

Computational Molecular Bioscience



Journal Editorial Board

ISSN: 2165-3445 (Print) ISSN: 2165-3453 (Online)

https://www.scirp.org/journal/cmb

Editorial Board

Dr. David R. Bevan Virginia Polytechnic Institute and State University, USA

Dr. Ajmal Rashid BhatUniversity of Kashmir, IndiaProf. Emilio GallicchioRutgers University, USA

Dr. Ian S. Haworth University of Southern California, USA

Prof. Srividhya JeyaramanIndiana University, USAProf. Cizhong JiangTongji University, ChinaDr. Daisuke KiharaPurdue University, USA

Prof. Jianyong Li Virginia Polytechnic Institute and State University, USA

Dr. Jose L. Medina-Franco Florida Atlantic University, USA
Dr. Oluwafemi Adeleke Ojo Landmark University, Nigeria

Dr. Sihua PengShanghai Ocean University, ChinaDr. Yuxing PengThe University of Chicago, USADr. Olli T. PentikäinenUniversity of Jyväskylä, Finland

Prof. Giulio Rastelli University of Modena and Reggio Emilia, Italy

Dr. A.H. Manjunatha Reddy RV College of Engineering, India

Prof. Igor A. TopolFrederick National Laboratory for Cancer Research, USADr. Ivanka TsakovskaInstitute of Biophysics and Biomedical Engineering, Bulgaria

Prof. Nagarajan VaidehiCity of Hope National Medical Center, USAProf. Dongqing WeiShanghai Jiao Tong University, China

Dr. Yasushige Yonezawa Kinki University, Japan



ISSN Online: 2165-3453 ISSN Print: 2165-3445

Table of Contents

Volume 12	Number 1	March 20)22
	ing and Molecular Dynami Mechanism of MTHFD2 I	nics Simulation Studies on the	
•			1
Rhenium Ligand	-	nd Core Canonical Pathways Involved in chymal Transition (EMT) Induced TTY Software System	
	•	Banerjee, S. Wisniewski, Q. Reaves, K. Dia, S. Brown, awat, S. Mandal, Z. Abedin, S. Ghosh, H. Banerjee	12
•	otranscriptomics Landscap ays in <i>Toxoplasma gondii</i> I	- ·	
T. Tarannum, M.	S. Alam, A. Rahman, S. Chakra	raborty, H. U. Shekhar, T. Rahman	20
Antibody-Like Ph	nosphorylation Sites. Them	ne for Studies of Cancer, Aging and Evolution	
J. Kubrycht, K. Siş	gler		58

Computational Molecular Bioscience (CMB) Journal Information

SUBSCRIPTIONS

The *Computational Molecular Bioscience* (Online at Scientific Research Publishing, https://www.scirp.org/) is published quarterly by Scientific Research Publishing, Inc., USA.

Subscription rates:

Print: \$79 per issue.

To subscribe, please contact Journals Subscriptions Department, E-mail: sub@scirp.org

SERVICES

Advertisements

Advertisement Sales Department, E-mail: service@scirp.org

Reprints (minimum quantity 100 copies)

Reprints Co-ordinator, Scientific Research Publishing, Inc., USA.

E-mail: sub@scirp.org

COPYRIGHT

Copyright and reuse rights for the front matter of the journal:

Copyright © 2022 by Scientific Research Publishing Inc.

This work is licensed under the Creative Commons Attribution International License (CC BY).

http://creativecommons.org/licenses/by/4.0/

Copyright for individual papers of the journal:

Copyright © 2022 by author(s) and Scientific Research Publishing Inc.

Reuse rights for individual papers:

Note: At SCIRP authors can choose between CC BY and CC BY-NC. Please consult each paper for its reuse rights.

Disclaimer of liability

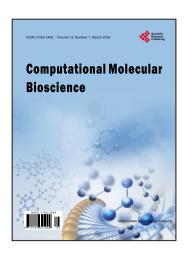
Statements and opinions expressed in the articles and communications are those of the individual contributors and not the statements and opinion of Scientific Research Publishing, Inc. We assume no responsibility or liability for any damage or injury to persons or property arising out of the use of any materials, instructions, methods or ideas contained herein. We expressly disclaim any implied warranties of merchantability or fitness for a particular purpose. If expert assistance is required, the services of a competent professional person should be sought.

PRODUCTION INFORMATION

For manuscripts that have been accepted for publication, please contact:

E-mail: cmb@scirp.org

Call for Papers



Computational Molecular Bioscience

ISSN: 2165-3445 (Print) ISSN: 2165-3453 (Online)

https://www.scirp.org/journal/cmb

Computational Molecular Bioscience (CMB) is an international journal dedicated to the latest advancement of Computational Molecular Bioscience. The goal of this journal is to provide a platform for scientists and academicians all over the world to promote, share, and discuss various new issues and developments in different areas of Computational Molecular Bioscience. All manuscripts must be prepared in English, and are subject to a rigorous and fair peer-review process. Accepted papers will immediately appear online followed by printed hard copy. The journal publishes original papers including but not limited to the following fields:

- ◆ Ab Initio and Density Functional Calculations of Biomolecules
- ◆ Atomistic and Coarse Grained Molecular Dynamics
- Combined Computational and Experimental Studies of Biomolecular Interactions
- ◆ Combined Quantum Mechanical and Molecular Mechanical Methods (QM/MM)
- ◆ Computational Chemistry of Biomolecules, Ligands and Drugs
- Computational Drug Design: Structure-Based; Ligand-Based; Rational; De Novo
- ◆ Computational Modelling of Biomolecular Structures Interactions and Processes
- ◆ Computational Systems Biology and Chemistry
- ◆ Development and Applications of Monte Carlo Methods
- ◆ Development and Design of New Biological and Chemical Databases and Data Mining Techniques
- ◆ Development, Testing and Applications to Biomolecular Systems
- ◆ Enzymatic Reaction Mechanisms and Inhibition
- ◆ High Performance Computing in Molecular and Biomolecular Sciences
- ◆ Ligand Binding and Free Energy Calculations
- ◆ Modelling of Membrane Processes and Protein-Membrane Interactions
- Modelling Protein Structure, Conformational Dynamics an Interactions
- ◆ Molecular Mechanics, Force Field Development and Evaluation
- ◆ Molecular Visualizations and Data Analysis
- ◆ Multilevel Computational Simulations
- ◆ Nucleic Acids Structure, Dynamics and Interactions with Ligands
- Protein Folding
- ◆ Protein Ligand Docking New Algorithm, Codes and Applications
- ◆ Protein-Nucleic Acids Interactions
- Quantitative Structure-Activity Relationships (QSAR)
- ◆ Semiempirical Electronic Structure Calculations
- ◆ Structural Bioinformatics and Homology Modelling

We are also interested in: 1) Short Reports—2-5 page papers where an author can either present an idea with theoretical background but has not yet completed the research needed for a complete paper or preliminary data; 2) Book Reviews—Comments and critiques.

E-mail: cmb@scirp.org

Website and E-Mail

https://www.scirp.org/journal/cmb

What is SCIRP?

Scientific Research Publishing (SCIRP) is one of the largest Open Access journal publishers. It is currently publishing more than 200 open access, online, peer-reviewed journals covering a wide range of academic disciplines. SCIRP serves the worldwide academic communities and contributes to the progress and application of science with its publication.

What is Open Access?

All original research papers published by SCIRP are made freely and permanently accessible online immediately upon publication. To be able to provide open access journals, SCIRP defrays operation costs from authors and subscription charges only for its printed version. Open access publishing allows an immediate, worldwide, barrier-free, open access to the full text of research papers, which is in the best interests of the scientific community.

- High visibility for maximum global exposure with open access publishing model
- Rigorous peer review of research papers
- Prompt faster publication with less cost
- Guaranteed targeted, multidisciplinary audience





Website: https://www.scirp.org Subscription: sub@scirp.org Advertisement: service@scirp.org