



X-ray Crystallography and Drug Discovery

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Message from the Guest Editor

Dear Colleagues,

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.





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Message from the Editor-in-Chief

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