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Rational Design of Pharmacologically Active Metal-Based Compounds

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Message from the Guest Editors

Metal-based biomolecules are involved in vital biochemical processes, being the active sites of metalloproteins, metalloenzymes, metal-containing and metal-binding drugs with a remarkable structural diversity and potential therapeutic and diagnostic applications. In recent years, the unique properties of metal-based compounds have tended to offer advantages in the discovery and development of new drugs. Much attention has focused on designing new structures with the desired composition and properties, e.g., coordination complexes, supramolecular structures as well as advanced nanomaterials with improved pharmacological properties and a broader range of activity.

This Special Issue focuses on recent advances in this multidisciplinary field with an emphasis on rational design, theoretical, analytical and physicochemical drug discovery strategies, related to biologically relevant applications. Original research articles, short communications and reviews highlighting the latest advances in the field will be considered for publication.











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Message from the Editor-in-Chief

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