



Molecular Dynamics Simulations of Metal-Binding Proteins and Nucleic Acids

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Message from the Guest Editor

More than one-third of all known proteins encoded need at least one metal ion to perform their biological function. Various metal-containing cofactors require dedicated biosynthetic enzymes for their assembly. Metal ions are also crucial to tune and stabilize the three-dimensional (3D) structure of nucleic acids, and to promote intermolecular interactions. To understand how the aforementioned processes work, it is necessary to investigate the 3D structure and mobility of the involved macromolecules at the atomic level. Molecular dynamics (MD) simulations complement experimental information and generate new hypotheses on the molecular and cellular functions of metal ions. Among the specific challenges posed by the MD of metal-binding macromolecular systems, a particularly relevant one is the parametrization of the metal site. This is obviously crucial to achieve an accurate interpretation of the data.





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Message from the Editor-in-Chief

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