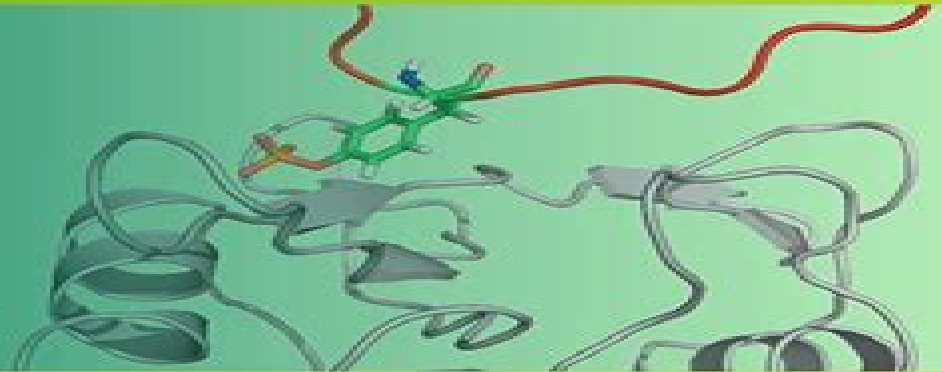


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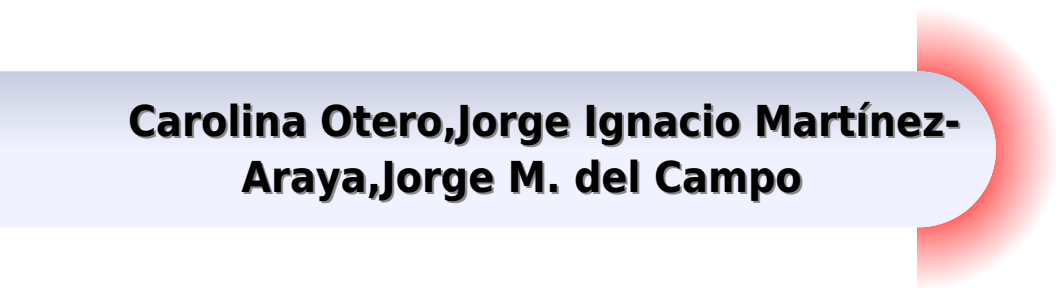


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Computational Peptidology Methods In Molecular Biology

**Carolina Otero, Jorge Ignacio Martínez-
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Computational Peptidology Peng Zhou,Jian Huang,2016-09-24 In this volume expert researchers detail in silico methods widely used to study peptides These include methods and techniques covering the database molecular docking dynamics simulation data mining de novo design and structure modeling of peptides and protein fragments Chapters focus on integration and application of technologies to analyze model identify predict and design a wide variety of bioactive peptides peptide analogues and peptide drugs as well as peptide based biomaterials Written in the highly successful Methods in Molecular Biology series format chapters include introductions to their respective topics lists of the necessary materials and reagents step by step readily reproducible laboratory protocols and key tips on troubleshooting and avoiding known pitfalls Authoritative and practical Computational Peptidology seeks to aid scientists in the further study into this newly rising subfield

Chagas disease novel drug targets and treatments Vilma G. Duschak,Gustavo Benaim,Alberto Enrique Paniz Mondolfi,2023-06-22 *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

Machine Learning for Peptide Structure, Function, and Design Ruiquan Ge,Chuan Dong,Juexin Wang,Yanjie Wei,2022-11-07 *Management of Fish Diseases* Sumanta Kumar Mallik,Neetu Shahi,Pramod Kumar Pandey,2025-03-22 This book covers various aspects of aquatic animal health such as pathogenic and beneficial microbes disease diagnosis treatment and preventive measures biosecurity disease management The environmental factors affecting aquatic animal well being and their nutritional requirements are also discussed Finally emerging trends and future research and management directions are also concluded in this book Aquatic animals are a crucial source of nutrition for people worldwide as they provide at least 20% of animal protein intake for over 3 billion individuals according to the Food and Agriculture Organization FAO Furthermore fishing and aquaculture industries generate employment and income for millions particularly in developing countries However pollution habitat destruction overfishing climate change and disease outbreaks pose a threat to aquatic animal health Disease outbreaks and pathogenic microbes can cause significant harm necessitating immediate attention Addressing this issue requires multifaceted approach that includes enhancing water quality managing animal stress levels improving biosecurity measures and practicing responsible aquaculture techniques Finally collaboration between government industry and researchers is critical to developing new and effective strategies for mitigating the impact of disease outbreaks on aquatic animal health This book provides concise information for students teachers researchers and academicians interested in the field of aquatic animal health It also serves as a reference book to administrators practitioners

stakeholders and non professionals interested in sustainable aquatic animal health management *Multiscale Modeling From Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations* Valentina Tozzini, Giulia Palermo, Matteo Dal Peraro, Alexandre M. J. J. Bonvin, Rommie E. Amaro, 2020-10-27 This eBook is a collection of articles from a Frontiers Research Topic Frontiers Research Topics are very popular trademarks of the Frontiers Journals Series they are collections of at least ten articles all centered on a particular subject With their unique mix of varied contributions from Original Research to Review Articles Frontiers Research Topics unify the most influential researchers the latest key findings and historical advances in a hot research area Find out more on how to host your own Frontiers Research Topic or contribute to one as an author by contacting the Frontiers Editorial Office frontiersin.org about contact

Advances in QSAR Modeling Kunal Roy, 2017-05-22 The book covers theoretical background and methodology as well as all current applications of Quantitative Structure Activity Relationships QSAR Written by an international group of recognized researchers this edited volume discusses applications of QSAR in multiple disciplines such as chemistry pharmacy environmental and agricultural sciences addressing data gaps and modern regulatory requirements Additionally the applications of QSAR in food science and nanoscience have been included two areas which have only recently been able to exploit this versatile tool This timely addition to the series is aimed at graduate students academics and industrial scientists interested in the latest advances and applications of QSAR

Endemic Plants: Experimental and Theoretical Insights Into Properties of Bioactive Metabolites With Therapeutic Potential Carolina Otero, Jorge Ignacio Martínez-Araya, Jorge M. del Campo, 2021-12-29

Artificial Protein and Peptide Nanofibers Gang Wei, Sangamesh G. Kumbar, 2020-07-28 Artificial Protein and Peptide Nanofibers Design Fabrication Characterization and Applications provides comprehensive knowledge of the preparation modification and applications of protein and peptide nanofibers The book reviews the synthesis and strategies necessary to create protein and peptide nanofibers such as self assembly including supramolecular assembly electrospinning template synthesis and enzymatic synthesis Then the key chemical modification and molecular design methods are highlighted that can be utilized to improve the bio functions of these synthetic fibers Finally fabrication methods for key applications such as sensing drug delivery imaging tissue engineering and electronic devices are reviewed This book will be an ideal resource for those working in materials science polymer science chemical engineering nanotechnology and biomedicine Reviews key chemical modification and molecular design methods to improve the bio functions of synthetic peptide and protein nanofibers Discusses the most important synthesis strategies including supramolecular assembly electrospinning template synthesis and enzymatic synthesis Provides information on fabrication of nanofibers for key applications such as sensing imaging drug delivery and tissue engineering

Computational Peptide Science Thomas Simonson, 2023-04-01 This volume details current and new computational methodologies to study peptides Chapters guide readers through antimicrobial peptides foldability amyloid sheet formation membrane active peptides organized peptide

assemblies protein peptide interfaces prediction of peptide MHC complexes advanced free energy simulations for peptide binding and methods for high throughput peptide or miniprotein design Written in the format of the highly successful Methods in Molecular Biology series each chapter includes an introduction to the topic lists necessary materials software and reagents includes tips on troubleshooting and known pitfalls and step by step readily reproducible protocols Authoritative and cutting edge Computational Peptides Science Methods and Protocols aims to provide concepts methods and guidelines to help both novices and experienced workers benefit from today s new opportunities and challenges

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