

عنوان مقاله:

In Silico Determination and Validation of FhuE Structure and Ligand Binding Site as a vaccine candidate in *Acinetobacter baumannii*

محل انتشار:

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خلاصه مقاله:

Acinetobacter baumannii is a gram-negative bacterium that causes serious infections in compromised patients. This pathogen grows under a wide range of conditions including iron-limiting conditions. Multidrug-resistant *Acinetobacter baumannii* is recognized to be among the most difficult antimicrobial-resistant gram negative bacilli to control and treat. One of the major challenges that the pathogenic bacteria face in their host is the scarcity of freely available iron. To survive in such conditions, bacteria express new proteins in their outer membrane and also secrete iron chelators called siderophores. In the case of human hosts, the free iron availability is 10-18M, which is far less than what is needed for the survival of the invading bacterial pathogen. To survive in such conditions, *Acinetobacter baumannii* expresses FhuE in its outer membrane. Evidence suggests that FhuE iron uptake protein is a useful antigen for inclusion in an effective vaccine, hence the identification of its structure is very important. Antibodies directed against these proteins associated with iron uptake exert a bacteriostatic or bactericidal effect, by blocking siderophore mediated iron uptake pathways. The structural homology displayed by these receptors permits modelling of the 3D structure of FhuE in the absence of crystallographic data.

کلمات کلیدی:

Acinetobacter baumannii, FhuE, 3D structure

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