Special Issue

Rational Design of Pharmacologically Active Metal-Based Compounds, 2nd Edition

Message from the Guest Editor

Metal-based biomolecules are involved in vital biochemical processes, being the active sites of metalloproteins, metalloenzymes, metal-containing and metal-binding drugs; in addition, they have 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. Additionally, the effects of metals can be highly specific and can be modulated to recognize specific metal-macromolecule interactions and to modify a number of properties including the charge, lipophilicity, lability, shapes and redox potentials. Much attention has focused on designing new structures with the desired composition and properties, e.g., coordination complexes and supramolecular structures, as well as advanced nanomaterials with improved pharmacological properties and a broader range of activity. A second volume has been launched to continue the discussion of this multidisciplinary field with an emphasis on rational design, theoretical, analytical and physicochemical drug discovery strategies related to biologically relevant applications.

Guest Editor

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Editor-in-Chief

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