J Mol Genet Med 2017, 11:4 (Suppl)
DOI: 10.4172/1747-0862-C1-022

Homology modeling, binding site identification and molecular docking of DNA polymerase delta in Plasmodium falciparum

Ikram Manzoor
Abdul Wali Khan University Mardan, Pakistan

Malaria is the world's most widespread disease caused by 5 species of the apicomplexan parasites genus *Plasmodium*. Annually, approximately 3.3 billion people are at risk in malaria. The sub Saharan African is the highest risk area of acquiring malaria about 80% cases and 90% of death, mostly affected by children and women. There are about 99 countries and territories with ongoing malaria transmission. The purpose of this study is to describe: Many DNA transactions, such as replication, repair and recombination involve DNA synthesis and consequently require the action of DNA synthesizing enzymes called DNA polymerases (Pol). Eukaryotic cells contain at least six different Pols, named alpha, beta, gamma, delta, epsilon, and zeta. Among them, Pol, delta occupies important roles in DNA replication, nucleotide excision repair, base excision repair and VDJ recombination. Therefore, in this study we modeled DNA polymerase delta of *Plasmodium falciparum* structure using homology modeling followed by identification and characterization of binding sites and thereby assessing druggability of the receptor. Homology models were constructed using MODELLER and I-TASSER server, refined and validated using PROCHECK in which 96.9% of 318 residues were present in the favored regions of the Ramachandran plots. Various drugs are available in the market as antihypertensive drug, so we have performed docking study with the binding site prediction algorithms to predict different binding pockets on the modeled proteins. The identification of 3D structures and binding sites for various known drugs will guide us for the structure-based drug design of novel compounds as DNA polymerase delta of *Plasmodium falciparum* antagonists for the treatment of malaria.

ikrambiochem2013@gmail.com