Special Issue

Biophysical Insights into Small Molecule Inhibitors

Message from the Guest Editor

This Special Issue aims to highlight recent advances in the study of small molecule inhibitors through a multidisciplinary biophysical lens. Emphasis will be placed on computational and experimental strategies that elucidate molecular recognition, binding mechanisms, and structure–activity relationships (SAR). Topics of interest include molecular dynamics simulations, free energy calculations, docking, QSAR modeling, and innovative descriptor-based approaches for rational drug design. Studies integrating traditional methods with novel computational or imaging-based descriptor extraction are particularly welcome, as they offer new perspectives for the characterization and optimization of inhibitors. Contributions spanning theory, methodology, and applied case studies are encouraged, with the ultimate goal of advancing drug discovery and providing deeper insights into molecular interactions.

Guest Editor

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