



Structure-based Drug Discovery

Harren Jhoti, Andrew R. Leach

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Structure-based drug discovery methods have been transformed in the last 5-10 years and are now having a major impact on the discovery of new drugs. Some of the most exciting developments in the field, such as Fragment-based methods, are described in this book. The book describes the latest developments in technologies that can be used to obtain the 3-D structures including the high profile structural genomics approaches being utilised worldwide. The use of 3-D protein structures in new, Fragment-based, approaches to drug discovery are described in some detail. This book includes experimental approaches using X-ray crystallography and NMR for Fragment-based screening as well as other biophysical methods for studying protein/ligand interactions. In addition, developments in computational chemistry methodology are covered together with an assessment of practical applications.

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