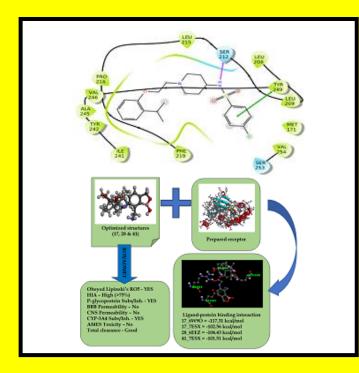
Journal of Molecular Docking

Volume 2 Issue 1 June 2022



Pharmacophore Based Virtual Screening and Docking of Different Aryl Sulfonamide Derivatives of 5HT7R Antagonist

In Silico Approach: Effect of the Oxidation Iron State (Heme-Group) in Steroidogenesis Pathways



Published by

Institute for Research and Community Services Universitas Muhammadiyah Palangkaraya

JOURNAL OF MOLECULAR DOCKING

J Mol Docking e-ISSN: 2798-138X

Volume 2 Issue 1 June 2022

Department of Pharmacy

Faculty of Health Sciences Universitas Muhammadiyah Palangkaraya, Indonesia

EDITOR-IN-CHIEF

Mohammad Rizki Fadhil Pratama Universitas Muhammadiyah Palangkaraya, Indonesia ORCID: 0000-0002-0727-4392

> Arif Nur Muhammad Ansori Universitas Airlangga, Indonesia

Sumera Zaib University of Central Punjab, Pakistan

Burak Tüzün Sivas Cumhuriyet Üniversitesi, Turkey

Yaseen Ali Mosa Mohamed Elshaier University of Sadat City, Egypt Lina Alekseevna Perekhoda National University of Pharmacy, Ukraine Anu Manhas Pandit Deendayal Energy University, India Muhammad Arba Universitas Halu Oleo, Indonesia

Cleydson Breno Rodrigues Dos Santos Universidade Federal do Amapá, Brazil

Pedro Jorge Silva Universidade Fernando Pessoa, Portugal

Siti Azma Jusoh Universiti Teknologi MARA, Malaysia Aisha Saddiqa Government College Women University Sialkot, Pakistan Sangita Kachhap

Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Poland Lalit Mohan Nainwal Harlal Institute of Management and Technology College of Pharmacy, India

EDITORIAL BOARDS

Arli Aditya Parikesit Indonesia International Institute for Life Sciences, Indonesia Tomasz M. Karpiński Poznań University of Medical Sciences, Poland **Renjith Thomas** St. Berchmans College, Mahatma Gandhi University, India Hassan Hadi Abdallah Salahaddin University-Erbil, Iraq Pavadai Parasuraman M.S.Ramaiah University of Applied Sciences, India Faizan Abul Qais Aligarh Muslim University, India

> Ahmad Ali University of Mumbai, India

INTERNATIONAL PEER-REVIEWERS

Geng Dong Shantou University Medical College, China Dede Mahdiyah Universitas Sari Mulia, Indonesia Monaj Kumar Sarkar SASTRA Deemed University, India

Rezi Riadhi Syahdi Universitas Indonesia, Indonesia

Amit Kumar Shrivastava Universal College of Medical Sciences, India Alan Carrasco-Carballo Benemérita Universidad Autónoma de Puebla, Mexico **Ahmed Hassen Shntaif** *University of Babylon, Iraq*

Mochammad Arfin Fardiansyah Nasution Universitas Indonesia, Indonesia

Kiran Bharat Lokhande Dr. D. Y. Patil Biotechnology and Bioinformatics Institute, India Fatahiya Mohamed Tap Universiti Teknologi MARA Cawangan Terengganu, Malaysia Nora Laref Centre Universitaire Relizane, Algeria

Eman Mohamed Abd El-Hameed El-Sayed Sarhan *City of Scientific Research and Technological Applications, Egypt* Jean-Paul Koto-te-Nyiwa Ngbolua University of Kinshasa, Democratic Republic of Congo Nursamsiar Sekolah Tinggi Ilmu Farmasi

Makassar, Indonesia Samir Chtita Université Hassan II de Casablanca, Morocco

Andhika Bintang Mahardhika Institut Teknologi Bandung, Indonesia

Saeful Amin Sekolah Tinggi Ilmu Kesehatan Bakti Tunas Husada, Indonesia Antônio Silva Machado Universidade Ceuma, Brazil

PUBLISHED BY



Institute for Research and Community Services Universitas Muhammadiyah Palangkaraya RTA Milono St. Km. 1,5 Palangka Raya 73111 jmd@umpr.ac.id https://journal.umpr.ac.id/index.php/jmd

EDITORIAL WORDS

apt. Mohammad Rizki Fadhil Pratama, S.Farm., M.Si. Editor in Chief J Mol Docking

Assalamu'alaikum Wr. Wb.

Alhamdulillahirabbil 'alamin. After a long wait for almost 1 years from the first planned, finally the new scientific journal of the Department of Pharmacy Universitas Muhammadiyah Palangkaraya can be published. This scientifc journal was named **Journal of Molecular Docking** (*J Mol Docking*), inspired by one of the most popular *in silico* methods in computer-aided drug design. Journal of Molecular Docking published every 6 months (2 issues/year) every June and December.

This edition contains five articles consisting of writings from three countries including India, Mexico, and Nigeria. The authors come from several institutions, including Maulana Azad National Urdu University, Osmania University, Osmania University College for Women, Vignan's Foundation for Science, Technology & Research, Ahmadu Bello University, Benemérita Universidad Autónoma de Puebla, Universidad Autónoma de Guerrero, The Tamil Nadu Dr. M.G.R. Medical University, and Anna University.

Editorial boards are fully aware that there are still room for improvement in this edition, hence with all humility willing to accept constructive suggestions and feedback for improvements to the publication for the next editions. The editorial board would like to thank all editors and reviewers, and contributors of the scientific articles who have provided the repetoire in this issue. We hope that all parties, especially the contributors of the articles, could re-participate for the the publication in the next edition on December 2022.

Wassalamu'alaikum Wr. Wb.

Palangka Raya, June 2022

Editor-in-Chief

Table of Contents JOURNAL OF MOLECULAR DOCKING

J Mol Docking – ISSN: 2798-138X (online)

Volume 2 Issue 1 June 2022

Sections: ORIGINAL RESEARCH ARTICLES

Pharmacophore Based Virtual Screening and Docking of Different Aryl Sulfonamide Derivatives of 5HT₇R Antagonist

Nahid Fatema / Maulana Azad National Urdu University & Osmania University, India Vijjulatha Manga / Osmania University & Osmania University College for Women, India Lingala Yamini / Osmania University College for Women, India Salman Ahmad Khan / Maulana Azad National Urdu University, India Qasim Ullah / Maulana Azad National Urdu University, India 1 - 15

Homology Modeling and Molecular Docking Studies of Selected Substituted Tetradecane on vlsE *Borrelia spielmanii*

Venu Paritala / Vignan's Foundation for Science, Technology & Research, India Harsha Thummala / Vignan's Foundation for Science, Technology & Research, India Talluri Naga Santosh Mohith / Vignan's Foundation for Science, Technology & Research, India 16 - 28

Molecular Docking Screening and Pharmacokinetic Studies of Some Boron-Pleuromutilin Analogues against Possible Targets of Wolbachia pipientis Fabian Audu Ugbe / Ahmadu Bello University, Nigeria Gideon Adamu Shallangwa / Ahmadu Bello University, Nigeria Adamu Uzairu / Ahmadu Bello University, Nigeria

Ibrahim Abdulkadir / Ahmadu Bello University, Nigeria 29 - 43

In Silico Approach: Effect of the Oxidation Iron State (Heme-Group) in Steroidogenesis Pathways David Mora-Martinez / Benemérita Universidad Autónoma de Puebla, Mexico Jorge Organista-Nava / Universidad Autónoma de Guerrero, Mexico Jesús Sandoval-Ramirez / Benemérita Universidad Autónoma de Puebla, Mexico Berenice Illades-Aguiar / Benemérita Universidad Autónoma de Puebla, Mexico Alan Carrasco-Carballo / Benemérita Universidad Autónoma de Puebla & Universidad Autónoma de Guerrero, Mexico 44 - 57

Comparative In-Silico Molecular Docking of Silymarin for SARS-CoV-2 Receptor Michael Antony Samy Amutha Gnana Arasi / The Tamil Nadu Dr. M.G.R. Medical University, India Sapthasri Ravichandran / The Tamil Nadu Dr. M.G.R. Medical University, India Irudayam Iayaraman / Anna University, India 58 - 67

Author Guidelines JOURNAL OF MOLECULAR DOCKING

J Mol Docking – ISSN: 2798-138X (online)

- 1. Writing is the result of original research and literature review in the field of pharmacy, chemistry, bioinformatics, and others using *Molecular Docking Simulation* as its main analysis method which have never been published in other scientific publication media.
- 2. Manuscripts that have been published in the form of a preprint on several platforms such as arXiv, SSRN, and ResearchGate are welcome to publish.
- 3. The manuscript is written in English with Book Antiqua font 10 pt, two-column, density 1.15 spaces, on A4 paper with a top-down margin of 2.5 cm and right-left margins 1.5 cm.
- 4. The manuscript is typed with MS-Word program using the provided template and saved in .doc or .docx format.
- 5. The manuscript is typed strictly with the following rules:
 - a. The title, short and clear, written in English. The title length does not exceed 20 words.
 - b. Authors, listed without mention of title or degree, under the name including the affiliation and complete address, and email of the corresponding author. The author's name, which consists of one word, must be repeated twice for first and last names. To author with names of more than two words, the author's last name consists of only one word, the rest is written as the first name.
 - c. Abstract, written in English which is a summary of the article. The abstract is created in one paragraph and a maximum of 250 words with Book Antiqua font 9 pt, single column, and space 1. Points that must be listed in the abstract include the research objectives, methods, results, conclusions, and keywords. The number of keywords is between three and five keywords.
 - d. Introduction, contain background, reasons for the importance of underlying research or hypotheses, general approaches and objectives of the research and relevant literature review. The number of paragraphs not restricted but the contents must include background, objectives, positions on previous research, as well as the novelty of the research. The little theoretical basis which indirectly related to the contents of the article could be included without sub-chapters required. Citation is written in the form of the last name followed by the year of publication. If the author numbered two people, the last names of the two writers were written separated by the "&". Citation of more than one author written in "et al".
 - e. Methodology, Research method consists of 2 sub-chapters including materials and methods. If data analysis is specific, or the way of analysis is novel, then data analysis subchapter could be added. The sub-chapters are written without numbering or bullet.
 - f. Results and Discussion, at least contain three subjects (1) description of results, (2) interpretation or explanation of results, and (3) comparative of results with previous studies results. If the subchapters very length could be made sub-sub-chapters with Arabic numbering. Description of the results can be in the form of tables and figures with a serial number (Table uses a sequence of Roman numerals and placed at the top, while figures using Arabic numeric sequence and placed in the below).
 - g. Conclusion, made in a single paragraph without the citation contains the final conclusion and suggestions for advanced research.
 - h. References, a list of recently selected topics is published last five years (minimum 75% of at least 10 references). The bibliography is written in appearance order chronologically with the serial number (Vancouver System) and suggested using a reference management application such as EndNote, Mendeley, Zotero, and other applications.
- 6. Authors whose manuscripts are published are free of charge for both Publication cost and article processing charge.
- 7. Authors will get full access to the article published on e-journal of Universitas Muhammadiyah Palangkaraya at the website https://journal.umpr.ac.id/index.php/jmd.

