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Protein Structure-Function Relationships and Inhibition: From Molecular Insights to Therapeutic Applications

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Message from the Guest Editors

Dear Colleagues,

Proteins are central players in all biological processes. A fundamental paradigm of structural biology assumes that the functionality of these macromolecules is strictly related to their three-dimensional structures. In this scenario, the understanding of protein structures is a prerequisite for modulating their activities and for developing new therapeutic agents targeting these giant biomolecules. The acquisition of atomic-level structural information about proteins is also fundamental for their modulation. For decades, this task has been extremely difficult due to the complex and time-consuming methodologies utilized to obtain experimental structural data. Very recently, the introduction of effective machine-learning-based approaches, such as Alpha Fold, has provided accurate structural information about proteins, starting from their amino acid sequences. This represents an extremely useful tool for the development of novel molecular entities aimed at enhancing or impairing protein functions.

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Message from the Editor-in-Chief

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