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Announcement

Drug research and discovery are of critical importance in human health care and are becoming increasingly expensive, while the need for new drugs is also increasing. Computational approaches for drug lead discovery and optimization have proven successful in many recent research programs. These methods have grown in their effectiveness not only because of improved understanding of the basic science – the biological events and molecular interactions that define a target for therapeutic intervention – but also because of advances in algorithms, representations, and mathematical procedures for studying such processes.

On April 7–11, 1997, the University of Minnesota Institute for Mathematics and its Applications (IMA) and Supercomputer Institute will bring together top researchers and interested newcomers for a workshop in computer-aided drug discovery and rational drug design. The workshop should be of interest to those whose speciality is computational chemistry, mathematics, or computer science as the goal is to promote interdisciplinary communication and collaboration. The workshop will present state-of-the-art research in both the science and the underlying mathematics, and it will attempt to identify new problems for possible collaborations. General subject areas of the workshop will include receptor-based applications such as binding energy approximations, molecular docking, and de novo design; non-receptor-based applications such as molecular similarity, conformational analysis, and structural diversity; molecular dynamics simulations and protein folding simulations; plus related issues such as drug delivery modeling and scientific visualization. The workshop will also focus on the mathematical procedures and algorithms upon which the scientific applications are based. The overall goal of the workshop is to bring together scientists and mathematicians to examine the current state of this very broad and interdisciplinary field of research, and to identify the areas where cross-fertilization of ideas and collaborative research might most effectively advance the field.

Organizing committee:
W. Jeffrey Howe, Upjohn Laboratories (chair)
Jeffrey M. Blaney, Chiron Corporation
Richard Dammkoehler, Washington University
Anton J. Hopfinger, University of Illinois at Chicago
Donald G. Truhlar, University of Minnesota

Confirmed speakers and their titles:
Overview: Garland Marshall, Washington University
Graph Theory: Peter Willett, University of Sheffield
Molecular Similarity: W. Graham Richards, Oxford University
Panel: Chaired by Jeff Howe and Tony Hopfinger
"What are the most important problems in drug design that may be computationally tractable?"

Panelists:
Dave Doherty, Minnesota Supercomputer Center, Inc.
Bill Dunn, University of Illinois at Chicago
W. Graham Richards, Oxford University
Doug Rohrer, Pharmacia & Upjohn
Conformational Analysis in Solution – Quantum Mechanical Representation: Christopher Cramer

Combinatorial Chemistry and Molecular Diversity: Robert Pearlman, University of Texas at Austin

Binding Energies: Colin McMartin, Ciba-Geigy Corporation
Docking: Regine Bohacek, Ciba-Geigy Corporation
Lattice Models, Protein Folding: Ken Dill, University of California at San Francisco

Molecular Dynamics Information Extraction: Dennis Sprous, Wesleyan University

Molecular Dynamics and Simulations: Thomas A. (Tom) Darden, National Institute of Environmental Health Science

Panel Discussion: Chaired by Jeff Blaney
"What are the new problems that should be addressed in the next ten years?"

Panelists:
Gordon Crippen, University of Michigan
Simon Kearsley, Merck
Garland Marshall, Washington University
Phil Portoghese, University of Minnesota

Neural Nets: Johann Gasteiger, University of Erlangen
Genetic Algorithms and Related Topics: David Rogers, Molecular Simulations Inc.
Optimization Techniques and Parallel Computing: Brian T. Luke, National Cancer Institute-Frederick Cancer Research and Development Center
Cell-Based Methods for Sampling in High-Dimensional Spaces: Jason Rush, Department of Mathematics, University of Washington
"There are more binding site models to explain our data than we ever thought possible": Gordon Crippen, University of Michigan

Scientific Visualization: Mike Pique, The Scripps Research Institute

Further information about this conference is available at the following URL:

http: //www2.msi.umn.edu/Symposia/Drug_design.html

For information on how to register, contact the IMA at:
Institute for Mathematics and its Applications
University of Minnesota
514 Vincent Hall
206 Church Street SE
Minneapolis, MN 55455, USA
Tel: 001 612 624-6066
E-mail: staff@ima.umn.edu