

Edited by  
Johann Gasteiger and Thomas Engel

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# Chemoinformatics

A Textbook



# Chemoinformatics A Textbook

**Johann Gasteiger, Thomas Engel**



## **Chemoinformatics A Textbook:**

*Chemoinformatics* Johann Gasteiger, Thomas Engel, 2003-11-07 This first work to be devoted entirely to this increasingly important field the Textbook provides both an in depth and comprehensive overview of this exciting new area Edited by Johann Gasteiger and Thomas Engel the book provides an introduction to the representation of molecular structures and reactions data types and databases data sources search methods methods for data analysis as well as such applications as structure elucidation reaction simulation synthesis planning and drug design A hands on approach with step by step tutorials and detailed descriptions of software tools and Internet resources allows easy access for newcomers advanced users and lecturers alike For a more detailed presentation users are referred to the Handbook of Chemoinformatics which will be published separately Johann Gasteiger is the recipient of the 1991 Gmelin Beilstein Medal of the German Chemical Society for Achievements in Computer Chemistry and the Herman Skolnik Award of the Division of Chemical Information of the American Chemical Society ACS in 1997 Thomas Engel joined the research group headed by Johann Gasteiger at the University of Erlangen Nuremberg and is a specialist in chemoinformatics

*Chemoinformatics* Johann Gasteiger, Thomas Engel, 2006

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*An Introduction to Chemoinformatics* Andrew R. Leach, V.J. Gillet, 2007-09-04 This book aims to provide an introduction to the major techniques of chemoinformatics It is the first text written specifically for this field The first part of the book deals with the representation of 2D and 3D molecular structures the calculation of molecular descriptors and the construction of mathematical models The second part describes other important topics including molecular similarity and diversity the analysis of large data sets virtual screening and library design Simple illustrative examples are used throughout to illustrate key concepts supplemented with case studies from the literature

**Chemoinformatics** Thomas Engel, Johann Gasteiger, 2018-05-18 This essential guide to the knowledge and tools in the field includes everything from the basic concepts

to modern methods while also forming a bridge to bioinformatics The textbook offers a very clear and didactical structure starting from the basics and the theory before going on to provide an overview of the methods Learning is now even easier thanks to exercises at the end of each section or chapter Software tools are explained in detail so that the students not only learn the necessary theoretical background but also how to use the different software packages available The wide range of applications is presented in the corresponding book Applied Chemoinformatics Achievements and Future Opportunities ISBN 9783527342013 For Master and PhD students in chemistry biochemistry and computer science as well as providing an excellent introduction for other newcomers to the field

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**Comprehensive Chemometrics** Steven Brown,Roma Tauler,Beata Walczak,2020-05-26 Comprehensive Chemometrics Second Edition Four Volume Set features expanded and updated coverage along with new content that covers advances in the field since the previous edition published in 2009 Subject of note include updates in the fields of multidimensional and megavariate data analysis omics data analysis big chemical and biochemical data analysis data

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*Comprehensive Chemometrics*, 2009-03-09 Designed to serve as the first point of reference on the subject Comprehensive Chemometrics presents an integrated summary of the present state of chemical and biochemical data analysis and manipulation The work covers all major areas ranging from statistics to data acquisition analysis and applications This major reference work provides broad ranging validated summaries of the major topics in chemometrics with chapter introductions and advanced reviews for each area The level of material is appropriate for graduate students as well as active researchers seeking a ready reference on obtaining and analyzing scientific data Features the contributions of leading experts from 21 countries under the guidance of the Editors in Chief and a team of specialist Section Editors L Buydens D Coomans P Van Espen A De Juan J H Kalivas B K Lavine R Leardi R Phan Tan Luu L A Sarabia and J Trygg Examines the merits and limitations of each technique through practical examples and extensive visuals 368 tables and more than 1 300 illustrations 750 in full color Integrates coverage of chemical and biological methods allowing readers to consider and test a range of techniques Consists of 2 200 pages and more than 90 review articles making it the most comprehensive work of its kind Offers print and online purchase options the latter of which delivers flexibility accessibility and usability through the search tools and other productivity enhancing features of ScienceDirect

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**Chemoinformatics: Theory, Practice, & Products** Barry A. Bunin, Brian Siesel, Guillermo Morales, Jürgen Bajorath,2006-11-28 Chemoinformatics is the use of information technology in the acquisition analysis and management of data and information relating to chemical compounds and their properties The purpose of this book is to provide computational scientists medicinal chemists and biologists with complete practical information and underlying theory relating to modern Chemoinformatics and related drug discovery informatics technologies This is an essential handbook for determining the right Chemoinformatics method or technology to use *Aslib Proceedings* ,2008 **European Journal of Inorganic Chemistry** ,2004 Choice ,2004

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