Fall 2023

Modeling Calcium Binding to Yersinia pestis Type III Secretion Needle

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Modeling Calcium Binding to *Yersinia pestis* Needle Protein YscF

PDB File: HexamerWTYscF.pdb

Primary Citation:

Mirdita M., Shutze K., Moriwaki Y., Heo L., Ovichinnikov S., Steinegger M. (2022) ColbFold: Making protein folding accessible to all. *Nature Methods,19*(6), 679-682, 10.1038/s41592-022-01488-1

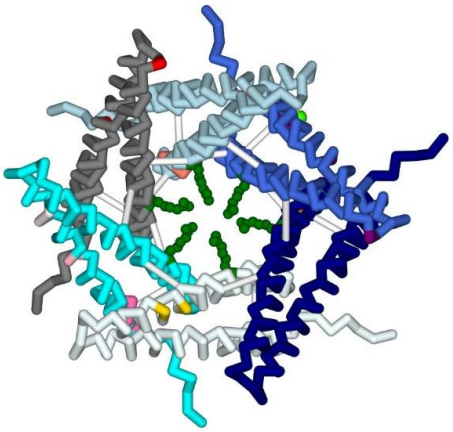
Description:

Yersinia pestis is the bacteria that causes the bubonic plague. The bacteria utilizes a type III secretion system (T3SS) through using an injectosome to insert toxins into host cells. The monomer protein YscF makes up the injectosome subunit of the *Yersinia pestis* T3SS. The Yop protein is the toxin released from the needle into host cells. It is thought that Yop (Yersinia Outer Proteins) secretion is regulated by the presence of calcium (Torruellas et al., 2005). Calcium presence will inhibit secretion of Yop, while the absence of calcium will encourage secretion of the Yop. The regulation of Yop secretion with calcium is refered to as regulated secretion (RS). In a 2005 experiment by Torruellas et. al, different mutations of the YscF protein in the needle of *Yersinia pestis* were created to understand regulation of the needle with calcium. The results determined what mutations lead to constitutive secretion (CS), no secretion (NS), or RS of the Yop toxin. CS refers to constant secretion of the Yop protein in the precense and absence of calcium. NS refers to no secretion of the Yop protein in the precense and absence of calcium. Our model shows a possible hexomer of the YscF *Y. pestis* needle subunit with the residue mutations that cause constitutive secretion of Yop and the residue mutations that cause no secretion, highlighted in their designated colors. The mutations that lead to CS are I13A, D17A, D28A, D46A, and will be highlighted in the model. The mutations that lead to NS are N31A, V34A, D77A, D77C, I82A, I82C will be highlighted in the model. The goal of our research is to understand how the mutations present in the wet lab experiment affect calcium binding to the YscF hexomer subunit.

Specific Model Details:

- The six (YscF) alpha helicies will be colored different colors to highlight different mutations and binding sites
    - Chain A is colored royal blue

    - Chain B is colored light blue
    - Chain C is colored gray
    - Chain D is colored cyan
    - Chain E is colored azure
    - Chain F is colored darkblue
- I13; D17; D28; D46 will be colored purple on chain A to indicate mutations that led to constitutive secretion of the Yop toxin
- N31; V34; D77; I82 will be colored salmon #FA8072 on chain B to indicate mutations that led to no secretion of the Yop toxin.
- The double mutant D28, D46 will be colored red on chain C to indicate a significant mutation discussed in the wet lab
- D73 will be colored green on each monomer to indicate a significant structural site that varies between single mutants discussed in the wet lab experiment
- Chain D will contain a calcium binding site (Asp 12, Asp 15, Leu 16) colored hotpink; (Asp 28, Asp 29) colored light pink; (Asp 36, Ser 37) colored lavenderblush
- Chain E will contain a Cu(II) (Mg and Zn also bind here regularly in the MIB2 binding simulation) His 56, Lys 60 [binding potential 7] binding site colored gold
- Chain F will contain an iron(III) binding site (Gln 80, Gln 84) colored darkorgange to show a binding site that is unique to Fe(III) MIB2 binding to the hexomer



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