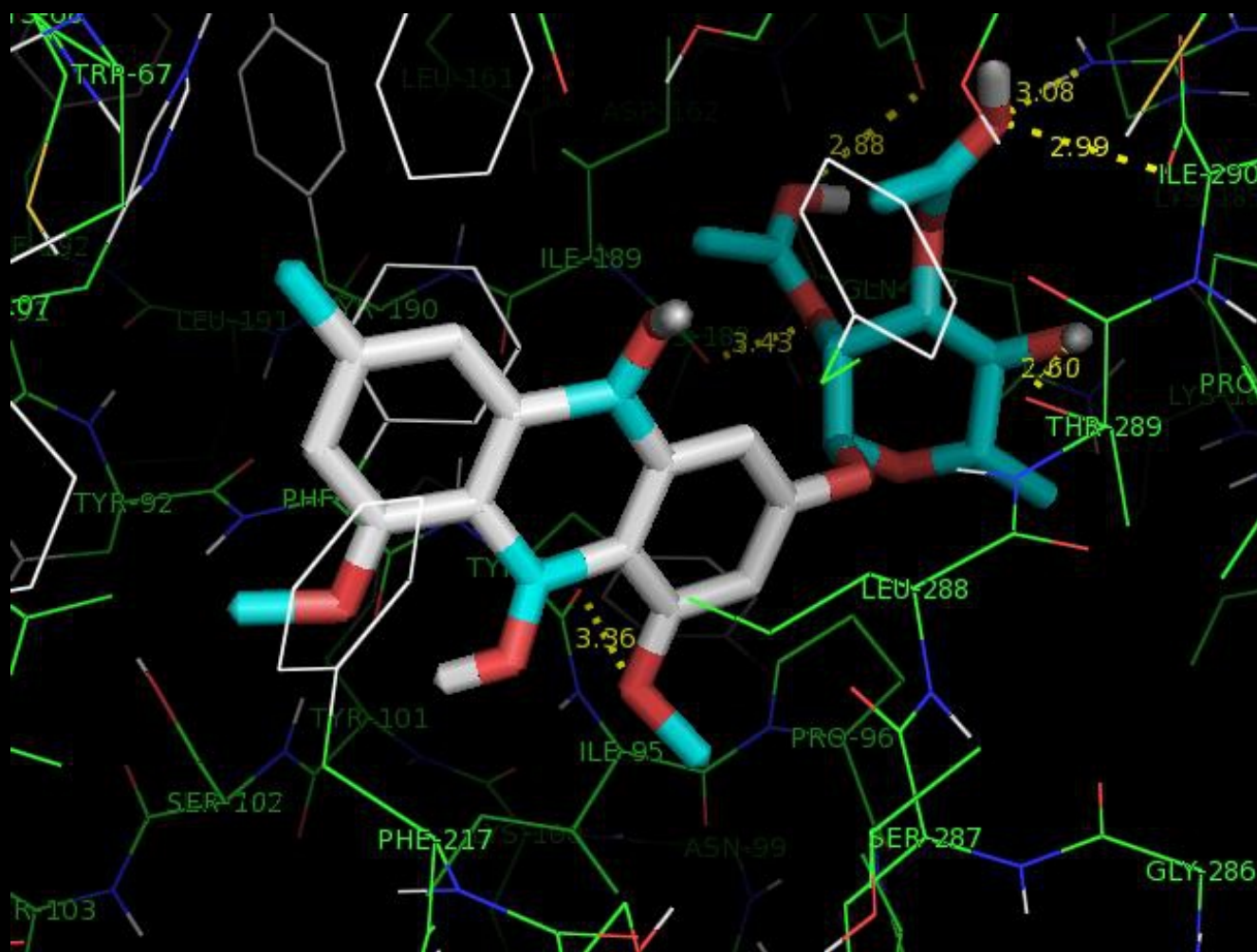


Computational Molecular Bioscience



ISSN: 2165-3445



Journal Editorial Board

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

<http://www.scirp.org/journal/cmb>

Editorial Board

Dr. David R. Bevan	Virginia Polytechnic Institute and State University, USA
Prof. Emilio Gallicchio	Rutgers University, USA
Prof. Juraj Gregan	University of Vienna, Austria
Dr. Ian S. Haworth	University of Southern California, USA
Prof. Srividhya Jeyaraman	Indiana University, USA
Prof. Cizhong Jiang	Tongji University, China
Dr. Daisuke Kihara	Purdue University, USA
Prof. Jianyong Li	Virginia Polytechnic Institute and State University, USA
Dr. Jose L. Medina-Franco	Florida Atlantic University, USA
Dr. Sihua Peng	Shanghai Ocean University, China
Dr. Olli T. Pentikäinen	University of Jyväskylä, Finland
Prof. Giulio Rastelli	University of Modena and Reggio Emilia, Italy
Prof. Igor A. Topol	Frederick National Laboratory for Cancer Research, USA
Dr. Ivanka Tsakovska	Institute of Biophysics and Biomedical Engineering, Bulgaria
Prof. Nagarajan Vaidehi	City of Hope National Medical Center, USA
Dr. Jinhua Wang	New York University Langone Medical Center, USA
Dr. Yanggan Wang	Emory University, USA
Prof. Dongqing Wei	Shanghai Jiao Tong University, China
Dr. Yasushige Yonezawa	Kinki University, Japan

Table of Contents

Volume 9 Number 1**March 2019****Bacterial Heavy Metal Resistance Genes and Bioremediation Potential**

H. Johnson, H. Cho, M. Choudhary.....1

Conceptual Density Functional Theory Study of the Chemical Reactivity Properties and Bioactivity Scores of the Leu-Enkephalin Opioid Peptide Neurotransmitter

J. Frau, N. Flores-Holguín, D. Glossman-Mitnik.....13

Spontaneous Unfolding and Refolding of Plantaricin α -Helix in Molecular Dynamics Simulation

S. M. Yan, G. Wu.....27

Computational Molecular Bioscience (CMB)

Journal Information

SUBSCRIPTIONS

The *Computational Molecular Bioscience* (Online at Scientific Research Publishing, 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 © 2019 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 © 2019 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.

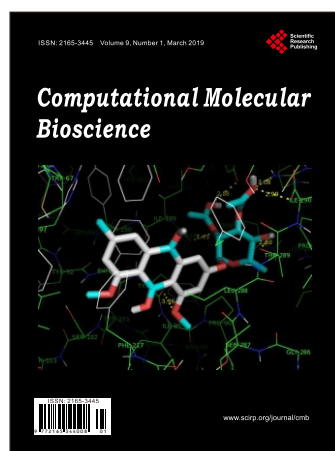
Disclaimer of liability

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



Computational Molecular Bioscience

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

<http://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 and 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.

Website and E-Mail

<http://www.scirp.org/journal/cmb>

E-mail: cmb@scirp.org

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



**Scientific
Research
Publishing**

Website: <http://www.scirp.org>

Subscription: sub@scirp.org

Advertisement: service@scirp.org