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STRUCTURAL PREDICTION AND ANALYSIS OF PUTATIVE DRUG TARGETS OF SHIGELLA FLEXNERI 2A, THE COMMONEST AGENT OF ENDEMIC SHIGELLOSIS IN DEVELOPING COUNTRIES

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Shigella causes common bacillary diarrhoea in humans which is termed as 'shigellosis'. While ***Shigella dysenteriae*** type 1 causes the most severe form of bloody dysentery and is responsible for outbreaks, ***S. flexneri***, ***S. sonnei*** and ***S. boydii*** causes endemic shigellosis. ***S. flexneri*** 2a is the commonest cause of bacillary diarrhoea in children of developing countries including India. Although not always recommended, antibiotics are used for empirical treatment. However, rapid emergence of antimicrobial resistance has resulted in the bacteria acquiring resistance to most available antimicrobials and therefore there is an immediate requirement of newer drugs effective against this pathogen. The proteome consisting of 4053 proteins of ***Shigella flexneri*** 2a str. 301 was retrieved from NCBI and CD HIT tool was used to remove paralogs/duplicates from the list. The resulting 3178 protein sequences were subjected to Blastp against human proteome to identify protein sequences non-homologous to humans. The resultant 1329 protein sequences were subsequently subjected to DEG Blastp that listed out 620 essential proteins of pathogens and sub-cellular localization were predicted using CELLO v.2.5 tool. 19 were identified as outer membrane proteins among which five (OMP F, thymidine kinase, porin, sorbitol-6-phosphate dehydrogenase, lipopolysaccharide 1,3-galactosyltransferase) were identified as pathogen specific. 3D structure analysis resulted in predicting binding pockets for these proteins which can serve as drug targets. SNP analysis of NGS data showed that the selected target proteins were not vulnerable to non-synonymous mutation during the course of time and therefore ideal candidates to be targeted with novel drugs.

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