Handbook of Chemoinformatics Algorithms (Chapman Hall/CRC Mathematical and Computational Biology)

Jean-Loup Faulon, Andreas Bender
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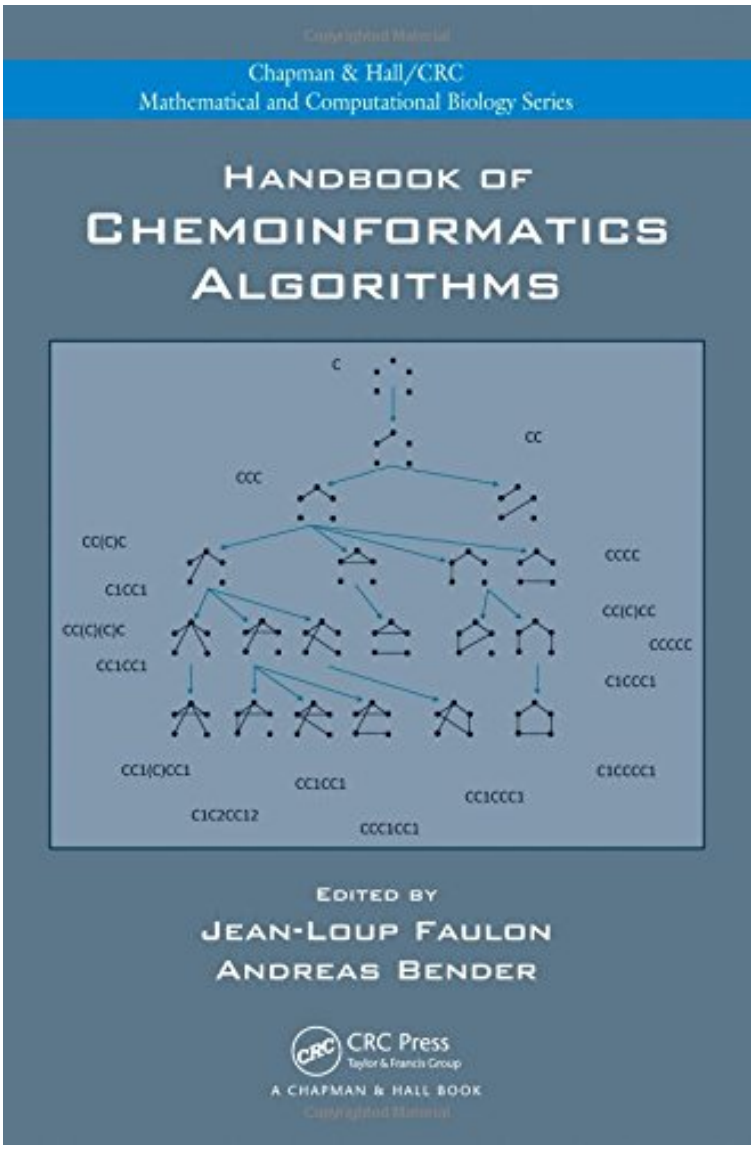

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Jean-Loup Faulon, Andreas Bender : Handbook of Chemoinformatics Algorithms (Chapman Hall/CRC Mathematical and Computational Biology) before purchasing it in order to gage whether or not it would be worth my time, and all praised Handbook of Chemoinformatics Algorithms (Chapman Hall/CRC Mathematical and Computational Biology):

0 of 0 people found the following review helpful. Excellent!By bbgunOne of the best chemoinformatics book so far! Cover algorithms for whoever want to implement their own chemoinformatics toolkit for drug discovery.

Unlike in the related area of bioinformatics, few books currently exist that document the techniques, tools, and algorithms of chemoinformatics. Bringing together worldwide experts in the field, the Handbook of Chemoinformatics Algorithms provides an overview of the most common chemoinformatics algorithms in a single source. After a historical perspective of the applications of algorithms and graph theory to chemical problems, the book presents algorithms for two-dimensional chemical structures and three-dimensional representations of molecules. It then focuses on molecular descriptors, virtual screening methods, and quantitative structureactivity relationship (QSAR) models, before introducing algorithms to enumerate and sample chemical structures. The book also covers computer-aided molecular design, reaction network generation, and open source software and database technologies. The remaining chapters describe techniques developed in the context of bioinformatics and computational biology and their potential applications to chemical problems. This handbook presents a selection of algorithms relevant in practice, making the book useful to those working in the field. It offers an up-to-date account of many algorithmic aspects of chemoinformatics.

About the AuthorJean-Loup Faulon is a professor in the Department of Biology at the University of Evry in France. Andreas Bender is an assistant professor in the Leiden/Amsterdam Center for Drug Research (LACDR) at Leiden University in the Netherlands.