Special Issue

Computational Design and Mechanistic Studies of Metal-Based Therapeutics

Message from the Guest Editors

The pivotal role of metal complexes in contemporary medicinal chemistry necessitates continued investigation, particularly through the lens of computational design and mechanistic elucidation. The considerable therapeutic promise of metal-based pharmaceuticals is evident in the extensive array of both platinum and non-platinum metallodrugs exhibiting a spectrum of biological activities. Computational methodologies are increasingly crucial in the rational design of metal-based therapeutics, enabling the precise manipulation of structural features to achieve desired biological outcomes and providing a rich chemical space for targeted computational drug development. This Special Issue aims to consolidate cutting-edge research focused on the computational design and mechanistic studies of metal-based medicinal complexes, integrating diverse computational approaches.

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Biomolecules is a multidisciplinary open-access journal that reports on all aspects of research related to biogenic substances, from small molecules to complex polymers. We invite manuscripts of high scientific quality that pertain to the diverse aspects relevant to organic molecules, irrespective of the biological question or methodology. We aim for a competent, fair peer review and rapid publication. Please look at some of the exciting work that has been published in *Biomolecules* so far. We would be delighted to welcome you as one of our authors.

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