Short Communication

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Journal of Medical Toxicology and Clinical Forensic Medicine

2021
Vol. 7 ISS. 2

In Silico Development of new Antimalarials with Molecular Docking as Inhibitor of Pv-DHFR

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Abstract

The process of discovering new drugs is long and very expensive. As a result, private investments have neglected tropical diseases and malaria, which mainly affect people in poor countries, which justifies the use of molecular modeling techniques and Virtual screening which have proved to be an effective strategy for the discovery and development of drug leads. It is estimated that this parasitic disease still affects more than 216 million people, and accounted for 445,000 deaths in 2016 The increasing prevalence of multidrug-resistant malaria has significantly reduced the effectiveness of current drugs. Thus, the DHFR enzyme has proven reliable and the best target for designing new antimalarial drugs. Aim: The purpose of our study is the identification of novel inhibitors of the P.vivax DHFR enzyme using Virtual Screening by Docking approach. Methods: A Virtual Screening by Docking has been carried out on a series of more than 10,000 molecules which represent the similar of 30 known molecules, in vitro, as inhibitors of Pv-DHFR (very low IC50), The chosen PDB is 2BL9 (Resolution = 1.9), the similar are downloaded from the PubChem database (Tanimoto 95%), the Molegro 6.0 Software has been used for the Virtual Screening process and its algorithm has been validated after obtaining RMSD = 0.8 (<2). A potential interaction was observed between several similar active compounds for example 53944258, 14570340 and 11451948 (hit compounds) and the enzyme Pv-DHFR, with a very low MolDock score (energy) compared to the reference ligand, with better interactions in the active site. The results of the physicochemical parameters (Lipinski's rule and ADMETox) suggest that all compound leads tend to be considered good candidates as drugs. In this study, we identified a new series of Pv-DHFR inhibitors using Molecular Docking, which tend to be considered good candidates as drugs, pending the completion of the bioassays

Biography

Faycal Layachi born in 1980 in Annaba (Algeria), is Assistant Master Hospital-University at the Faculty of Medicine of Annaba since 2011. He obtained his diploma of specialist in Therapeutic Chemistry from the University of Algiers in 2008, to practice at the CHU of Bab el Oued as Resident and Tizi Ouzou University Hospital as a specialist practitioner. He is interested in the research and development of new drugs through drug discovery approaches.