Advances in Computational Methods for Macromolecular Modeling

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3 The workshop on Methods for Macromolecular Modeling (M), held at New York University on 12- 14 October 2000, attracted 187 participants from Eu rope, Asia, the Americas, and the Middle East. (see monod.biomath .nyu.eduj rvhganjconfOO.html for more information). The exciting program was made possible by the dedicated work of the international advisory committee whose members were P. Deuflhard, J. Hermans, B. Leimkuhler, A. E. Mark, S. Reich, T. Schlick, and R. Skeel. We are indebted to the following agen cies and institutions for their generous support: the Burroughs Wellcome Fund, Department of Energy, National Science Foundation, National Insti tutes of Health, Computational Biomedicine Initiative at Mount Sinai School of Medicine, and NYU's Courant Institute of Mathematical Sciences, Depart ment of Chemistry, and Science Council. This volume is a collection of 19 review and original articles by the speak 3 ers and participants of the M workshop. The topics covered include molecu lar dynamics methods, Monte Carlo methods, other conformational sampling methods, free energy methods, long range interactions and fast electrostatics, and statistical approaches to protein structures. A perspective article intro duces the contributions in this volume and reflects on future prospects in macromolecular modeling.

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