Special Issue

Application of Computational Studies for Elucidation of Protein Structure and Function

Message from the Guest Editor

Nowadays, computational techniques are widely applied to various problems including biological systems. In particular, many computer simulation techniques are applied to protein dynamics and folding. Bioinformatics techniques are also applied to extract various information from amino acid sequences and evolutional results. Artificial intelligence techniques have been developed in the field of protein structure prediction. Thus, we are planning this Special Issue regarding new applications of various computational techniques to solve problems related to protein structures and functions. It should be noted that pure theoretical works are important to solve protein problems. We are also interested in very complicated protein systems and drug discovery.

Guest Editor

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As the premier open access journal dedicated to molecular chemistry, now in its 29th 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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