

# Topics in Current Chemistry

**174**

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## **Molecular Similarity II**



**Springer**

# Molecular Similarity Ii Topics In Current Chemistry Vol 174

**Ensheng Dong**



## **Molecular Similarity Ii Topics In Current Chemistry Vol 174:**

*Advances in Molecular Similarity* R. Carbó-Dorca,P.G. Mezey,1999-02-18 This volume highlights some of the advances in molecular similarity Molecular similarity research is a dynamic field where the rapid transfer of ideas and methodologies from the theoretical quantum chemical and mathematical chemistry disciplines to efficient algorithms and computer programs used in industrially important applications is especially evident These applications often serve as motivating factors toward new advances in the fundamental and theoretical fields and the combination of intellectual challenge and practical utility provides mutual advantages to theoreticians and experimentalists The aim of this volume is to present an overview of the current methodologies of molecular similarity studies and to point out new challenges unsolved problems and areas where important new advances can be expected *Adaptive Systems in Drug Design* Gisbert Schneider,Sung-Sau

So,2002-10-01 A brief history of drug design presented to make clear that there are fashions in this important field and that they change rather rapidly This is due in part to the fact that the way that a new paradigm is accepted in a drug company often does not depend on its scientific merit alone *Indian Journal of Biochemistry and Biophysics* ,1996 Indian Journal of Biochemistry & Biophysics ,1999 *Contributions to Science* ,1999 **Subject Guide to Books in Print** ,1997

*International Books in Print*, 1995 Barbara Hopkinson,[Anonymus AC01401231],1995 *Books in Print* ,1991

*Reviews in Computational Chemistry, Volume 16* Kenny B. Lipkowitz,Donald B. Boyd,2009-09-22 Volume 16 Reviews In Computational Chemistry Kenny B Lipkowitz and Donald B Boyd The focus of this book is on methods useful in molecular design Tutorials and reviews span 1 methods for designing compound libraries for combinatorial chemistry and high throughput screening 2 the workings of artificial neural networks and their use in chemistry 3 force field methods for modeling materials and designing new substances and 4 free energy perturbation methods of practical usefulness in ligand design From Reviews of the Series This series spans all the subdisciplines in the field from techniques to practical applications and includes reviews from many of the acknowledged leaders in the field the reviews cross many subdisciplines yet are both general enough to be of wide interest while including detailed information of use to workers in particular subdisciplines *Journal of the American Chemical Society* **Topics in Current Chemistry** Jürgen Rohr,1973 **The Organic Chemistry of Drug Design and Drug Action** Richard B. Silverman,Mark W. Holladay,2014-03-29 The Organic Chemistry of Drug Design and Drug Action Third Edition represents a unique approach to medicinal chemistry based on physical organic chemical principles and reaction mechanisms that rationalize drug action which allows reader to extrapolate those core principles and mechanisms to many related classes of drug molecules This new edition includes updates to all chapters including new examples and references It reflects significant changes in the process of drug design over the last decade and preserves the successful approach of the previous editions while including significant changes in format and coverage This text is designed for undergraduate and graduate students in chemistry studying medicinal chemistry or

pharmaceutical chemistry research chemists and biochemists working in pharmaceutical and biotechnology industries

Updates to all chapters including new examples and references

Chapter 1 Introduction Completely rewritten and expanded as an overview of topics discussed in detail throughout the book

Chapter 2 Lead Discovery and Lead Modification Sections on sources of compounds for screening including library collections virtual screening and computational methods as well as hit to lead and scaffold hopping expanded sections on sources of lead compounds fragment based lead discovery and molecular graphics and deemphasized solid phase synthesis and combinatorial chemistry

Chapter 3 Receptors Drug receptor interactions cation  $\pi$  and halogen bonding atropisomers case history of the insomnia drug suvorexant

Chapter 4 Enzymes Expanded sections on enzyme catalysis in drug discovery and enzyme synthesis

Chapter 5 Enzyme Inhibition and Inactivation New case histories for competitive inhibition the epidermal growth factor receptor tyrosine kinase inhibitor erlotinib and Abelson kinase inhibitor imatinib for transition state analogue inhibition the purine nucleoside phosphorylase inhibitors forodesine and DADMe ImmH as well as the mechanism of the multisubstrate analog inhibitor isoniazid for slow tight binding inhibition the dipeptidyl peptidase 4 inhibitor saxagliptin

Chapter 7 Drug Resistance and Drug Synergism This new chapter includes topics taken from two chapters in the previous edition with many new examples

Chapter 8 Drug Metabolism Discussions of toxicophores and reactive metabolites

Chapter 9 Prodrugs and Drug Delivery Systems Discussion of antibody drug conjugates

**International Aerospace Abstracts** ,1968      *Medical Books and Serials in Print* , 1979 R. R. Bowker LLC,1979-05      **Deutsche Nationalbibliographie und Bibliographie der im Ausland erschienenen deutschsprachigen Veröffentlichungen** ,1995      The Molecular Biology of Flowering Brian R. Jordan,1993 The transition from vegetative to reproductive growth is one of the most important developmental changes in plants Although the physiology of the process has been well documented the molecular basis has only recently begun to be determined This book reviews our current knowledge of the molecular biology and genetics of flowering a subject that is rapidly being recognized for both its fundamental importance and its biotechnological exploitation It will interest research workers and advanced students in plant genetics and plant molecular biology      Physics Briefs ,1990      *Medical Times* ,1843      *The Medical Times and Gazette* ,1843      *American Scientist* ,1942      **Nature** Sir Norman Lockyer,1869

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