



MENU

[Smart Search](#) > [Results for Analogues of Ox...](#) >

Analogues of Oxamate, Pyruvate, and Lactate as Potential Inhibitors of Plas...

[Free Full Text from Publisher](#) [View Full Text on ProQuest](#)[Full Text Links](#) ▾[Export](#) ▾[Add To Marked List](#)< 1 of 100 >

Analogues of Oxamate, Pyruvate, and Lactate as Potential Inhibitors of *Plasmodium knowlesi* Lactate Dehydrogenase Identified Using Virtual Screening and Verified via Inhibition Assays

By

Fuad, FAA (Fuad, Fazia Adyani Ahmad) ^[1]; Salim, NO (Salim, Nurhainis Ogu) ^[2][View Web of Science ResearcherID and ORCID](#) (provided by Clarivate)

Source

PROCESSES

[← View Journal Impact](#)

Volume: 10 Issue: 11
DOI: 10.3390/pr10112443

Article Number 2443

Published NOV 2022

Indexed 2022-12-23

Document Type Article

Jump to [↓ Enriched Cited References](#)

Abstract

Malaria management remains a challenge, due to the resistance of malaria parasites to current antimalarial agents. This resistance consequently delays the global elimination of malaria throughout the world. Hence, the demand is increasing for new and effective antimalarial drugs. The identification of potential drugs that target Pk-LDH can be obtained through virtual screening analyses, as this has been previously applied to discover Pf-LDH inhibitors. In this study, the selected candidates from our virtual screening analyses were subsequently tested against purified Pk-LDH, and verified through an inhibition of Pk-LDH via enzymatic activity assays. Virtual screening analysis from this study showed that 3,3-Difluoropyrrolidine hydrochloride and 3-hydroxytetrahydrofuran exhibited binding affinity values of -3.25 kcal/mol and -3.74, respectively. These compounds were selected for evaluation towards inhibitory activity against Pk-LDH assays, including two compounds from a previous study which are oxalic acid and glycolamide. The earlier compounds were structurally similar to lactate and pyruvate, and the latter two compounds were structurally similar to a known LDH inhibitor, oxamate. Among all of the compounds tested, oxalic acid showed the highest inhibition activity at 54.12%; interestingly, this correlated well with the virtual screening analyses, which showed that this compound was the best among the oxamate analogues, with a binding affinity value of -2.59 kcal/mol. Hence, further exploration and development of this compound may result in a promising antimalarial drug for malaria treatment, especially for infection involving *P. knowlesi*.

Keywords

Author Keywords: [malaria](#); [Plasmodium knowlesi](#); [lactate dehydrogenase](#); [virtual screening](#); [inhibition assay](#)

Author Information

Corresponding Address: Fuad, Fazia Adyani (corresponding author)

Int Islamic Univ Malaysia, Dept Chem Engn & Sustainabil, Kulliyyah Engn, Jalan Gombak, Selangor 53100, Malaysia

E-mail Addresses :

fazia_adyani@iium.edu.my

Addresses :

¹ Int Islamic Univ Malaysia, Dept Chem Engn & Sustainabil, Kulliyyah Engn, Jalan Gombak, Selangor 53100, Malaysia

² Natl Inst Hlth, Inst Med Res, Parasitol Unit, Minist Hlth, NIH Complex, Bandar Setia Alam, Shah Alam 40170, Selangor, Malaysia

E-mail Addresses :

fazia_adyani@iium.edu.my

Categories/ Classification

Research Areas: Engineering

Citation 1 Clinical & Parasitology - Malaria, 1.217.59
Topics: Life Sciences, Toxoplasmosis & Coccidiosis, Malaria
Sustainable Development Goals: 03 Good Health and Well-being

Web of Science Categories

Engineering, Chemical

Funding

View funding text

Funding agency	Grant number
International Islamic University Malaysia Research Initiative Grants	RIGS15-141-0141

+ See more data fields

Journal information

PROCESSES

[← View Journal Impact](#)

eISSN 2227-9717

Current Publisher MDPI, MDPI AG, Grosspeteranlage 5, CH-4052 BASEL, SWITZERLAND

Research Areas Engineering

Web of Science Categories Engineering, Chemical

2.8

Journal
Impact
Factor™
(2024)

0.41

Journal
Citation
Indicator™
(2024)

Citation Network

In Web of Science Core Collection

4

Citations

[🔔 Create citation alert](#)

5

Times Cited in All Databases

[+ See more times cited](#)

23

Cited References

Use in Web of Science

0

Last 180 Days

1

Since 2013

[Learn more →](#)

This record is from:

Web of Science Core Collection

- Science Citation Index Expanded (SCI-EXPANDED)