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Structural and Mechanistic Enzymology: Bringing Together Experiments and Computing (Advances in Protein Chemistry and Structural Biology)

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Both strategies for investigation (computational and experimental) in structural and mechanistic Enzymology have developed to some extent independently. However, over the last few years a trend has emerged for strengthening their integration. This combination not only brings together computations and experiments focused on the same enzymatic problems, but also provides complementary insights into the investigated properties and has a powerful synergy effect. This thematic volume of *Advances in Protein Chemistry and Structural Biology* focuses on the recent success in structural and mechanistic enzymology and has its main emphasis on explaining the enzyme phenomena by using both the experimental and computational approaches. The selected contributions demonstrate how the application of a variety of experimental techniques and modeling methods helps further the understanding of enzyme dynamics, mechanism, inhibition, and drug design.

Focuses on the recent success in structural and mechanistic enzymology.

Has its main emphasis on explaining the enzyme phenomena by using both the experimental and computational approaches.

Demonstrates how the application of a variety of experimental techniques and modeling methods helps further the understanding of enzyme dynamics, mechanism, inhibition, and drug design.



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