

Numerous essential biological functions involve metalloproteins; therefore, understanding metalloproteins and how to manipulate them is significant in the biological and medical fields. An examination of current research, **Metalloproteins: Theory, Calculations, and Experiments** explores the interplay between theory and experiment, detailing the role of theoretical modeling in the field and explaining how it aids experiments. The text also presents the current state of computational protein modeling, enabling researchers to adopt computation as an integral component of their studies.

Features

- Discusses the interplay between theory and experiment in the field of metalloproteins
- Analyzes structure, function, and interactions
- Provides theoretical and experimental points of view
- Details the computational chemical aspects of metalloproteins

This book addresses two different aspects on metalloproteins in unison. It reviews the development of theoretical and computational methods for metalloprotein simulation with specific examples. The authors also present some of the most intriguing and important experimental results on metalloprotein systems. Although a connection can be made between these two aspects of the research, the authors do not do so explicitly. Rather, they provide the platform required to ignite further collaboration between experimentalists and theoreticians.

A collection of works from top researchers in this field, the text presents diverse subjects that comprehensively reflect the current state of metalloprotein research. With these advances in structural information, theory and computation are starting to play a more significant role, particularly in identifying the reaction mechanism. The book summarizes some of the recent progress in both experiments and theory/computation, showing the synergy that is now developing.



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