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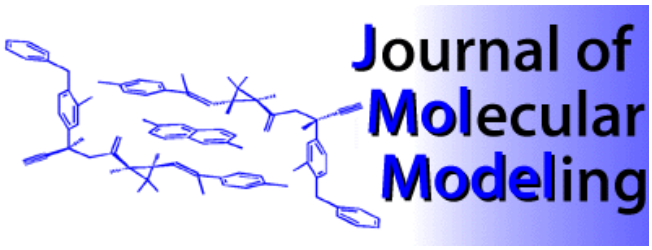

Book review

Reviews in Computational Chemistry, Volume 9

Edited by K.B. Lipkowitz and D.B. Boyd, VCH Publishers, New York, 1996. ISBN 1-56081-930-8. US $ 110.–

Received: 1 October 1997 / Published: 7 November 1997

As in previous volumes, the editors discuss the importance of computational chemistry in the preface. This time they use a literature survey to answer the questions "Which countries publish the most, and what are the *epicenters* of computational chemistry?"

The central theme of volume 9 of the *Reviews in Computational Chemistry* is molecular modelling. The five reviews deal with different topics ranging from theoretical approaches to applications in drug design.

The first chapter, written by James R. Damewood Jr., looks at applications of molecular modelling methods from an industrial point of view. A large number of case studies are described, in which molecular modelling was successfully used in peptide mimetic design to develop new drugs.

The following chapter reviews theoretical and practical aspects of the important subject of free energy calculations. T.P. Straatsma explains the underlying statistical thermodynamical background in a clear and understandable way. A list of recommendations to follow when doing free energy calculations conclude this chapter.

In many biological processes, like for example cell-cell recognition, carbohydrates play a vital role. The various available computational methods to study the conformations of oligosaccharides are described by Robert J. Woods in chapter 3.

A large number of force fields is nowadays available and can easily be applied using sophisticated graphics interfaces. But what method should be used? Ingrid Pettersson and Tommy Liljefors try to answer this question in chapter 4. They summarize and discuss articles were different force fields were compared.

The final chapter is somewhat different from the others. Gustavo A. Arteca surveys the large variety of molecular shape descriptors. He classifies the different descriptors according to the dimensionality of the molecular represenation in a hierarchical scheme. The chapter ends with some comments on descriptors for dynamical changes of shape and for relative shapes between two molecules.

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