

***In silico* Structure Analysis of *Acinetobacter baumannii* Outer Membrane Protein, BtuB, as a Potential vaccine candidate**

Parisa Ghasemi^{1*}, Fatemeh Sefid²

¹Department of Biology, Tarbiat Modares University, Tehran, Iran

²Department of Biology, Shahed University, Tehran-Qom Express Way, Iran

*parisa.ghasemi@modares.ac.ir

Abstract: *Acinetobacter baumannii* is a Gram-negative aerobic bacterium, This is recognized as a notorious opportunistic pathogen mainly prevalent in hospital settings. *A. baumannii*'s ability to adapt and survive in a range of environments has been a key feature for its persistence and success as an opportunistic pathogen. Gram-negative bacteria possess specialized active transport systems that function to transport organometallic cofactors or carriers, such as cobalamins, siderophores, and porphyrins, across their outer membranes. Cobalamins bind to BtuB with nanomolar affinity. BtuB is a β -barrel membrane protein that facilitates transport of cobalamin (vitamin B12) from the extracellular medium across the outer membrane of *Escherichia coli*. It is thought that binding of B12 to BtuB alters the conformation of its periplasm-exposed N-terminal residues (the TonB box), which enables subsequent binding of a TonB protein and leads to eventual uptake of B12 into the cytoplasm.

Here we describe the topology and 3D structure of a novel antigen which was discovered by mining the bacterial genome and that is very effective in inducing bactericidal antibodies. This antigen is a very good candidate for inclusion in universal vaccines against *Acinetobacter baumannii*.

Keywords: *Acinetobacter baumannii*, BtuB; 3D structure

References

- [1] Doi Y, Murray GL, Peleg AY, *Acinetobacter baumannii*: evolution of antimicrobial resistance-treatment options, *Semin Respir Crit Care Med*, 36 (2015) 085-098.
- [2] Peleg AY, Paterson DL, Multidrug-resistant *Acinetobacter*: a threat to the antibiotic era, *Internal Medicine Journal*, 36 (2006) 479-482.
- [3] Peleg AY, Seifert H, Paterson DL, *Acinetobacter baumannii*: emergence of a successful pathogen, *Clin Microbiol Reviews*, 21 (2008) 538-582.
- [4] Mills A, Le HT, Duong, TonB-dependent ligand trapping in the BtuB transporter, *Biochimica et Biophysica Acta (BBA) – Biomembranes*, 12 (2016) 3105-3112.
- [5] L. Dijkshoorn, A. Nemeč, and H. Seifert, An increasing threat in hospitals: multidrug-resistant *Acinetobacter baumannii*, *Nature Reviews Microbiology*, 5 (2007) 939-951.
- [6] F. Perez, A. M. Hujer, K. M. Hujer, B. K. Decker, P. N. Rather, and R. A. Bonomo, Global challenge of multidrug-resistant *Acinetobacter baumannii*, *Antimicrobial agents and chemotherapy*, 51 (2007) 3471-3484.
- [7] P. E. Fournier, H. Richet, and R. A. Weinstein, The epidemiology and control of *Acinetobacter baumannii* in health care facilities, *Clinical infectious diseases*, 42 (2006) 692-699.
- [8] L. V. Bentancor, A. Routray, C. Bozkurt-Guzel, A. Camacho-Peiro, G. B. Pier, and T. Maira-Litran, Evaluation of the trimeric autotransporter Ata as a vaccine candidate against *Acinetobacter baumannii* infections, *Infection and immunity*, 80 (2012) 3381-3388.
- [9] T. Hoda, S. L. M. Gargari, M. J. Nadoushan, and S. D. A. Astaneh, Characterization of the *Salmonella typhi* outer membrane protein C, *..*, 41 (2013) 128-134.
- [10] David P. Chimento^{1,2}, Arun K. Mohanty^{1,3}, Robert J. Kadner² & Michael C. Wiener³ Substrate-induced transmembrane signaling in the cobalamin transporter BtuB *Nature Structural & Molecular Biology* 10 (2003) 394 – 401.