

Type-I peptidomimetics or pseudopeptides

- These are synthesized by structure based drug design. These peptidomimetics are closely similar to peptide backbone while retaining functional groups that makes important contacts with binding sites of the receptors.
- Some units mimic shortportions of secondary structure of peptide for example β-turns and have been used to generate lead compounds. Many early protease inhibitors were designed from substrate product mimetics of the peptide bond in a transition state or product state for the enzyme-entalyzed reaction.
- For example Pyrrolinones contains peptide-like side-chains that fit the active sites of most peptidases and also these are resistant to normal proteolysis because they replace amide bonds with metabolically stable units on amino acid unit of parent peptides

Pseudopeptides In Drug Discovery

Michael D. Taylor

Pseudopeptides In Drug Discovery:

Pseudo-peptides in Drug Discovery Peter E. Nielsen, 2006-03-06 Peptides are among the most versatile bioactive molecules yet the do not make good drugs because they are quickly degraded or modified in the body To overcome this problem stable and at the same time biologically active pseudo peptides have been developed These novel compounds open up new perspectives in drug design by providing an entire range of highly specific and non toxic pharmaceuticals This is the first work devoted to the topic and draws together knowledge gained on different types of peptidomimetics and other pseudo peptides with drug properties As such it includes peptoids beta peptides polyamide DNA binders as well as peptide nucleic acids The expert authors and editor discuss chemical properties and stability biological activity and reactivity as well as practical aspects of synthesis making this a prime resource for drug developers and bioorganic chemists working with these compounds **Computational Drug Discovery** Pooja A. Chawla, Dilpreet Singh, Kamal Dua, Muralikrishnan Dhanasekaran, Viney Chawla, 2024-10-07 Computational methods and understanding computational models are important in modern drug discovery The book focuses on computational approaches that can improve the development of in silico methodologies It includes lead hit methods docking algorithms computational chiral compounds structure based drug design GROMACS and NAMD structural genomics toxicity prediction enzyme inhibitors and peptidomimetic therapeutics

Hydrolysis in Drug and Prodrug Metabolism Bernard Testa, Joachim M. Mayer, 2003-08 Many drugs and other xenobiotics e g preservatives insecticides and plastifiers contain hydrolyzable moieties such as ester or amide groups In biological media such foreign compounds are therefore important substrates for hydrolytic reactions catalyzed by hydrolases or proceeding non enzymatically Despite their significance until now no book has been dedicated to hydrolysis and hydrolases in the metabolism of drugs and other xenobiotics. This work fills a gap in the literature and reviews metabolic reactions of hydrolysis and hydarion from the point of views of enzymes substrates and reactions **Advances in Drug Research** ,1997-07-21 This volume continues the trend for Advances in Drug Research of shorter but more frequent volumes In line with the tradition of the series chapters on general themes are interspersed with chapters on specific drug classes and Computer Aided Drug Design in Industrial Research E.C. Herrmann, R. Franke, 2013-03-09 The Ernst targets Schering Research Foundation sponsored its 15th workshop in Berlin on October 19 21 1994 Leading scientists from Europe and North America were invited to discuss computer aided drug design in industrial research Computer aided drug design is a very exciting field and an intellec tual challenge like playing chess But these reasons are no longer sufficient to justify using this method in industry if they ever were Fig 1 The participants of the workshop VI Preface Therefore when we together with Prof Hoyer started to think about this workshop our intentions quickly became clear We were not so much interested in the very latest developments of methods or in computer aided drug design itself enough conferences have dealt with these topics However we were very interested in the usefulness and limitations of computer aided drug design in the

indu strial research process A lot has changed in the pharmaceutical industry recently These changes are gaining momentum so it is the right time to think about the role of computer aided drug design in this changing environment 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 p 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 European Journal of Organic Chemistry, 2007 **Green Approaches in Medicinal Chemistry for** Sustainable Drug Design Bimal Banik, 2024-06-01 Extensive experimentation and high failure rates are a well recognised downside to the drug discovery process with the resultant high levels of inefficiency and waste producing a negative environmental impact Sustainable and Green Approaches in Medicinal Chemistry Second Edition reveals how medicinal chemistry can play a direct role in addressing this issue After providing essential context to the growth of green chemistry in relation to drug discovery the book goes on to identify a broad range of practical techniques and useful insights revealing how medicinal chemistry techniques can be used to improve efficiency mitigate failure and increase the environmental

benignity of the entire drug discovery process Drawing on the knowledge of a global team of experts Sustainable and Green Approaches in Medicinal Chemistry 2e encourages the growth of green medicinal chemistry and supports medicinal chemists drug discovery researchers pharmacologists and all those in related fields across both academia and industry in integrating these approaches into their own work This first volume of the second edition covers synthesis methods following green chemistry principles contributing to sustainability by saving energy using lesser toxic reagents solvents catalysts and environmentally benign sources including plants and agricultural materials Highlights the need for the adoption of sustainable and green chemistry pathways in drug development Reveals risk factors associated with the drug development process and the ways sustainable approaches can help address these factors Identifies novel and cost effective green medicinal chemistry approaches for improved efficiency and sustainability **Current Pharmaceutical Design**, 1995-08

Drug Discovery and Development Omboon Vallisuta, Suleiman Olimat, 2015-06-03 It is very important for scientists all over the globe to enhance drug discovery research for better human health This book demonstrates that various expertise are essential for drug discovery including synthetic or natural drugs clinical pharmacology receptor identification drug metabolism pharmacodynamic and pharmacokinetic research The following 5 sections cover diverse chapter topics in drug discovery Natural Products as Sources of Leading Molecules in Drug Discovery Oncology and Drug Discovery Receptors Involvement in Drug Discovery Management and Development of Drugs against Infectious Diseases Advanced Methodology

<u>Drug Discovery</u> Hany El-Shemy, 2013-01-23 Natural products are a constant source of potentially active compounds for the treatment of various disorders The Middle East and tropical regions are believed to have the richest supplies of natural products in the world Plant derived secondary metabolites have been used by humans to treat acute infections health disorders and chronic illness for tens of thousands of years Only during the last 100 years have natural products been largely replaced by synthetic drugs Estimates of 200 000 natural products in plant species have been revised upward as mass spectrometry techniques have developed For developing countries the identification and use of endogenous medicinal plants as cures against cancers has become attractive Books on drug discovery will play vital role in the new era of disease treatment using natural products **Privileged Scaffolds in Drug Discovery** Bin Yu, Ning Li, Caiyun Fu, 2023-07-19 Privileged Scaffolds in Drug Discovery is the most complete and up to date work in the area Covering a wide range of privileged structures it is a perfect reference for scientists involved in targeted drug development The editors recruited epserts from several prestigious Chinese institutions to cover the areas of antiviral drugs chalcone pyrimidine benz imidazoles natural product derived privileged scaffolds N Sulfonyl carboxamides kinase inhibitors antitumor molecules antineurodegenerative drugs triazoles oxazolidinone indole and indoline scaffolds tigliane diterpenoids peptide and peptide based drugs guassinoids and others including pseudonatural products macrocycles stable peptides and peptidomimetics The book also explores scaffolds in drug molecules approved in recent years Privileged Scaffolds in Drug Discovery is a complete

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Approaches to Rational Drug Design David B. Weiner, William V. Williams, 2020-12-17 This book is the first to provide both a broad overview of the current methodologies being applied to drug design and in depth analyses of progress in specific fields It details state of the art approaches to pharmaceutical development currently used by some of the world s foremost laboratories The book features contributors from a variety of fields new techniques previously unpublished data and extensive reference lists Biomedical Index to PHS-supported Research, 1993 Biomedical Index to PHS-supported Research: pt. A. Subject access A-H, 1992

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