Abstract

Toll like receptors (TLRs) play a key role in the innate immune response to infectious agents. The Mycobacterium tuberculosis bacilli and its antigens interaction with TLR-2-1 and TLR-4-MD2 were shown to activate intracellular signalling which determines the outcome of the disease. Present study focused on two new antigens Rv0679c and Rv0180c of M.tb H37Rv and their interactions with human and mouse TLRs using computational approach. Structures of Rv0679c and Rv0180c antigens of M.tb were generated using I-TASSER and docked with TLR-2-1 and TLR-4-MD2 complexes of human and mouse using Cluspro2.0. Rv0180c antigen has better binding energy to both human and mouse TLR-2-1 and TLR-4-MD2 compared to Rv0679c and other mycobacterial antigens. The Rv0679c and Rv0180c antigens have better binding energy to TLR 4-MD2 complex compared to TLR-2-1 in both human and mouse. Both antigens has better binding energy to mouse TLRs compared to human except where Rv0180c has better binding to human TLR-2-1. Our findings suggest that Rv0180c might be the preferred for binding to TLRs than Rv0679c and within TLRs, TLR-4-MD2 for interaction.
References


**Index Terms**

Computer Science

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**Keywords**

Mycobacterium tuberculosis, toll like receptors, invasion, I-TASSER, docking, ClusPro