In Silico Epitope Mapping of Acinetobacter Baumannii Outer Membrane Protein, FilF, As a Potential Vaccine Candidate

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Abstract: Introduction: *Acinetobacter baumannii* is an important pathogen causing a variety of infections. *A. baumanni*'s ability to survive for long period of time on environmental surfaces makes it a frequent cause for healthcare-associated infections led to multiple outbreaks. As recently multidrug resistance has been increased. Therefore new strategies against its infections are needed. Outer membrane proteins are involved in nutrient uptake so they are good vaccine candidates. In this study we exploited bioinformatic tools to determination and validation of ligand binding site *baumannii* fimbrial protein, FilF, that recently was predicted as a potential vaccine candidate.
Methods: FilF potentially B-cell epitopes were predicted by using Ellipro software. In addition ligand binding sites determined using COFACTOR software. Dogsitescore server was used to protein drugability assessment and functionally and structurally important residues were identified.
Results: linear and discontinuous epitopes with their protrusion index (PI) as well as some of the main linear epitope parameters including accessibility, antigenicity, beta-turn, bepipred linear epitope, flexibility and hydrophilicity are shown in the paper. Ligand binding sites determined using COFACTOR software, indicate involvement of conserved residues include 537, 540 and 58 in binding site with the highest $Cscore^{LB}$. Pockets and descriptors calculated for FilF are presented in the article. Functional residues on the 3D structure of FilF predicted by Auto Patch Analysis are: 521, 523,572, 573, 574, 575, 576, 578 and 589.

Keywords: Acinetobacter baumannii; Vaccine candidate; FilF; Epitope; Bioinformatic

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