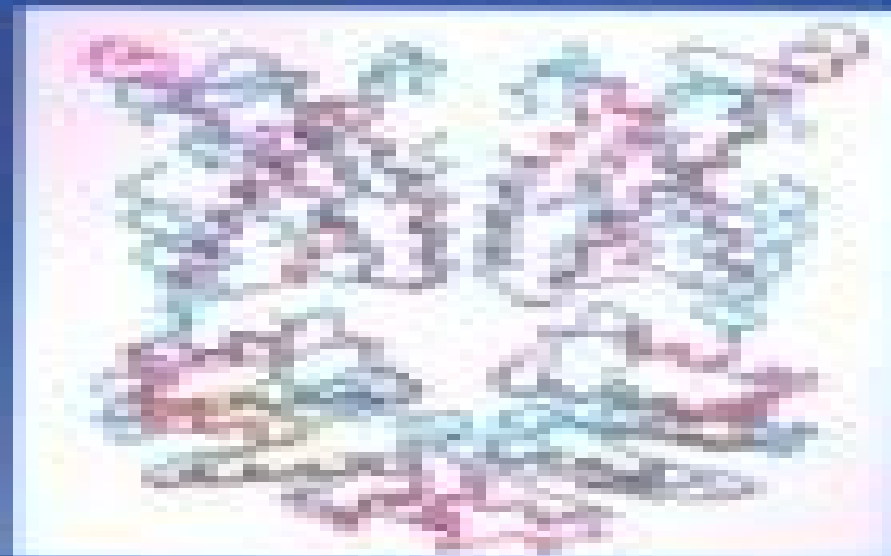




VIRTUAL ADMET ASSESSMENT IN TARGET SELECTION AND MATURATION

William A. Miller
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Virtual Admet Assessment In Target Selection And Maturation

B. Maisch,R. Oelze



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Virtual ADMET Assessment in Target Selection and Maturation B. Testa, Lechoslaw Turski, 2006-12-15 Today biologists and medicinal chemists realize that there is a strong relationship between pharmacodynamic what the drug does to the organism and pharmacokinetic what the organism does to the drug effects A significant contributing factor to the evolution in drug discovery was the methodological and technological revolution with the advent of combinatorial chemistry high throughput screening and profiling and in silico prediction of target based activity and ADMET absorption distribution metabolism excretion and toxicity properties High throughput screening and in silico methods have accelerated the process towards drugability of new chemical structures Another component of the revolution in drug discovery is the replacement of the disease indication based approach by a target based approach A better understanding of pathophysiology of diseases and the underlying biological processes of diseases combined with explosive development of genomics and proteomics have been instrumental in the birth of this new paradigm This volume summarizes discussions of these three aspects of modern drug discovery i e priority for targets early ADMET assessment and in silico screening We trust that readers from academia as well as from industry will benefit from these studies

Virtual ADMET Assessment in Target Selection and Maturation Bernard Testa, Lechoslaw Turski, 2006 A significant contributing factor to the evolution in drug discovery was the methodological and technological revolution with the advent of combinatorial chemistry This volume summarizes discussions of three aspects of modern drug discovery that is priority for targets early ADMET assessment and in silico screening , *Predictive ADMET* Jianling Wang, Laszlo Urban, 2014-02-28 This book helps readers integrate in silico in vitro and in vivo ADMET absorption distribution metabolism elimination and toxicity and PK pharmacokinetics data with routine testing applications so that pharmaceutical scientists can diagnose ADMET problems and present appropriate recommendations to move drug discovery programs forward The book introduces the current clinical practice for drug discovery and development along with the impact on early risk assessment consolidates the tools and models to intelligently integrate existing in silico in vitro and in vivo ADMET data and demonstrates successful cases and lessons learned from real drug discovery and development In short it is a book aimed to provide a practical road map for drug discovery and development scientists to generate efficacious and safe drugs for unmet medical needs

In Silico Toxicology Mark T. D. Cronin, Judith C. Madden, 2010 In Silico methods to predict toxicity have become increasingly important recently particularly in light of European legislation such as REACH and the Cosmetics Regulation They are also being used extensively worldwide e g in the USA Canada Japan and Australia In assessing the risk that a chemical may pose to human health or to the environment focus is now being directed towards exploitation of in silico methods to replace in vivo or in vitro techniques A prediction of potential toxicity requires several stages 1 Collation and organisation of data available for the compound or if this is not available information for related compounds 2 An assessment of the quality of the data 3 Generation of additional

information about the compound using computational techniques at various levels of complexity calculation of physico chemical properties 2 D 3 D MO descriptors and specific receptor modelling interaction 4 Use of an appropriate strategy to predict toxicity ie a statistically valid method which makes best use of all available information mechanism of action activity for related compounds extrapolation across species and endpoints likely exposure scenario amounts over time etc 5 Consideration then needs to be given to how this information is used in the real world ie use of expert systems tools as relevant to assessors if sufficiently different to previous weight of evidence approaches 6 Finally evidence should be presented from case studies within this area No other publication brings together information on all of these areas in one book and this publication is unique in that it provides a logical progression through every one of these key stages and defines the use of computational approaches to predict the environmental toxicity and human health effects of organic chemicals The volume is aimed at the developers and users of in silico toxicology and provides an analysis of all aspects required for in silico prediction of toxicology including data collation quality assessment and computational approaches The contributions from recognised leaders in each of these areas include evidence of the use and applicability of approaches using real world case studies concerning both environmental and human health effects The book provides a very useful single source reference for people working in this area including academics professionals under and post graduate students as well as Governmental Regulatory Scientists involved in chemical risk assessment and REACH

Drug Bioavailability Han van de Waterbeemd, Bernard Testa, 2009-09-18 The gold standard for industrial research now completely revised in line with current trends in the field with all contributions extensively updated or rewritten In 21 chapters readers can benefit from the key working knowledge of today s leading pharmaceutical companies including Pfizer AstraZeneca and Roche Drug developers from industry and academia present all the factors governing drug bioavailability complete with practical examples and real life data Part I focuses on in vitro and in vivo measurements of physicochemical properties such as membrane permeability and ionization Part II discusses solubility and gastrointestinal absorption while the third part is devoted to metabolism and excretory mechanisms The much revised and expanded part IV surveys current in silico approaches to predict drug properties needed to estimate the bioavailability of any new drug candidate The final part shows how poor bioavailability may be improved by various approaches during the development process No other publication offers the same level of treatment on this crucial topic in modern drug development

Nuclear Receptors as Molecular Targets for Cardiometabolic and Central Nervous System Diseases Jean-Louis Junien, B. Staels, 2008 Focuses on the mechanistic involvement of nuclear receptors in cardiological metabolic and neurological disorders This book also focuses on possible explanation of pathways involved in pathogenesis on susceptibility to and prevention of metabolic and neurological disorders and on the aspects of drug finding

Pulmonary Arterial Hypertension Jochen Antel, M. B. Hesselink, R. T. Schermuly, 2010 Pulmonary hypertension is a fatal lung and heart disease It is characterized by shortness of breath fatigue and fainting It is exacerbated

by an increase of the pressure in the lung vasculature through exercise leading to progressive worsening of hemodynamics right ventricular hypertrophy right heart insufficiency and finally right heart failure This book focuses on pulmonary arterial hypertension a rare and progressive subgroup of pulmonary hypertension which is today incurable and terminally faal Classification of pulmonary arterial hypertension its pathology and strategies for future therapy will be of interest both to those suffering from the disease and those who take care of patients This volume will also engage physicians and other scientists contributing to an understanding of the pathophysiology of pulmonary arterial hypertension and attempting to extend life of humans with pulmonary arterial hypertension by developing causal and curative therapies Cardiovascular Benefits of Omega-3 Polyunsaturated Fatty Acids B. Maisch,R. Oelze,2007-01-18 Solvay Pharmaceuticals Conferences

Human Papillomaviruses and Cervical Cancer Magnus von Knebel Doeberitz,N. Wentzensen,2007 Contains twelve articles which explore the epidemiology of HPV testing strategies for HPV infections new HPV detection methods and other potential biomarkers that might prove useful in cervical cancer diagnosis This book includes articles which address the research on biomarkers for cervical cancer

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