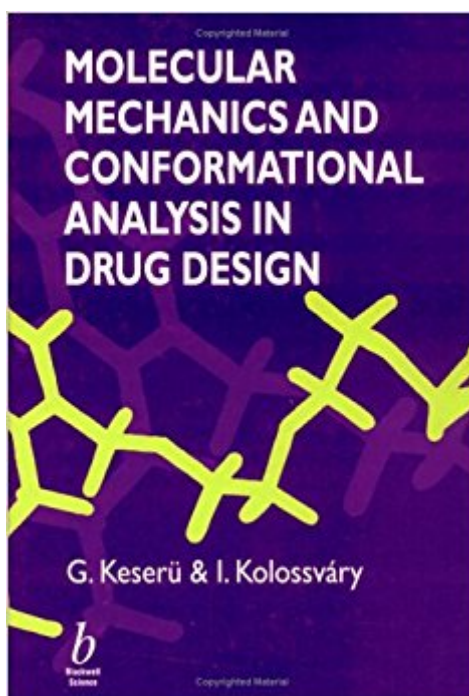


The book was found

# Molecular Mechanics And Conformational Analysis In Drug Design



## Synopsis

Molecular modelling truly has come of age. Computational chemistry techniques are now routinely used to simulate chemical and physical properties before synthesis. The widespread availability of high-performance computer processing power combined with an abundance of computational chemistry software has allowed non-specialists to do modelling previously reserved for specialists. But the software has not yet evolved to the point where its results can be taken on faith. All outputs are highly dependent on the inputting assumptions, so an understanding of these are fundamental to any serious studies. This book provides clear descriptions of the theoretical background to molecular mechanics-based conformational energy calculations. Although the book is written primarily for the non-specialist, there is enough rigour to serve as an essential reference for experts. Using real examples, the emphasis is on demonstrating how the calculations relate to actual studies. The non-specialist can omit certain sections and still get a working knowledge of all the important methods.

## Book Information

Hardcover: 176 pages

Publisher: Blackwell Publishing; 1 edition (March 29, 1999)

Language: English

ISBN-10: 0632052899

ISBN-13: 978-0632052899

Product Dimensions: 0.8 x 6.8 x 9.8 inches

Shipping Weight: 1.3 pounds (View shipping rates and policies)

Average Customer Review: Be the first to review this item

Best Sellers Rank: #8,529,518 in Books (See Top 100 in Books) #34 in [Books > Medical Books > Pharmacology > Molecular](#) #550 in [Books > Medical Books > Pharmacology > Chemistry](#) #1087 in [Books > Computers & Technology > Programming > Software Design, Testing & Engineering > Structured Design](#)

## Customer Reviews

Molecular modelling has truly "come to age". Computational chemistry techniques are now routinely used to simulate chemical and physical properties before synthesis. The widespread availability of high-performance computer processing power combined with an abundance of computational chemistry software has allowed non-specialists to do modelling previously reserved for specialists. However, the software has not yet evolved to the point where its results can be taken on faith. All

outputs are highly dependent on the inputting assumptions,

[Download to continue reading...](#)

Molecular Mechanics and Conformational Analysis in Drug Design Conformational Analysis of Medium-Sized Heterocycles (Methods in Stereochemical Analysis) The Nuclear Overhauser Effect in Structural and Conformational Analysis, 2nd Edition The Conformational Analysis of Heterocyclic Compounds Advanced Molecular Quantum Mechanics: An Introduction to Relativistic Quantum Mechanics and the Quantum Theory of Radiation (Studies in Chemical Physics) Mechanics of Materials (Computational Mechanics and Applied Analysis) Graphic Design Success: Over 100 Tips for Beginners in Graphic Design: Graphic Design Basics for Beginners, Save Time and Jump Start Your Success (graphic ... graphic design beginner, design skills) Reinforced Concrete: Mechanics and Design (4th Edition) (Civil Engineering and Engineering Mechanics) Cellular and Molecular Immunology: with STUDENT CONSULT Online Access, 7e (Abbas, Cellular and Molecular Immunology) Cellular and Molecular Immunology, 8e (Cellular and Molecular Immunology, Abbas) Bacteriophages: Methods and Protocols, Volume 2: Molecular and Applied Aspects (Methods in Molecular Biology) Hemoglobin Disorders: Molecular Methods and Protocols (Methods in Molecular Medicine, Vol. 82) Molecular Simulation Studies on Thermophysical Properties: With Application to Working Fluids (Molecular Modeling and Simulation) Molecular Biology (WCB Cell & Molecular Biology) Current Topics in Computational Molecular Biology (Computational Molecular Biology) Molecular Visions (Organic, Inorganic, Organometallic) Molecular Model Kit #1 by Darling Models to accompany Organic Chemistry Organic Chemistry Molecular Model Set: Molecular Model Set Molecular Visions Organic Model Kit with Molecular Modeling Handbook Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics Computational Fluid Mechanics and Heat Transfer, Third Edition (Series in Computational and Physical Processes in Mechanics and Thermal Sciences)

[Contact Us](#)

[DMCA](#)

[Privacy](#)

[FAQ & Help](#)