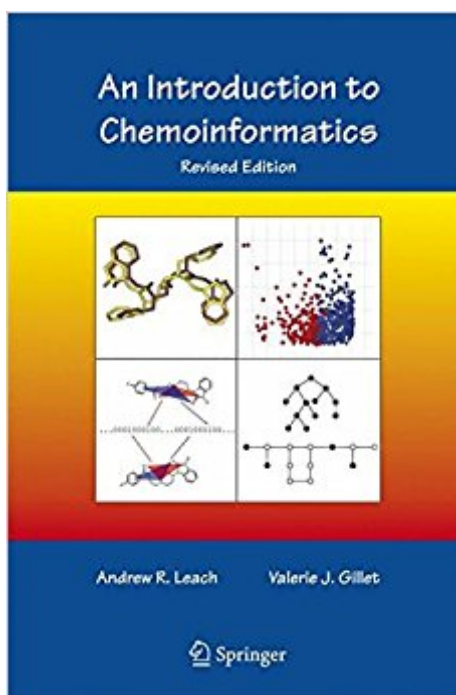


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An Introduction To Chemoinformatics



Synopsis

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.

Book Information

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Customer Reviews

This is a rather remarkable little book. Just as its title promises, it provides an introduction to a very wide variety of chemoinformatic and CADD topics. Although the book is written for beginning graduate students and advanced undergraduates, it could certainly provide a very helpful overview for professionals with no prior knowledge of the subject matter. Robert S. Pearlman, University of Texas at Austin. J.Am. Chem. Soc., Vol 126, No. 4, 2004.

This is really a great book. It is well organized and clearly written. The authors do a particular good job of explaining how the techniques discussed work. Having read the book you'll feel you could implement the techniques discussed yourself. I would recommend this book to anyone with moderate knowledge of chemistry who wants an understanding of the major aspects of

chemoinformatics.

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