



Molecular Dynamics: Applications in Molecular Biology (Topics in Molecular & Structural Biology)

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In the introduction to this series in "Topics in Molecular Biology" in 1980, great emphasis was placed on the importance of molecular structure for understanding biological phenomena. At this time, the emphasis was on the three-dimensional models determined from experimental methods such as x-ray crystallography. More speculative model building and conformational analysis was mentioned only in passing. In the decade since this was written, the original emphasis on molecular structure has increased with many new structures being solved. Along with the accumulation of new three-dimensional structures, there has been an awareness that it is not the static picture alone but also the dynamics of macro-molecules which are important. Although x-ray crystallography can model some aspects of atomic motion, it has been the extension of computer simulation techniques such as molecular dynamics from physics and chemistry to molecular biology which has provided an overall picture of macromolecular dynamics. The aim of this book is to review the uses of molecular dynamics and related modelling techniques as applied to biological macro-molecules. It is particularly suited for those who have not specialized in simulation techniques. As well as describing applications to proteins, nucleotides and carbohydrates, we have also reviewed the exciting possibilities which emerge from the use of free energy perturbation methods in protein engineering and drug designs. Recently, molecular dynamics has started to play a direct role in the determination of macro-molecular structures themselves when simulated annealing protocols are used in combination with experimental data from x-ray crystallography or nmr spectroscopy.

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