Special Issue

Metal Complexes Containing Bioactive Ligands: Structure and Biological Evaluation

Message from the Guest Editor

This Special Issue aims to illuminate and present modern synthetic procedures used for the chemical modification of bioactive compounds, with a clear outline of the mechanism of modification and complete chemical characterization of intermediates and products. This research topic also covers the theoretical methods used for the prediction of the reaction mechanism, stability of compounds, complexation modes, and interactions through DFT, Natural Bond Orbital, and Quantum Theory of Atoms in Molecules Analyses. Articles, including those on Molecular Docking and Molecular Dynamics and SARS studies, are also welcome if they include the prediction of the physicochemical properties, binding modes, toxicity, or biological activity of compounds based on natural products and their transition metal complexes.

Keywords:

- bioactive ligands
- transition metal complexes
- dft
- molecular dynamics
- cytotoxicity
- antioxidant activity

Guest Editor

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