

Book Review of Chemical Library Design

Chemical Library Design. Edited by Joe Zhongxiang Zhou. Humana Press, New York, NY. 2011. x + 362 pp. 18.5 × 26 cm. ISBN 9781607619307. \$209.00.

This book contains 18 chapters divided into five sections. Section I covers General Topics, including a historical overview of chemical library design, an informative chapter on chemoinformatics and library design, molecular library design using multiobjective optimizations, scaleable approaches to combinatorial library design, and application of Free–Wilson selectivity for combinatorial library design, and two chapters highlighting application of QSAR, shape pharmacophore modeling, and pharmacophore fingerprinting to combinatorial library design. Section II focuses on structure-based library design, with chapters on structure-based library design and docking methods and a chapter describing methods used in a library designed for identification of 11 β -HSD1 adamantyl amide inhibitors. Section III explores fragment-based library design in three chapters, including the design of screening collections, and a fascinating chapter on the use of the Pfizer Global Virtual Library Space for generation of library design ideas. Section IV of the text consists of a single chapter on the design, annotation, and application of a kinase-targeted library. The final section of this work contains four chapters highlighting the use of computer-based library design tools to streamline and design syntheses. Two of these chapters highlight further use of the Pfizer Global Virtual Library Space for design and synthesis of libraries and single compounds, as well as a design of a library focused against human Chk1 kinase. The final two chapters describe two separate tools, GLARE (Global Library Assessment of REagents) and CLEVER (Chemical Library Editing, Visualizing, and Enumerating Resource). These chapters outline the use and implementation of these two separate web-based or downloadable program suites that should be of great interest to investigators designing and synthesizing chemical libraries.

The “General Topics” section of this book is extremely useful; it provides a broad view of chemical library design. The selection of different approaches in the seven chapters of this section provides a good review of several major methods to apply to library design. Likewise, the two sections on Structure-based and Fragment-based library design, which contain three chapters each, cover concepts with sufficient depth to satisfy experts in the field, while remaining accessible to those with less experience in chemical library design.

The inclusion of several chapters highlighting computational tools provides insight into technological development and tools for chemical library design. However, the chapters demonstrating the use of the Pfizer Global Library Virtual Space may prove to be little use to the majority of readers, as this is a tool available only internally at Pfizer. While perhaps lacking utility for a broader audience, the chapters highlighting the Pfizer tool would be exceedingly useful to programmers or designers interested in developing combinatorial chemical library software utilities and,

as such, will appeal to that audience. The description of the two “freeware tools,” GLARE and CLEVER, should prove to be very useful to a broad audience interested in chemical library design and provide an excellent description and demonstration of the implementation of those programs.

The format of the book is well designed, and it is easy to read. The chapters are well written by experts in the field. A few of the chapters contain rich color illustrations, while others convey information in sharp black-and-white or greyscale. Each chapter is extensively referenced and includes keywords and abstracts.

In summary, Chemical Library Design is a high-quality addition to the Methods in Molecular Biology series. The quality of writing, organization, and topic selection form a valuable resource that should be educational and serve as a good resource for those interested in Chemical Library Design.

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