Available online at **www.joac.info**

ISSN: 2278-1862

Journal of Applicable Chemistry

2018, 7 (5): 1373-1380

(International Peer Reviewed Journal)

Molecular Docking Studies of Hydroxamic acid Derivatives with *Plasmodium falciparum* Dihydrofolate Reductase-Thymidylate Synthase (PfDHFR-TS)

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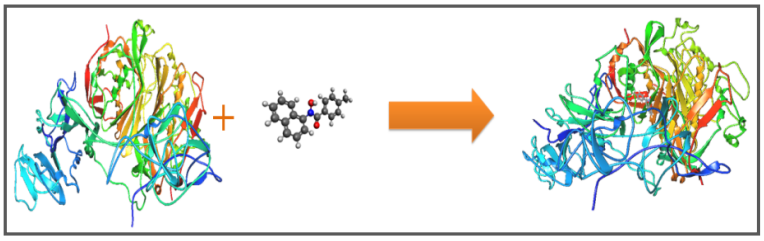
Accepted on 20th August, 2018

ABSTRACT

Malaria caused by protozoa of the genus Plasmodium is a major global health concern. The Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) enzyme obtained from malarial parasites acts as a target for various drugs. Therefore, molecular docking studies of hydroxamic acid derivatives with PfDHFR-TS have been done using Ascore method from Argus Lab 4.0.1. The receptor structure was obtained from Protein Data Bank (PDB No. 1J3I). N-arylhydroxamic acid derivatives interact with PfDHFR-TS to form a complex. The Ascore energies vary between -8.86 to -13.02 Kcal mol^{-1}. N-1-naphthyl-p-methylbenzohydroxamic acid, N-p-MBHA shows the highest binding energy with the receptor. This binding depends on the hydrogen bond donor ability of the compound.

Graphical Abstract



Keywords: *Plasmodium falciparum* dihydrofolate reductase-thymidylate synthase (PfDHFR-TS), Molecular Docking Studies, N-arylhydroxamic acid, ArgusLab 4.0.1 software.