# Book review

**QSAR: Hansch Analysis and Related Approaches** by Hugo Kubinyi, VCH, 1996. DM 198 (xii + 240 pages) ISBN 3 527 3035 X

The study of quantitative structure–activity relationships (QSAR) is a widely mistrusted discipline. On the one hand, certain properties of molecules, such as their heats of formation, can be well correlated with the presence or absence of certain descriptors, such as functional groups or chain branching. On the other hand, *in vivo* activity is a much more complicated 'property' that generally defies prediction. Experienced pharmaceutical and agricultural researchers know that, in most cases, QSAR is not highly predictive and can be hard to use, and that, depending on exactly which parameters are chosen, a wide range of answers is possible. Thus many researchers shun QSAR entirely.

For this reason *QSAR: Hansch Analysis and Related Approaches*, the first volume in a series entitled *Methods and Principles in Medicinal Chemistry*, is a very important book. It provides an excellent introduction to the field of QSAR analysis. The author, Dr Hugo Kubinyi, has many years of experience in the field of traditional QSAR (Hansch analysis) and knows well the strengths and weaknesses of these methods. The book contains many examples of the use of QSAR methods and more than 1,100 references spanning the entire field of QSAR. The index is excellent.

The book provides a thorough grounding in traditional QSAR methods and points out many of the pitfalls. Many different *in vitro* properties that can be correlated using QSAR are discussed, and many of the 'buzzwords' that surround the field of QSAR, such as partial least squares (PLS), principal component analysis (PCA) and D-optimal design, are described. A very important message of this book is that QSAR is not primarily about prediction. Because of the complexity of predicting *in vivo* properties, the author contends, the correct view of QSAR is that it helps in making sense of the general trends in research data, hence contributing to the 'big picture', rather than allowing the scientist simply to plug all of the data into an equation and predict the next blockbuster drug. This perspective on QSAR is valuable because many researchers have a very different expectation (either much higher or much lower) of what QSAR can accomplish. Perhaps for this reason, 'success stories' in QSAR are generally given short shrift in this book, although many references both to the success stories and reviews on the topics are provided. More coverage of such real-world examples would have been useful.

Towards the end of the book is a chapter on 3D QSAR. This short chapter suffers from being rather dated, because the book was written in 1993. However, many of the basic topics in the field are discussed, such as comparative molecular field analysis (CoMFA), conformational generation, 3D database searching and *de novo* drug design.

This book will certainly be worthwhile reading for many scientists. For the novice, the book provides a fast but thorough introduction to the field of QSAR; the book will help anyone who has already dabbled in QSAR to achieve deeper understanding, and the collection of references will be invaluable even for the expert. The book provides valuable insights into the many properties that can be studied via QSAR methods. Overall, the book does an excellent job of pointing out the potential applications of these powerful techniques.

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