Special Issue

Computational Approaches for Protein Design

Message from the Guest Editors

Computational approaches for protein design, as demonstrated by AI-based technologies, have shown high efficiency in protein design and accurate prediction of molecular structures. These approaches are particularly attractive when solutions for complex problems are designed using transferable learning and pre-trained models, enabling computational biologists to find explanatory models in the presence of uncertainties existing in molecular data. Discovering new insights in molecular data is a key area of research within deep learning frameworks based on hierarchical feature representation. This approach has demonstrated high efficiency in learning explanatory models from underdetermined or imbalanced data.

Authors are invited to contribute research and review articles to this Special Issue to be considered for publication. The main focus of this Special Issue is on new theoretical results and reproducible applications that demonstrate the advantages of computational approaches in protein design and the prediction of molecular structures.

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The *International Journal of Molecular Sciences* (*IJMS*) 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, and molecular biophysics. *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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