World Academy of Science, Engineering and Technology
International Journal of Pharmacological and Pharmaceutical Sciences
Vol:18, No:02, 2024

Combating Malaria: A Drug Discovery Approach Using Thiazole Derivatives Against Prolific Parasite Enzyme PfPKG

Authors : Hari Bezwada, Michelle Cheon, Ryan Divan, Hannah Escritor, Michelle Kagramian, Isha Korgaonkar, Maya MacAdams, Udgita Pamidigantam, Richard Pilny, Eleanor Race, Angadh Singh, Nathan Zhang, LeeAnn Nguyen, Fina Liotta

Abstract : Malaria is a deadly disease caused by the Plasmodium parasite, which continues to develop resistance to current antimalarial drugs. In this research project, the effectiveness of numerous thiazole derivatives was explored in inhibiting the PfPKG, a crucial part of the Plasmodium life cycle. This study involved the synthesis of six thiazole-derived amides to inhibit the PfPKG pathway. Nuclear Magnetic Resonance (NMR) spectroscopy and Infrared (IR) spectroscopy were used to characterize these compounds. Furthermore, AutoDocking software was used to predict binding affinities of these thiazole-derived amides in silico. In silico, compound 6 exhibited the highest predicted binding affinity to PfPKG, while compound 5 had the lowest affinity. Compounds 1-4 displayed varying degrees of predicted binding affinity. In-vitro, it was found that compound 4 had the best percent inhibition, while compound 5 had the worst percent inhibition. Overall, all six compounds had weak inhibition (approximately 30-39% at 10 μM), but these results provide a foundation for future drug discovery experiments.

Keywords : Medicinal Chemistry, Malaria, drug discovery, PfPKG, Thiazole, Plasmodium
Conference Title : ICOSMC 2024 : International Conference on Organic Synthesis and Medicinal Chemistry
Conference Location : Washington, United States
Conference Dates : February 26-27, 2024