Special Issue

X-ray Crystallography and Drug Discovery

Message from the Guest Editor

High-resolution protein structures obtained by X-ray crystallography are a powerful tool in the drug discovery process. The atomic information about the target protein structure or the knowledge of the interaction of protein–ligand complexes contributes to driving the design of a new drug. Hence, structure-based drug discovery (SBDD) requires the use of structural information in drug development. In order to achieve this goal is essential to make high-ordered crystals keeping their quality unaltered from crystallization to data acquisition. Crystallization tips such as co-crystallization induced by streak seeding, microseeding, macroseeding, etc. can help to attain suitable reproducibility of crystals that diffract at high resolution. Finally, in the drug discovery process, the synergy between the X-ray crystallography scientists and the medicinal chemistry and computational chemistry researchers is necessary to merge all information acquired for proposing new (or optimized) ligands as drug candidate molecules.

Guest Editor

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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.

Editor-in-Chief

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