



*molecules*

IMPACT  
FACTOR  
**4.2**

Indexed in:  
**PubMed**

CITESCORE  
**7.4**

*Special Issue Reprint*

## **Molecular Modeling in Drug Design**

[www.mdpi.com/books/reprint/1187](http://www.mdpi.com/books/reprint/1187)

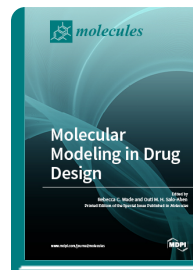
Edited by

Rebecca Wade

Outi Salo-Ahen

ISBN 978-3-03897-614-1 (Softback)

ISBN 978-3-03897-615-8 (PDF)



Since the first attempts at structure-based drug design about four decades ago, molecular modelling techniques for drug design have developed enormously, along with the increasing computational power and structural and biological information of active compounds and potential target molecules. Nowadays, molecular modeling can be considered to be an integral component of the modern drug discovery and development toolbox. Nevertheless, there are still many methodological challenges to be overcome in the application of molecular modeling approaches to drug discovery. The eight original research and five review articles collected in this book provide a snapshot of the state-of-the-art of molecular modeling in drug design, illustrating recent advances and critically discussing important challenges. The topics covered include virtual screening and pharmacophore modelling, chemoinformatic applications of artificial intelligence and machine learning, molecular dynamics simulation and enhanced sampling to investigate contributions of molecular flexibility to drug–receptor interactions, the modeling of drug–receptor solvation, hydrogen bonding and polarization, and drug design against protein–protein interfaces and membrane protein receptors.



Order Your Print Copy

You can order print copies at

[www.mdpi.com/books/reprint/1187](http://www.mdpi.com/books/reprint/1187)

MDPI Books offers quality open access book publishing to promote the exchange of ideas and knowledge in a globalized world. MDPI Books encompasses all the benefits of open access – high availability and visibility, as well as wide and rapid dissemination. With MDPI Books, you can complement the digital version of your work with a high quality printed counterpart.



## Open Access

Your scholarly work is accessible worldwide without any restrictions. All authors retain the copyright for their work distributed under the terms of the Creative Commons Attribution License.



## Author Focus

Authors and editors profit from MDPI's over two decades of experience in open access publishing, our customized personal support throughout the entire publication process, and competitive processing charges as well as unique contributor discounts on book purchases.



## High Quality & Rapid Publication

MDPI ensures a thorough review for all published items and provides a fast publication procedure. State-of-the-art research and time-sensitive topics are released with a minimum amount of delay.



## High Visibility

Due to our global network and well-known channel partners, we ensure maximum visibility and broad dissemination. Title information of books is sent to international indexing databases and archives, such as the Directory of Open Access Books (DOAB), and the Verzeichnis Lieferbarer Bücher (VLB).



## Print on Demand and Multiple Formats

MDPI Books are available for purchase and to read online at any time. Our print-on-demand service offers a sustainable, cost-effective and fast way to publish MDPI Books printed versions.