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Structural analysis of major translocator – chaperone interaction from Ysa-Ysp T3SS of *Yersinia enterocolitica*

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Abstract

Certain serotypes of *Yersinia enterocolitica* Biovar 1B possess *Yersinia* secretion apparatus- *Yersinia* secretion protein (Ysa-Ysp) Type III Secretion System (T3SS), which is responsible for the gastrointestinal phase of *Y. enterocolitica* infection. *Y. enterocolitica* is an opportunistic pathogen which infects immune-compromised individuals to cause gastroenteritis, mesenteric adenitis and other nosocomial infections. Enhanced virulence of *Y. enterocolitica* Biovar 1B is attributed to the activation of Ysa-Ysp T3SS, which is further regulated by the formation of functional injectisome. YspB is a major hydrophobic translocator protein responsible for the formation of functional translocon at the tip of the needle. YspB is a highly unstable protein recalcitrant to recombinant expression. Its cognate class II chaperone SycB imparts stability to YspB. Like other major translocator proteins YspB possesses a highly helical structure and transmembrane helices required for its translocation through the narrow conduit of the needle and its interaction with the host cell plasma membrane. Being a translocator protein it has to interact with chaperones, other translocators and host cell plasma membrane, which is evident from the existence of intramolecular coiled-coil regions in YspB structure. Due to high hydrophobicity and presence of intrinsically disordered regions YspB could not be expressed to the extent required for experimental three dimensional structure determinations. Therefore, a homology model of YspB was generated by threading algorithm of I-TASSER server. This model depicted an all helical star shaped structure with alpha helices interspersed by random coil regions. The inner concave core of SycB forms the interface of interaction with YspB. This interaction is polar or ionic in nature and mediated predominantly by tyrosine residues present in the first two TPRs of SycB. The bulky nature of YspB molecule results in dissociation of the dimeric state of SycB during YspB-SycB interaction. ConSurf analysis predicted that the evolutionarily conserved residues are mostly present in the helices and random coil regions of YspB involved in interaction with SycB. Understanding the mechanism of YspB-SycB interaction would enable us to decipher the regulation of Ysa- Ysp T3SS and further to design drugs for the inhibition of YSa-Ysp T3SS.

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