## Poster I-35

**Structural Analysis of the Protein Twitching Motility**


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**Short Abstract:** We have concentrated our effort in understanding some crucial features of protein Twitching Motility of Xylella fastidiosa. Our study is based on the model of this protein, constructed by homology modeling in which we used the crystallographic structure of a Víbrio cholerae homologous protein as a mold.

**Long Abstract:**
A laboratory consortium in Sao Paulo, Brazil, has published the X. fastidiosa genome, lineage 9a5c, revealing 2,679,305 pairs of bases in the main chromosome and other two plasmids: one with 51,158 and the other with 1,285 pairs of bases. In total, 2,905 genes were identified. The proteome project of X. fastidiosa revealed over 800 expressed proteins, where 112 of them were identified. Some of the 112 proteins are potentially involved in the pathogenic processes of this bacterium in citrus.
The goal of this research is to analyze the tridimensional structure of the PilT protein identified by the proteome, a product of XF1633 gene. Such a protein is associated with adhesion systems and it is a fimbria of type IV, which is supposed to be responsible for the setting of the bacterium in the vascular system of the plant. Our study is based on the model of this protein, constructed by comparative modeling where we used the crystallographic structure of a Víbrio cholerae homologous protein (PDB code: 1p9w) as a template.
We hope that we can put forward a new insight into understanding specificity that PilT protein has associated with adhesion systems supposed to be responsible for the setting of the bacterium in the vascular system of the plant and can help in the design of mutagenesis experiments aimed at elucidating the mechanism of action of the PilT protein associated with adhesion systems and setting of the bacterium.
Analysis of the model structure using Star Sting software indicates that some amino acids present energy of contacts higher than those on the average. Those residues can have an important role in the stability of this protein when crossreferenced with the residues showing

order of cross presence and cross link higher than the usual measures.
In terms of functionality, we are identifying the residue ensemble 19, 21, 64, 67, 82, 84, 99, 181, 183, 185, 200, 206, 208, 231 within the “hot-spots” – the hydrophobic patches at the protein surface. Among those residues, we show that residues 19, 82, 183,206, 208 and 231 have the highest energy of internal contacts found in this protein.
Only the residues 54, 94, 96, 127, 201, 203, 217, 227, 229 satisfy the condition of having a very high order of cross presence (co-location of residues in 3D environment, although they are separated in the primary sequence by the least amino-acids; the order of cross presence/link is a measure of how many times the primary sequence comes back within a given sphere in 3D fold.