Structure-Based Drug Discovery: An Overview (RSC Biomolecular Sciences)

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Structure-based drug discovery is a collection of methods that exploits the ability to determine and analyse the three dimensional structure of biological molecules. These methods have been adopted and enhanced to improve the speed and quality of discovery of new drug candidates. After an introductory overview of the principles and application of structure-based methods in drug discovery, this book then describes the essential features of the various methods. Chapters on X-ray crystallography, NMR spectroscopy, and computational chemistry and molecular modelling describe how these particular techniques have been enhanced to support rational drug discovery, with discussions on developments such as high throughput structure determination, probing protein-ligand interactions by NMR spectroscopy, virtual screening and fragment-based drug discovery. The concluding chapters complement the overview of methods by presenting case histories to demonstrate the major impact that structure-based methods have had on discovering drug molecules. Written by international experts from industry and academia, this comprehensive introduction to the methods and practice of structure-based drug discovery not only illustrates leading-edge science but also provides the scientific background for the non-expert reader. The book provides a balanced appraisal of what structure-based methods can and cannot contribute to drug discovery. It will appeal to industrial and academic researchers in pharmaceutical sciences, medicinal chemistry and chemical biology, as well as providing an insight into the field for recent graduates in the biomolecular sciences.

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