

Abstract Type : Poster

Abstract Submission No. : PO-1032

Molecular Modeling and structural analysis of the Neisseria meningitidis 3-oxoacyl synthase II and Dihydropteroate synthase proteins to inhibit cardiovascular deficiency using Insilico approach.

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Objectives: *Neisseria meningitidis* (NM) is foremost causative agent of bacterial meningitis. Meningitis disease may existing as a fulminant gram-negative sepsis with well-known cardiovascular deficiency and disseminated intravascular coagulation, threatening ischemic tissue damage. The most communal reason of death in patients with meningitis was cardiorespiratory failure, stroke, status epilepticus or brain herniation. The two very important protein has been selected for the study of homology modeling and structural validation in *Neisseria meningitidis*. The 3-oxoacyl (acyl carrier protein) synthase II (3OASII) enzyme which involved in fatty acid biosynthesis of *Neisseria meningitidis*. This enzyme in fatty acid synthesis and target for discovery of novel antibacterial agent. Dihydropteroate synthase (DHPS), an enzyme plays an acute role in the bacterial folate metabolism which catalyzes the development of 7, 8- dihydropteroate from paminobenzoic acid (pABA) and 6-hydroxymethyl-7, 8-dihydropterin-pyrophosphate (DHPP). The absence of the folate pathway in higher eukaryotes makes it an attractive drug target.

Methods: In current study, a complete 3 oxoacyl (acyl carrier protein) synthase II and Dihydropteroate synthase protein structure model was generated using Modeller V9.12 software so as to understand the mechanistic detail of its functioning. The energy minimization analysis using YASARA and the stereo chemical quality of the models was checked by Rampage, Verfy3D, Errat, ProSA and QMEAN servers.

Results: The analysis of present studies provide three dimensional (3D) structure of 3 oxoacyl synthase II and dihydropteroate synthase protein will be helpful for the advance study of drug designing in meningitis disease.

Conclusions: The current study showed that 3 oxoacyl synthase II and Dihydropteroate synthase modeled protein is highly reliable and stable, so it will use to identifying the drug designing research of meningitis disease.