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Huma M. Lodhi, Yoshihiro Yamanashi

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Chemoinformatics and Advanced Machine Learning Perspectives: Complex Computational Methods and Collaborative Techniques Lodhi, Huma, Yamanishi, Yoshihiro, 2010-07-31 This book is a timely compendium of key elements that are crucial for the study of machine learning in chemoinformatics giving an overview of current research in machine learning and their applications to chemoinformatics tasks Provided by publisher **Tutorials in Chemoinformatics** Alexandre Varnek, 2017-08-14 30 tutorials and more than 100 exercises in chemoinformatics supported by online software and data sets Chemoinformatics is widely used in both academic and industrial chemical and biochemical research worldwide Yet until this

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Chemoinformatics and Advanced Machine Learning Perspectives Huma M. Lodhi, Yoshihiro Yamanashi, 2011 This book is a timely compendium of key elements that are crucial for the study of machine learning in chemoinformatics giving an overview of current research in machine learning and their applications to chemoinformatics tasks Provided by publisher

Applied Chemoinformatics Thomas Engel, Johann Gasteiger, 2018-04-19 Edited by world famous pioneers in chemoinformatics this is a clearly structured and applications oriented approach to the topic providing up to date and focused information on the wide range of applications in this exciting field. The authors explain methods and software tools such that the reader will not only learn the basics but also how to use the different software packages available Experts describe applications in such different fields as structure spectra correlations virtual screening prediction of active sites library design the prediction of the properties of chemicals the development of new cosmetics products quality control in food the design of new materials with improved properties toxicity modeling assessment of the risk of chemicals and the control of chemical processes The book is aimed at advanced students as well as lectures but also at scientists that want to learn how chemoinformatics could assist them in solving their daily scientific tasks Together with the corresponding textbook Chemoinformatics Basic Concepts and Methods ISBN 9783527331093 on the fundamentals of chemoinformatics readers will *Bioinformatics and the Cell* Xuhua Xia,2010 Chemoinformatics and have a comprehensive overview of the field Bioinformatics in the Pharmaceutical Sciences Navneet Sharma, Himanshu Ojha, Pawan Raghav, Ramesh K. Goyal, 2021-05-21 Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences brings together two very important fields in pharmaceutical sciences that have been mostly seen as diverging from each other chemoinformatics and bioinformatics As developing drugs is an expensive and lengthy process technology can improve the cost efficiency and speed at which new drugs can be discovered and tested This book presents some of the growing advancements of technology in the field of drug development and how the computational approaches explained here can reduce the financial and experimental burden of the drug discovery process This book will be useful to pharmaceutical science researchers and students who need basic knowledge of computational techniques relevant to their projects Bioscientists bioinformaticians computational scientists and other stakeholders from industry and academia will also find this book helpful Provides practical information on how to

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