Lecture Notes
in Computational Science
and Engineering 24

3rd International Workshop
on Algorithms for Macromolecular Modeling

Organizing Committee

Springer-Verlag Berlin Heidelberg GmbH

Tamar Schlick
Hin Hark Gan
Editors

Computational Methods for Macromolecules: Challenges and Applications

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

With 128 Figures, 14 in Color, and 55 Tables

Springer

Editors

Tamar Schlick
Hin Hark Gan

Department of Chemistry
Courant Institute of Mathematical Sciences
New York University
and Howard Hughes Medical Institute
251 Mercer Street
New York, NY 10012, USA
e-mail: schlick@nyu.edu
hgan@biomath.nyu.edu

Cataloging-in-Publication Data applied for

Die Deutsche Bibliothek - CIP-Einheitsaufnahme

Computational methods for macromolecules : challenges and applications ;
proceedings of the 3rd International Workshop on Algorithms for Macromolecular Modeling,
New York, October 12 - 14, 2000 ; with 55 tables / Tamar Schlick ; Hin Hark Gan, ed.. -
Berlin ; Heidelberg ; New York ; Barcelona ; Hong Kong ; London ; Milan ; Paris ; Tokyo :
Springer, 2002
(Lecture notes in computational science and engineering ; Vol. 24)

Cover figure: Washington Square Arch, Greenwich Village, New York City
(photo by Hin Hark Gan)

Mathematics Subject Classification (2000):
92-XX, 34-XX, 35-XX, 41-XX, 60-XX, 70-XX, 82-XX

ISSN 1439-7358

ISBN 978-3-540-43756-7 ISBN 978-3-642-56080-4 (eBook)
DOI 10.1007/978-3-642-56080-4

http://www.springer.de

Originally published by Springer-Verlag Berlin Heidelberg New York in 2002

Cover Design: Friedhelm Steinen-Broo, Estudio Calamar, Spain
Cover production: *design & production*
Typeset by the authors using a Springer TEX macro package

Printed on acid-free paper SPIN: 10859427 46/3142/LK - 5 4 3 2 1 0

Preface

The workshop on Methods for Macromolecular Modeling (M^3), 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/~hgan/conf00.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 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^3 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.

Tamar Schlick and Hin Hark Gan
New York
November 20, 2001

Table of Contents

VII STATISTICAL APPROACHES TO PROTEIN STRUCTURES