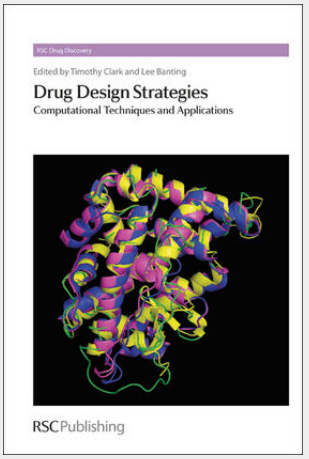
Banting / Clark

Drug Design Strategies

Computational Techniques and Applications



This book documents the latest research into the theory and application of force-fields, semi-empirical molecular orbital, density functional and ab initio calculations, Quantum Mechanical (QM) based modelling, Atoms in Molecules (AIM) approach, and biomolecular dynamics. It also covers theory and application of 2D cheminformatics, QSAR/QSPR, ADME properties of drugs, drug docking/scoring protocols and approaches, topological methodology, and modelling accurate inhibition constants of enzymes. Finally, the book gives the theory and applications of multiscale modelling of proteins and biomolecular systems. The information need for a book in this area is due to the continuing rapid advance of firstly theoretical approaches, secondly software/hardware and lastly the successful application of the technology and this book fills a gap in the literature. The co-editors have extensive experience of teaching and researching in the field and the book includes contributions from cutting-edge academic and industrial researchers in their respective fields. It is essential reading for medicinal chemists, computational chemists and those in the pharmaceutical industry.

Drug Design Strategies: Computational Techniques and Applications documents the latest research into the theory and application of force-fields, semi-empirical molecular orbital, density functional and ab initio calculations, Quantum Mechanical (QM) based modelling, Atoms in Molecules (AIM) approach, and biomolecular dynamics. It also covers theory and application of 2D cheminformatics, QSAR/QSPR, ADME properties of drugs, drug docking/scoring protocols and approaches, topological methodology, and modelling accurate inhibition constants of enzymes. Finally, the book gives the theory and applications of multiscale modelling of proteins and biomolecular systems. The information need for a book in this area is due to the continuing rapid advance of firstly theoretical approaches, secondly software/hardware and lastly the successful application of the technology and this book fills a gap in the literature. The co-editors have extensive experience of teaching and researching in the field and the book includes contributions from cutting-edge academic and industrial researchers in their respective fields. It is essential reading for medicinal chemists, computational chemists and those in the pharmaceutical industry.

193,50 €
180,84 € (zzgl. MwSt.)

Lieferfrist: bis zu 10 Tage

Artikelnummer: 9781849731676
Medium: Buch
ISBN: 978-1-84973-167-6
Verlag: RSC Publishing
Erscheinungstermin: 18.01.2012
Sprache(n): Englisch
Auflage: Erscheinungsjahr 2012
Serie: Drug Discovery
Produktform: Gebunden
Gewicht: 526 g
Seiten: 239
Format (B x H): 162 x 241 mm