

## COMPUTER SIMULATION OF BIOMOLECULAR SYSTEMS%0A

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Computer Simulation of Chemical and Biomolecular Systems Vol. 482 (1986) ANNALS OF THE NEW YORK ACADEMY OF SCIENCES Free Energy Simulations a M. Mezei and D.L. Beveridge b Chemistry Department Hunter College of the City University of New York New York, NY 10021 INTRODUCTION. Monte Carlo or molecular dynamics simulations involve the numerical determinations of the statistical thermodynamics and

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Computer Simulation of Biomolecular Systems: Where Do We Stand? Wilfred F. van Gunsteren and Daan P. Geerke Laboratory of Physical Chemistry, Swiss Federal Institute of Technology, ETH, 8093 Zurich, Switzerland E-mail: wfvgn@igc.phys.chem.ethz.ch The four major aspects that determine the quality of the ensemble of molecular conformations as obtained from biomolecular simulation are reviewed

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