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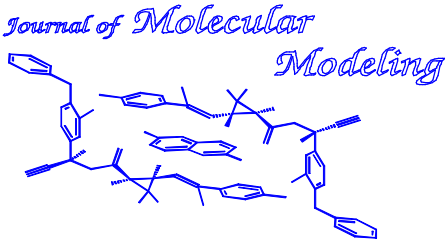

Book review

Computer Aided Molecular Design — Applications in Agrochemicals, Materials, and Pharmaceuticals

Edited by Charles H. Reynolds, M. Katherine Holloway, and Harold K. Cox. Washington, D. C., The American Chemical Society, 1995. x + 428 pp. 15.5 x 23 cm. ISBN 0-8412-3160-5. US $ 99.95.

This book was developed from a symposium of the American Chemical Society, sponsored by the Division of Computers In Chemistry and The Division of Agrochemicals, at the 207th National meeting of the ACS, held in San Diego, California, March 13 - 17, 1994. The book addresses the editors' stated goal of providing answers to two questions, which might be asked by practicing scientists — viz. (1) What new product have arisen from Computer Aided Molecular Design (CAMD) ? and (2) How can the many non-specialist scientists apply modeling and computational techniques to their work ?

The first question is the harder to answer. Molecular modeling / computational chemistry / CAMD techniques have become a part of the team effort of most industrial research projects. The general field has matured so much in the past ten years, that its application is as commonplace as, say, spectroscopic methods. Thus the attribution of a breakthrough discovery exclusively to CAMD is difficult to do in practice, although in most cases, the rest of the team would ratify the importance of the computational component of the work.

To answer the second question, the book is organized into 28 chapters, which are deemed to be case studies in the application of computational chemistry techniques to real-world research problems, in three sections: (1) Pharmaceuticals, (2) Agrochemicals, and (3) Materials.

Volume 589 of the ACS Symposium Series continues the excellent tradition of its predecessors, by offering the reader comprehensive, and current information on subjects of importance to specialists incomputational chemistry as well as their experimental colleagues. Each of the 28 chapters is written by well-known leaders in their respective fields who provide fascinating demonstrations of their extensive expertise. The breadth of computational topics covered makes the volume important to those wishing to gain insight outside of their core area of expertise. The utility of the work is all the more apparent when one considers that most of the techniques described and applied in each of the three topical sections could just as well be applied in either of the other two.

The volume contains three indices: An author index, an affiliation index, and a subject index. Each chapter contains an extensive bibliography. The price is reasonable. It is recommended for individuals, researchers, and institutional libraries.

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