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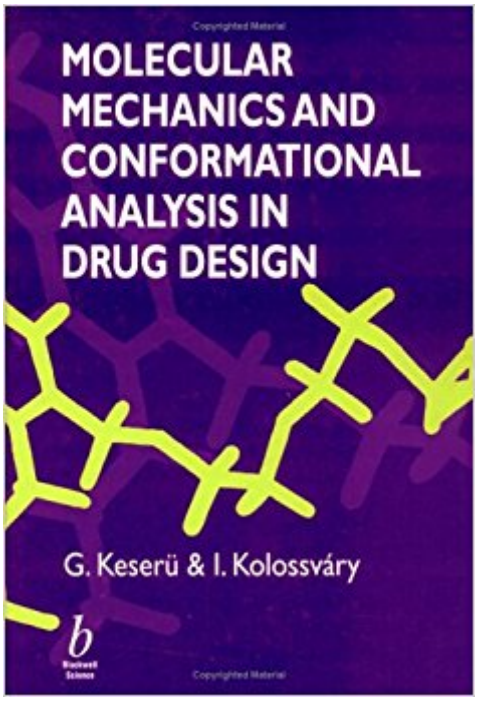

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Synopsis

Molecular modelling truly has come of age. Computational chemistry techniques are now routinely used to simulate chemical and physical properties before synthesis. The widespread availability of high-performance computer processing power combined with an abundance of computational chemistry software has allowed non-specialists to do modelling previously reserved for specialists. But the software has not yet evolved to the point where its results can be taken on faith. All outputs are highly dependent on the inputting assumptions, so an understanding of these are fundamental to any serious studies. This book provides clear descriptions of the theoretical background to molecular mechanics-based conformational energy calculations. Although the book is written primarily for the non-specialist, there is enough rigour to serve as an essential reference for experts. Using real examples, the emphasis is on demonstrating how the calculations relate to actual studies. The non-specialist can omit certain sections and still get a working knowledge of all the important methods.

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