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In-silico methods of drug designing against *Burkholderia pseudomallei*

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ABOUT THE STUDY

A respiratory infection called melioidosis, often known as Whitmore's disease, is brought on by the Gram-negative, intracellular bacterium *Burkholderia pseudomallei*. The bacteria are widely distributed in tropical regions, particularly in Southeast Asia and northern Australia. They flourish on muddy ground and filthy water, and they directly infect their hosts. Percutaneous inoculation is thought to be the main route of infection in endemic areas after exposure to contaminated muddy ground or surface water, such as in agricultural fields (Patel et al., 2013). Tropical storms, cyclones, typhoons, and floods are just a few of the environmental factors that are frequently thought to cause melioidosis, which has inhalation as its primary mechanism of pathogenesis. None of these events are uncommon.

This idea is supported by the fact that melioidosis may become more severe during the rainy season as a result of prolonged exposure to the pathogen as a result of higher risk of infection. The dose of infection frequently increases as a result of the potential for recurrent inhalation of fomites caused by heavy rain and winds that produce aerosols. We now consider this airborne disease to be a potential biological weapon because we were unable to defeat it. It is included on the list of category B agents maintained by the US Centers for Disease Control and Prevention. Co-administering a variety of antibiotics is the recommended treatment plan for melioidosis. Unfortunately (Currie et al., 2008), the lack of vaccinations against *B. pseudomallei* has caused the disease to relapse and reactivate after the cessation of antibiotic therapy due to the pathogen's natural resistance pattern to a variety of medicines.

Intracellular infections evade the immune system by hiding inside certain host cells. Another widely held belief is that cellular immunity, particularly that involving $CD4^+$ and $CD8^+$ T cells, is essential for the defence against intracellular bacterial infections. The implication that particular immune responses are required for defence against various diseases is a crucial consideration in deciding the type of vaccination that should be created (Wiersinga et al., 2006). To give an example, vaccinations based on slain entire cells or separated protein or polysaccharide fractions of cells may cause robust antibody reactions but may be ineffective at promoting cell-mediated immunity.

To use the notion of docking simulation to have a good understanding of the production of a peptide vaccine against *B. pseudomallei*. Finding a bacterial component that we can produce an effective vaccination against is quite difficult, as seen in the cases of intracellular Gram-negative Category B pathogens. PAMPs (Pathogen Associated Molecular Patterns) such as lipid-A, lipopolysaccharide (LPS), flagellin, peptidoglycan, DNA, and Type III Secretion System (TTSS) are present in *B. pseudomallei* and may be well recognised by several TLRs (Toll-like Receptors) (Currie et al., 2000). We selected the most virulent proteins from the immunesera generated during infection after carefully analysing the probable immunogenic proteins allowing *B. pseudomallei* to possess a wide range of cellular function and invasion methods.

In order to stimulate cell-mediated immunity, the production of a peptide vaccine included simulations of docking and dynamics between a target epitope obtained from a chosen immunogenic protein and a class 1 MHC molecule. We would get a 3D mechanism and a range of vaccine efficacy through a docking and molecular dynamics simulation study (Moore et al., 2003), according to system biology. Our study's main goal was to find a potential vaccination candidate that would survive several

immunoinformatic screening processes as well as molecular docking and dynamics simulation to demonstrate the candidates' efficacy as *B. pseudomallei* vaccines.

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