Results

MOLECULAR MODELING & COMPUTATIONAL CHEMISTRY

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About 100 papers from 25 journals are cited.

Editorial and News

I am the new Editor for MMCC Results, the Molecular Modeling and Computational Chemistry News Letter. I took this project responsibility from Prof. David Busath starting from this year. I have worked two years as an Assistant Editor of MMCC Results under the previous Editor, Prof. David Busath. We have covered more than 25 journals every month and selected the more interesting articles for each issue of this newsletter.

I sincerely hope that all the scientists from acdemic and industrial background will give their full support to this project.

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David Busath,M.D.
Dr. Gelin was founder of MMCC Results and edited volumes 1-6.
Dr. David Busath edited volumes 7-14

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Marginal symbols indicate that the authors acknowledged the use of a software package from a commercial sourse. **A** refers to Accelrys Inc. and **T** to Tripos Inc. Other companies are denoted by their name in a box. Papers of special interest are marked by an exclamation point [**!**].

List of the Journals covered in MMCC Results Newsletter

(1) European Journal of Biophysics

(2) European Journal of Medicinal Chemistry

(3) Molecular Simulation

(4) Journal of Molecular Modeling

(5) Journal of Molecular Graphics & Modeling

(6) Bioorganic & Medicinal Chemistry

(7) Current Opinion in Structural Biology

(8) Current Opinion in Chemical Biology

(9) PNAS (USA)

(10) Journal of Biochemistry

(11) Journal of Biophysical Chemistry

(12) Journal of Chemical Theory & Computation

(13) Theoretical Chemistry Accounts: Theory, Computation, & Modeling

(14) Journal of Biomolecules

(15) Journal of Medicinal Chemistry

(16) Journal of American Chemical Society

(17) Proteins: Structure, Function and Bioinformatics

(18) Journal of Computer-Aided Molecular Design

(19) Journal of Computational Chemistry

(20) Journal of Physical Chemistry-B

(21) Biophysical Journal

(22) Journal of Chemical Information and Modeling

(23) Journal of Chemical Physics

(24) Trends in Biochemical Sciences

(25) Journal of Biomolecular Structure and Dynamics

(26) Journal of Molecular Biology

(27) Biopolymers

(28) Protein Engineering & Design

(29) Bioinformatics

(30) Nature

1. APPLICATIONS

Small Molecules

Biopolymers

Threading and Fold Recognition

Protein Structure Prediction

Comparative or Homology Modeling

Protein Side-Chain Conformation Prediction

Peptide Conformational Analysis

Protein Structure Analysis

Protein Engineering

Protein Hydration

Protein Electrostatics and Titration

Protein Dynamics

Free Energy Calculations

Ligand Binding

Enzyme Catalysis

Protein-Protein Interactions

Membrane Proteins and Lipid-Peptide Interactions

Proteins and Surfaces

Protein Design

Protein Folding

Protein-Nucleic Acid Interactions
Nucleic Acids

Lipids and Surfactants

Carbohydrates

Polymers

Surfaces, Catalysts, and Materials Subjects

2. METHODOLOGY

Quantitative Structure-Activity Relations

Conformational Search and Analysis

Structure-Based Focussing

Potentials and Parameters

Solvation Energy

Global Energy Minimization

Normal Modes Analysis

Molecular Dynamics

Monte Carlo

Free Energy Perturbation

QM/MM

Secondary Structure Prediction

Comparative or Homology Modeling

Peptide Conformational Analysis

Side Chain Structure Prediction

Protein Structure Prediction

Threading or Fold Prediction

Surface and Volume Determination

Structural Similarity Analysis

Protein Folding

Ligand Docking

Structure Determination

3. JOURNAL REVIEWS

Journal of Computational Chemistry 20(11), August, 1999

Journal of Computational Chemistry 20(12), September, 1999

Bioinformatics 15(5) May, 1999

Bioinformatics 15(7) July, 1999

Bioinformatics 15(8) August, 1999

4. BOOK REVIEWS

5. SOFTWARE/NETWARE REVIEWS

6. EMPLOYMENT OPPORTUNITIES

Ads for this section cost $200 and run for three months unless withdrawn. There is no size limit, but each ad can fully describe only one specific position with additional positions described only in general terms and as a group. Alternative formats will be accommodated within reason. Email or mail your text to the editor by the third Saturday of the month prior to publication (*N.B.*: no issues in August and January).

SYLVIA HONEYCUTT INFO HERE!

7. UPCOMING MEETINGS

8. ADDRESSES OF PRINCIPAL AUTHORS

The production sites for the corresponding or principal authors are given in brackets in the citations. When not designated by the publisher, the first author is assumed to be the principal. Current addresses are listed here.

Temple F. Smith

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