

Special Issue

Synthesis, Structure, Molecular Modeling, and Bioactivity of Metal Complexes

Message from the Guest Editor

Bioinorganic and Computational Chemistry have reached a level of maturity and are now considered central scientific disciplines in the pharmaceutical industry. They involve exploring the applications of metal compounds in vital biological mechanisms and pathways, such as biological signaling, molecular recognition, and biocatalysis, in combination with computational contributions to optimize cost-effective synthetic routes and screen extensive databases. Additionally, they entail proposing hypotheses regarding the potential mechanisms of action of drugs in biological systems. This Special Issue of *Molecules* is dedicated to showcasing the application of these methods in medicinal computational chemistry. We warmly invite fellow scientists to submit original papers or reviews that will undoubtedly enhance cutting-edge knowledge in this field.

Guest Editor

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 30th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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