

From Medicinal Chemistry to Food Science

A Transfer of *In Silico* Methods Applications

Pietro Cozzini
Editor

Food Science
and Technology

NOVA



Medicinal Chemistry Food Science Applications

Jiyuan Zhang



Medicinal Chemistry Food Science Applications:

Application of Nanotechnology in Food Science, Processing and Packaging Chukwuebuka Egbuna, Jaison Jeevanandam, Kingsley C. Patrick-Iwuanyanwu, Eugene N. Onyeike, 2022-05-03 This book entitled Application of Nanotechnology in Food Science Processing and Packaging presents up to date information on the emerging roles of nanotechnology in food industry its fundamental concepts techniques and applications The application of nanotechnology in the food industry is an emerging area which has found tremendous use in improving food quality through the enhancement of food taste texture colour and flavour Also its application has improved the bioavailability and target delivery of certain bioactive food ingredients through controlled release of nutrients a feature that is impossible with the conventional methods of food processing The application of nanotechnology in food packaging for the detection of contaminants pathogens biotoxins and pesticides through nanosensor safety evaluations has led to the increase in shelf life of products and quality assurance through the detection and monitoring of toxins This book taps from the experience of subject experts from key institutions around the world The users of this book will benefit greatly as the chapters were simplified and arranged carefully to aid proper understanding consistency and continuity

Foodinformatics Karina Martinez-Mayorga, José Luis Medina-Franco, 2014-11-21 The explosion in the generation of information parallels the explosion of computational resources The use of computers to collect store and manipulate chemical information is at the heart of chemoinformatics These methodologies whose main target thus far has been the pharmaceutical field are general and can be applied to other types of chemical data sets such as those containing food chemicals While the use of chemical information methodologies to address food related challenges is still in its infancy interest is growing and will continue to do so as the methods prove useful particularly for providing practical solutions to food industry challenges Foodinformatics gives an overview of basic concepts applications tools and perspectives of the emerging field of foodinformatics The book is an important addition to the literature and will be of interest of food chemists nutritionists informaticians and scientists of related fields About the Editors Karina Martinez-Mayorga Instituto de Química UNAM Mexico City Mexico and Torrey Pines Institute for Molecular Studies Port St Lucie FL USA José Luis Medina-Franco Instituto de Química UNAM Mexico City Mexico and Torrey Pines Institute for Molecular Studies Port St Lucie FL USA

From Medicinal Chemistry to Food Science Pietro Cozzini, 2015 The aim of this book is to illustrate the big opportunity to transfer computational techniques well accepted and used in medicinal chemistry to food science through this we hope to discover new pollutants possible dangerous food additives contaminants from industries xenoestrogens etc The paradigm is if a molecule can interact with a receptor i.e. a Nuclear Receptor it can modify the signaling pathway and should be investigated to discover negative effects on food The interaction can be predicted using in silico techniques well known by medicinal chemists to discover new lead compounds or to study the behavior of a protein ligand interaction The book starts with an introduction about the computational methods applied to

food safety by authors coming from a big food company who elucidate the importance of this approach for industries and food agencies In Chapter Two the authors give an overview of in vivo tests for food contaminant and toxin evaluation In Chapter Three in vitro and in silico models of digestion are compared In Chapter Four the authors belonging both to an in silico lab and a wet lab use a case study of poliphenols to show how to merge in silico prediction and in vitro controls to gain time and money in estrogen receptors Additionally poliphenol binding studies use a molecule modeling approach In Chapter Five a non typical docking approach is presented a reverse docking approach Chapter Six and Seven introduce the problem of receptor flexibility and how to treat this important characteristic that must be considered in computational simulations Chapter Eight is a review about QSAR methods well considered in this approach Chapter Nine show a non conventional informatics approach to ab initio in silico protein structure prediction The last chapter is dedicated to the informatics requirements for in silico simulations to help researchers approaching this field Annals of Chemical Medicine, Including the Application of Chemistry to Physiology, Pathology, Therapeutics, Pharmacy, Toxicology, & Hygiene ... ,1881

Application of Chemical Engineering Zhong Cao,Ying He He,Li Xian Sun,Xue Qiang Cao,2011-05-12 Selected peer reviewed papers from the 2011 International Conference on Chemical Engineering and Advanced Materials CEAM 2011 28 30 May 2011 Directory of Research Grants ,1993 **New Scientist and Science Journal** ,1989-09 **Chemical News and Journal of Industrial Science** ,1898 New Scientist ,1989 *The Chemical News and Journal of Physical Science* ,1898 *Chemical News and Journal of Physical Science* ,1893 *British Medical Journal* ,1890 **The Chemical News and Journal of Industrial Science** ,1898 **Pacific Medical Journal** ,1897 **Topics in Medicinal Chemistry** Ralph M. Myerson,Joseph L. Rabinowitz,1967 *The Medical Times and Gazette* ,1878 The Druggists' Circular and Chemical Gazette ,1890 Includes Red book price list section title varies slightly issued semiannually 1897 1906

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