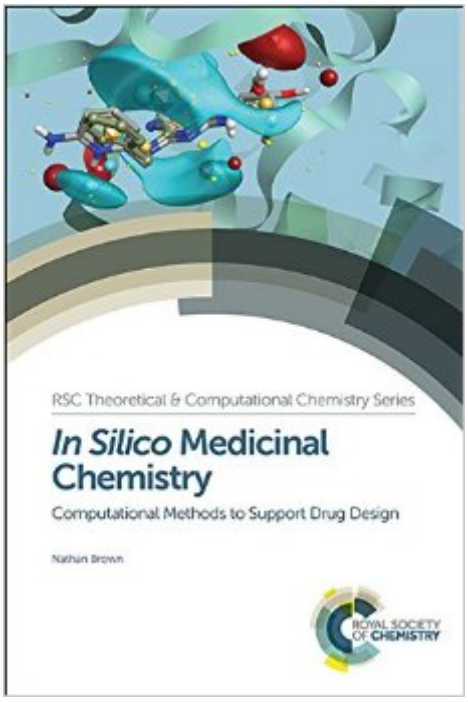
In Silico Medicinal Chemistry: Computational Methods To Support Drug Design (Theoretical And Computational Chemistry Series)



Synopsis

Covering computational tools in drug design using techniques from chemoinformatics, molecular modelling and computational chemistry, this book explores these methodologies and applications of in silico medicinal chemistry. The first part of the book covers molecular representation methods in computing in terms of chemical structure, together with guides on common structure file formats. The second part examines commonly used classes of molecular descriptors. The third part provides a guide to statistical learning methods using chemical structure data, covering topics such as similarity searching, clustering and diversity selection, virtual library design, ligand docking and de novo design. The final part of the book summarises the application of methods to the different stages of drug discovery, from target ID, through hit finding and hit-to-lead, to lead optimisation. This book is a practical introduction to the subject for researchers new to the fields of chemoinformatics, molecular modelling and computational chemistry.

Book Information

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