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Structural Biology in Drug Discovery Jean-Paul Renaud, 2020-01-27 With the most comprehensive and up-to-date overview of structure-based drug discovery covering both experimental and computational approaches, *Structural Biology in Drug Discovery: Methods, Techniques, and Practices* describes principles, methods, applications, and emerging paradigms of structural biology as a tool for more efficient drug development. Coverage includes successful examples, academic and industry insights, novel concepts, and advances in a rapidly evolving field. The combined chapters, by authors writing from the frontlines of structural biology and drug discovery, give readers a valuable reference and resource that: Presents the benefits, limitations, and potentiality of major techniques in the field such as X-ray crystallography, NMR, neutron crystallography, cryo-EM, mass spectrometry and other biophysical techniques, and computational structural biology Includes detailed chapters on druggability, allostery, complementary use of thermodynamic and kinetic information, and powerful approaches such as structural chemogenomics and fragment-based drug design Emphasizes the need for the in-depth biophysical characterization of protein targets as well as of therapeutic proteins, and for a thorough quality assessment of experimental structures Illustrates advances in the field of established therapeutic targets like kinases, serine proteinases, GPCRs, and epigenetic proteins, and of more challenging ones like protein-protein interactions and intrinsically disordered proteins

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LanguageBeyond the One-Electron DescriptionIndex Readership: Physicists and chemists, graduate and undergraduate students in chemical physics.
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Molecular Dynamics Simulations of Disordered Materials Carlo Massobrio,Jincheng Du,Marco Bernasconi,Philip S. Salmon,2015-04-22 This book is a unique reference work in the area of atomic-scale simulation of glasses. For the first time, a highly selected panel of about 20 researchers provides, in a single book, their views, methodologies and applications on the use of molecular dynamics as a tool to describe glassy materials. The book covers a wide range of systems covering traditional network glasses, such as chalcogenides and oxides, as well as glasses for applications in the area of phase change materials. The novelty of this work is the interplay between molecular dynamics methods (both at the classical and first-principles level) and the structure of materials for which, quite often, direct experimental structural information is rather scarce or absent. The book features specific examples of how quite subtle features of the structure of glasses can be unraveled by relying on the predictive power of molecular dynamics, used in connection with a realistic description of forces.

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