Special Issue

Application of Computational Methods and Biomolecular Structural Modeling to the Investigation of Metalloproteins

Message from the Guest Editors

The structural bioinformatics of metalloproteins is important for providing links between 3D structure and biological function, with particular focus on the role of metal ions and how this role has evolved and become diversified among organisms. In this Special Issue, we wish to cover the most recent advances in all these aspects of computational methods for the study of metalloproteins by hosting a mix of original research articles and short critical reviews.

Guest Editors

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Deadline for manuscript submissions

closed (31 August 2021)

Molecules

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Impact Factor 4.6
CiteScore 8.6
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mdpi.com/si/45417

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As the premier open access journal dedicated to molecular chemistry, now in its 29th 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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