molecular dynamic simulation, and the prediction of functions. The accumulation of structural, functional and evolutionary knowledge of protein domains is still being continued and is providing an important basis for structure-guided drug discovery, protein therapeutics, genome-based diagnosis, designed proteins, molecular beacons and sensors, and synthetic biology. This Special Issue focuses on recent advances in the domain-centric analysis of proteins in the field of biochemistry, bioinformatics and biophysics. In addition, either the analysis of natural domain pairs (architectures) or the design of artificial multi-domain proteins are in focus. Original research papers, concise reviews, and perspectives are welcome.

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 30th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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