MODERN CONCEPTS IN MOLECULAR MODELING

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Computational methods to predict and analyze the structural and energetic properties of small or macromolecules and their interactions play an increasingly important role in chemistry and biology. The wealth of available sequences, structures, and mutagenesis data provide an enormous database for computational efforts to predict structures, simulate molecular interactions, and understand them in quantitative energetic terms.

The field of molecular modeling is very diverse and difficult to define. Primary goals of the workshop, **Modern Concepts in Molecular Modeling,** were to highlight major directions of computer modeling efforts and to reflect the diversity of current research. How are molecular structures and properties analyzed? How are biomolecules and their interactions modeled and energetically characterized? What are the successes, caveats, and limitations?

The majority of contributions to the session have focused on the development and application of various energy functions to study the structure, energetics, and dynamics of proteins and their interactions with ligands. These include molecular dynamics, free energy calculations and empirical free energy functions, quantum mechananics, and molecular field analysis.

Others contributions have targeted structure comparison, prediction, and assessment.

In aggregate, these studies provide an exciting view of current developments in computer-aided molecular modeling and theoretical analysis or biological molecules. The research presented in this session certainly contributes to the wide spectrum of methods and applications in the biocomputing arena.

Participants in this workshop included: **B. Hess**, University of Groningen, *Model for the Long Term Dynamics of Proteins;* **P. A. Kollman**, University of California, San Francisco, *Molecular Dynamics and Free Energy Calculations;* **T. P. Lybrand**, University of Washington, *Evaluation of Three-Dimensional Models for Proteins and Protein-Ligand Complexes;* **G. M. Maggiora**, Pharmacia & Upjohn, *MIMIC: A Field-Based Approach to Molecular Similarity with Applications to Small Molecules and Proteins;* **T. Mirzadegan**, Roche Bioscience, *Homology Modeling of Immunoglobulins;* **J. Novotny**, Bristol-Myers Squibb Research Institute, *Empirical Free Energy Calculations on Mutants of the HyHEL-10-Lysozyme Complex;* **R. E. Stenkamp**, University of Washington, *Protein Superfamilies as Targets for Computer Modeling: The Carbohydrate Recognition Domain of a Macrophage Lectin; and,* **A. Tempzcyk**, Agouron Pharmaceuticals, Inc., *Combined Quantum and Molecular Mechanics: Catalytic Mechanism of the Protein Serine/Threonine Phosphatase Family.*

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