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Sinopsis

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"This book provides an excellent introduction to the modeling of biomolecular structures and dynamics. It is subdivided into three parts covering relatively broad topics: (1) molecular structure and modeling, inclusive of current problems and state of computation (Chapters 1-6); (2) molecular mechanics: force field origin, composition, and evaluation techniques (Chapters 7-9); and (3) simulation techniques: conformational sampling by geometry optimization, Monte Carlo, and molecular dynamics approaches (Chapter 10-13). The last chapter (Chapter 14) is devoted to discussing the similarity and diversity problems in chemical design. The book's appendices complement the material in the main text through homework assignments, reading lists, and other information useful for teaching molecular modeling.\par The book is intended for students of an interdisciplinary graduate course in molecular modeling as well as for researchers (physicists, mathematicians and engineers) to get them started in computational molecular biology."