



In Silico Structural Analysis of *Acinetobacter baumannii* Outer Membrane Protein, FilF, As a Potential Vaccine Candidate

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Abstract: Introduction: *Acinetobacter baumannii* is the third most common gram-negative bacteria causing a variety of infections. Resistance to various antibiotics is a susceptible factor for development of infections. As recently multidrug resistance has been increased. Therefore treatment of *A. baumannii* infections has become a considerable health care challenge. Outer membrane proteins are involved in antibiotic resistance so they are good vaccine candidates. In this study we exploited bioinformatic tools to better understanding and characterizing a *baumannii* fimbrial protein, FilF, structure that recently was predicted as a potential vaccine candidate.

Methods: FilF sequence availability and homology was studied and CLCsequenceViewer software was used to alignments analysis. Primary sequence analysis was performed by Protparam and subcellular localization as well as topology of protein was predicted. Secondary and 3D structures were predicted by various bioinformatic servers. In addition 3D structure evaluation and orientation of the protein structure in membrane were studied.

Results: FilF sequence alignment between *A. baumannii* and other *Acinetobacter* species showed no significant difference. Primary structure characteristics including molecular weight, theoretical pI, Atomic composition, instability and aliphatic index were computed. FilF subcellular localization predicted by CELLO was OuterMembrane with the highest reliability. The schematic results of protein secondary and 3D structures prediction are illustrated in the paper. The Z-score value for average FilF structure was -2.11, which is within the range observed for native set of proteins of same size. In addition Ramachandran plot analysis provides evidence that the predicted model has good quality.

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

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