Special Issue

Transition Metal Complexes with Heterocyclic Ligands: Structural Insights, Biological Potential, and Computational Perspectives

Message from the Guest Editors

This Special Issue, titled “Transition Metal Complexes with Heterocyclic Ligands: Structural Insights, Biological Potential, and Computational Perspectives”, brings together contributions on the synthesis, structural characterization, and biological evaluation of transition metal–heterocyclic complexes. Special emphasis is placed on the role of advanced spectroscopic and crystallographic techniques (XRD, NMR, FTIR, and related methods) in elucidating the molecular architecture and reactivity patterns of these compounds. In addition, computational approaches ranging from density functional theory (DFT) calculations to molecular docking and molecular dynamics simulations provide valuable mechanistic insights into their interaction with biomolecular targets, complementing experimental findings.

Guest Editors

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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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