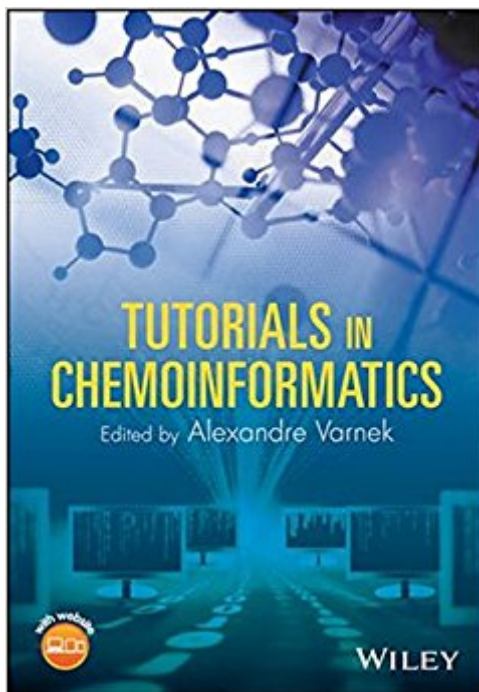


The book was found

Tutorials In Chemoinformatics



Synopsis

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 unique guide, there were no books offering practical exercises in chemoinformatics methods. Tutorials in Chemoinformatics contains more than 100 exercises in 30 tutorials exploring key topics and methods in the field. It takes an applied approach to the subject with a strong emphasis on problem-solving and computational methodologies. Each tutorial is self-contained and contains exercises for students to work through using a variety of software packages. The majority of the tutorials are divided into three sections devoted to theoretical background, algorithm description and software applications, respectively, with the latter section providing step-by-step software instructions. Throughout, three types of software tools are used: in-house programs developed by the authors, open-source programs and commercial programs which are available for free or at a modest cost to academics. The in-house software and data sets are available on a dedicated companion website. Key topics and methods covered in Tutorials in Chemoinformatics include: Data curation and standardization Development and use of chemical databases Structure encoding by molecular descriptors, text strings and binary fingerprints The design of diverse and focused libraries Chemical data analysis and visualization Structure-property/activity modeling (QSAR/QSPR) Ensemble modeling approaches, including bagging, boosting, stacking and random subspaces 3D pharmacophores modeling and pharmacological profiling using shape analysis Protein-ligand docking Implementation of algorithms in a high-level programming language Tutorials in Chemoinformatics is an ideal supplementary text for advanced undergraduate and graduate courses in chemoinformatics, bioinformatics, computational chemistry, computational biology, medicinal chemistry and biochemistry. It is also a valuable working resource for medicinal chemists, academic researchers and industrial chemists looking to enhance their chemoinformatics skills.

Book Information

Hardcover: 488 pages

Publisher: Wiley; 1 edition (August 14, 2017)

Language: English

ISBN-10: 1119137969

ISBN-13: 978-1119137962

Product Dimensions: 6.7 x 1.1 x 9.6 inches

Shipping Weight: 2.3 pounds (View shipping rates and policies)

Average Customer Review: Be the first to review this item

Best Sellers Rank: #777,328 in Books (See Top 100 in Books) #62 in Books > Science & Math > Chemistry > Clinical #226 in Books > Science & Math > Chemistry > Analytic #2546 in Books > Textbooks > Science & Mathematics > Chemistry

Customer Reviews

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 unique guide, there were no books offering practical exercises in chemoinformatics methods. Tutorials in Chemoinformatics contains more than 100 exercises in 30 tutorials exploring key topics and methods in the field. It takes an applied approach to the subject with a strong emphasis on problem-solving and computational methodologies. Each tutorial is self-contained and contains exercises for students to work through using a variety of software packages. The majority of the tutorials are divided into three sections devoted to theoretical background, algorithm description and software applications, respectively, with the latter section providing step-by-step software instructions. Throughout, three types of software tools are used: in-house programs developed by the authors, open-source programs and commercial programs which are available for free or at a modest cost to academics. The in-house software and data sets are available on a dedicated companion website. Key topics and methods covered in Tutorials in Chemoinformatics include: Data curation and standardization Development and use of chemical databases Structure encoding by molecular descriptors, text strings and binary fingerprints The design of diverse and focused libraries Chemical data analysis and visualization Structure-property/activity modeling (QSAR/QSPR) Ensemble modeling approaches, including bagging, boosting, stacking and random subspaces 3D pharmacophores modeling and pharmacological profiling using shape analysis Protein-ligand docking Implementation of algorithms in a high-level programming language Tutorials in Chemoinformatics is an ideal supplementary text for advanced undergraduate and graduate courses in chemoinformatics, bioinformatics, computational chemistry, computational biology, medicinal chemistry and biochemistry. It is also a valuable working resource for medicinal chemists, academic researchers and industrial chemists looking to enhance their chemoinformatics skills.

Edited by Alexandre Varnek, PhD, is a professor of theoretical chemistry at The University of

Strasbourg, France where he heads the Laboratory of Chemoinformatics, and is Director of two MSc programs: Chemoinformatics and In Silico Drug Design. Professor Varnek's research focuses on developing new approaches and tools for virtual screening and "in silico" design of new compounds and chemical reactions.

[Download to continue reading...](#)

Tutorials in Chemoinformatics Autodesk Maya 138 Tutorials and Tips by Antonio Bosi: 138 useful Maya tutorials (tips & tricks) for experts and beginners An Introduction to Chemoinformatics The Silver Way: Techniques, Tips, and Tutorials for Effective Character Design How to Draw Cartoon Characters with Colored Pencils: in Realistic Style, Step-By-Step Drawing Tutorials How to Draw Superheros and Movie Characters, Learn to Draw Batman, Spider-Man 3, Superman How To Draw: The Complete Starter Course on How To Draw - Easy Drawing Tutorials on How To Draw Manga Like A Pro! Colored Pencil Guide - How to Draw Realistic Objects: with colored pencils, Still Life Drawing Lessons, Realism, Learn How to Draw, Art Book, Illustrations, Step-by-Step drawing tutorials, Techniques Big Book on How to Draw Animals with Colored Pencils: Drawing tutorials, How to draw Braids, Buns, and Twists!: Step-by-Step Tutorials for 82 Fabulous Hairstyles ATI TEAS Secrets Study Guide: TEAS 6 Complete Study Manual, Full-Length Practice Tests, Review Video Tutorials for the Test of Essential Academic Skills, Sixth Edition No Shenanigans! Mixed media painting: No-nonsense tutorials from start to finish to release the artist in you! Ultimate Ableton Live 9 & 8 Course - 66 Detailed & Easy to Follow Training Video Tutorials Learn Guide (Music Habits) Dance Tutorials For Hip Hop GMATÂ Test Prep:Â GMATÂ Secrets Study Guide: Complete Review, Practice Tests, Video Tutorials for the Graduate Management Admission Test Ultimate Slime: DIY Tutorials for Crunchy Slime, Fluffy Slime, Fishbowl Slime, and More Than 100 Other Oddly Satisfying Recipes and Projects--Totally Borax Free! NCLEX-RN Premier 2017 with 2 Practice Tests: Online + Book + Video Tutorials + Mobile (Kaplan Test Prep) ACT Prep Book: ACT Secrets Study Guide: Complete Review, Practice Test, Video Tutorials for the ACT Test SAT Prep Book: SAT Secrets Study Guide: Complete Review, Practice Tests, Video Tutorials for the New College Board SAT Exam How to draw Superheroes: with Colored Pencils in Realistic Style, Learn to Draw Cartoon and Movie Characters, Step-by-Step Drawing Tutorials, How to Draw Batman, Superman, Spider-Man 2, Marvel, DC NCLEX-PN Premier 2017 with 2 Practice Tests: Online + Book + Video Tutorials + Mobile (Kaplan Test Prep)

Contact Us

DMCA

Privacy

FAQ & Help