Cheminformatics without Formulas

Virtual Screening in Drug Discovery

Edited by *Juan Alvarez* and *Brian Schoichet*.

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The main question posed in any review on scientific text books is: Who is the audience—well-educated laymen, students or professionals? In my view *Virtual Screening in Drug Discovery* provides an easy-to-read introduction to the field of cheminformatics, in particular virtual screening, for students and those medicinal chemists starting to become familiar with this topic. The book has five parts with 16 chapters altogether. The first two parts (five chapters) explain algorithms of structure-based virtual screening. Part III deals with ligand-based virtual screening, and Parts IV and V describe modifications of established molecular-docking tools. Having thoroughly read the book, my major criticism is that the editors did not elucidate the concept they wanted to follow. I felt somehow lost in a diverse compilation of individual contributions. My particular impression was that it is a great endeavour to edit a multiauthor book on virtual screening and not to discourage an audience of chemists and pharmacists—either students or professionals—who may not like complicated mathematics but try to understand the fascination of virtual screening. Several chapters of this book come very close to this ambitious goal, like Chapter 13 by Juan Alvarez on pharmacophore-based docking, or those by Gerd Klebe (Chapter 1) and Matthias Rarey (Chapter 2) on structure-based screening. These latter ones are my favourite articles, I have to admit. In addition, I learned much about data mining from reading Chapter 6 by Nikolay Savchuk and Konstantin Balakin. But still: overall the volume would have benefited from more rigorous editing to clarify the whole idea of the book.

Certainly the demand for medicinal chemists with an expert knowledge who apply and improve current virtual-screening tools is coupled with a permanent need for the education of computational chemists and virtual screeners. Does the book by Alvarez and Shoichet support modern education in this complex subject by combining chemistry and pharmacy with physics and computer science? In such a compilation of expert contributions, the reader expects detailed explanations of virtual-screening tools including some basic formulae for molecule representations, molecular similarity and structure of chemical space as well as the basic physical formulae describing protein–ligand interactions and scoring functions. It is indeed astonishing that there are no mathematical equations presented at all, except in Chapter 10. However, this lack is compensated for by a clear and scientifically correct text is in most parts. There is no doubt that many aspects of structure-based screening as docking methods are well explained in words. Although, surprisingly, some important standard terms like "Tanimoto similarity" are neither explained nor even mentioned in the book's index!

Some of the most challenging aspects of virtual screening, like ADMETox predictions and modern approaches for de novo design, are completely omitted in the present edition. Such topics should be added in an extended edition.

Despite my picky points of criticism, I do recommend the book for progressed and progressive novices in the field of virtual screening and drug discovery.

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