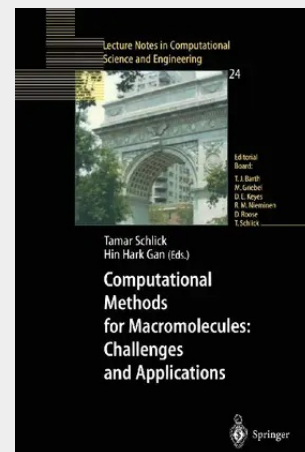


Computational Methods for Macromolecules: Challenges and Applications

Proceedings of the 3rd International Workshop on Algorithms for Macromolecular Modeling, New York, October 12-14, 2000

The workshop on Methods for Macromolecular Modeling (M), held at New York University on 12-14 October 2000, attracted 187 participants from Europe, Asia, the Americas, and the Middle East. (see monod.biomath.nyu.edu/rvhganjconfOO.html for more information). The exciting program was made possible by the dedicated work of the international advisory committee whose members were P. Deuffhard, J. Hermans, B. Leimkuhler, A. E. Mark, S. Reich, T. Schlick, and R. Skeel. We are indebted to the following agencies and institutions for their generous support: the Burroughs Wellcome Fund, Department of Energy, National Science Foundation, National Institutes of Health, Computational Biomedicine Initiative at Mount Sinai School of Medicine, and NYU's Courant Institute of Mathematical Sciences, Department of Chemistry, and Science Council. This volume is a collection of 19 review and original articles by the speakers and participants of the M workshop. The topics covered include molecular 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 introduces the contributions in this volume and reflects on future prospects in macromolecular modeling.

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