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Insilico structural analysis of Afimbrial adhesin virulence protein of uropathogenic *Escherichia coli*

M.Abhilash^{1*}, S.Uma Maheshwari², H.K.Makari³, H.S.Ravikumar Patil³¹Department of Biotechnology, The Oxford college of Engineering, Bangalore, (INDIA)²Department of Nanotechnology, Karunya University, Coimbatore, (INDIA)³Department of Biotechnology, G.M.Institute of Technology, Davangere, (INDIA)

E-mail : abhibiotek@gmail.com

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ABSTRACT

Fimbrial adhesion is a Virulence Determinant which is classified under Adhesins category of virulence factor of uropathogenic *Escherichia coli*. Afimbrial adhesin Protein with swissprot accession number P08180 was selected for analysis using Bioinformatics tools. Analysis included Secondary structure prediction and calculation of important structural properties.

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KEYWORDS

Uropathogenic *E.coli*;
Fimbrial adhesion;
Secondary structure prediction;
Structural properties
calculations.

INTRODUCTION

E.coli is responsible for three types of infections in humans: urinary tract infections (UTI), neonatal meningitis, and intestinal diseases (gastroenteritis). These three diseases depend on a specific array of pathogenic (virulence) determinants which renders it pathogenic. One such virulence protein is fimbrial adhesion as seen in Uropathogenic *Escherichia coli*. Fimbrial adhesion of pathogenic *E.coli* mediate adherence to the upper urinary tract. These adhesins bind to the Dr blood group antigen and also agglutinate human erythrocytes in the presence of D-mannose (mannose-resistant hemagglutination (MRHA)).

Among various organisms which are known to cause Urinary tract infections, *Escherichia coli* is the most predominant pathogen being isolated in 70-90% of cases. It has been accepted that UTI caused by *E.coli* is an ascending infection caused by the strains originating in the intestinal tract, because a high similarity exists be-

tween *E.coli* strains from urine and faeces of infected individuals.

Different virulence factors of *E.coli* which are thought to have a role in the pathogenesis of Urinary Tract Infections are O Antigens, K Antigens, Hemolysins, Serum resistance, Adhesins, Capacity to produce mannose sensitivity and resistant haemagglutination. fimbrial adhesion is a Virulence Determinant which is classified under Adhesins category of virulence factor.

Adhesins-fimbriae

The term adhesin has been described as a microbial surface component that mediates specific attachment to eukaryotic cell membrane and encompasses well known fimbriae as well as other poorly characterized and undefined structures.

Adherence is facilitated by *E.coli* Fimbriae which are proteinaceous fibers on the bacterial cell wall. Fimbriae produce adhesins that bind to specific carbohydrate receptors present on uroepithelial cells^[6]. Many

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bacteria are known to be adhesive, attaching to and living in close association with various surfaces in their natural habitat. The ability of many pathogenic bacteria to adhere to specific host tissues is a factor of primary importance in diseases such as bacterial diarrhea, gonorrhoea and Urinary Tract Infections. This specific adherence plays two important roles

1. It allows the bacteria to resist and circumvent the flushing and cleansing mechanisms that protect many epithelial surfaces in higher animals.
2. It determines the site of microbial infection by facilitating specific surface interaction between the bacteria and host epithelium.

Many studies^[2,3] have shown that bacterial adherence is an essential virulence factor in the pathogenesis of community acquired Urinary Tract Infections. Duguid et al.^[1] studied fimbriae of *E.coli* in great detail and classified them into three groups depending upon their haemagglutinating properties as the MSHA (Mannose Sensitive Haemagglutinating) type, MRHA (Mannose Resistant Haemagglutinating) type and non-fimbrial haemagglutinin type.

MATERIALS AND METHODS

Protein with swiss-prot primary accession number P08180, of length 161 amino acids was selected for analysis.

Sequence used for analysis

>sp|P08180|AFAE1_ECOLX Afimbrial adhesin AFA-I OS=*Escherichia coli*
 MKKLAIIGATSVMMMTGTAQANFTSSGTNGKV
 DLITTEECR_xVTVESKSESFLRSGLVANRHITNLGIQS
 TGCGTGQRVALKLGAGSYDDTNGAHMTHENGTDKL

LVSMGSATGDGTQDGGVYYINRDGNWNGQMVF
 VRNDQQHLPTGKYTLNLEGGFWTK

Tool used for protein analysis

- Gor IV secondary structure prediction tool
- Pep tool

RESULTS AND DISCUSSION

Protein structure analysis

Secondary structure prediction of modeled virulence protein was carried out using Gor iv secondary structure prediction tool (Figure 1).

Description of the result

Sequence length : 161

GOR4:

Alpha helix	(Hh)	: 22 is 13.66%
3 ₁₀ helix	(Gg)	: 0 is 0.00%
Pi helix	(Ii)	: 0 is 0.00%
Beta bridge	(Bb)	: 0 is 0.00%
Extended strand	(Ee)	: 49 is 30.43%
Beta turn	(Tt)	: 0 is 0.00%
Bend region	(Ss)	: 0 is 0.00%
Random coil	(Cc)	: 90 is 55.90%
Ambiguous states	(?)	: 0 is 0.00%
Other states		: 0 is 0.00%

Amino acid frequency plot (Figure 2), obtained from pep tool

Beta staircase model

The beta staircase graphically displays (Figure 3) the disposition of amino acid side chains about an assumed alpha helix. The view is always along the central axis of the helix from N to C-terminus. The helical wheel is an effective method for displaying the symmetry of hydrophobic/hydrophilic side chains of AFIMBRIAL

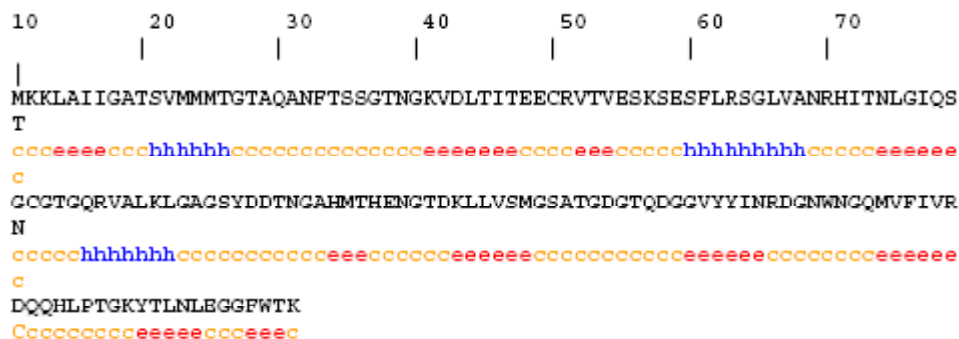


Figure 1: Output of GOR iv secondary structure prediction

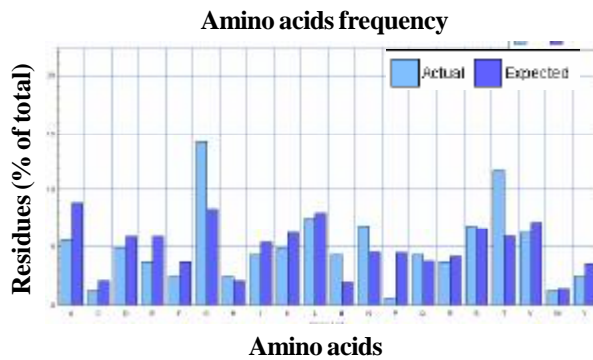


Figure 2: Amino acid frequency plot of Afimbrial adhesin (*Escherichia coli*)

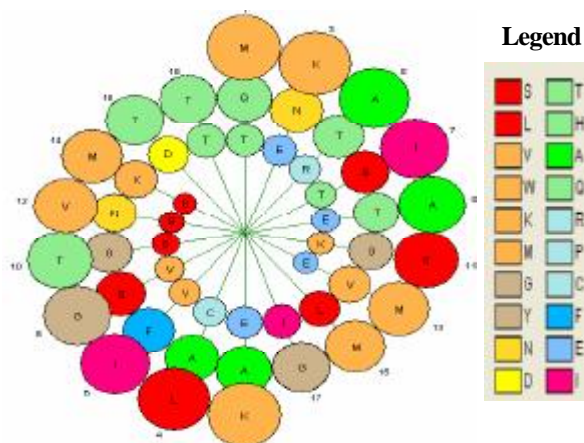


Figure 3: Beta staircase model of Afimbrial adhesin (*Escherichia coli*) obtained from pep tool

TABLE 1: Molecular properties of Afimbrial adhesin protein (*Escherichia coli*) obtained using pep tool

Molecular weight (Daltons)	17184.313
Number of amino acids	161
Mean amino acid weight(Daltons)	106.735
Average hydrophobicity	-0.36087
Ratio of hydrophilicity to hydrophobicity	1.35255
Percentage of hydrophilic amino acids	50.3106
Percentage of hydrophobic amino acids	49.6894
Ratio of % hydrophilic to hydrophobic	1.0125
Mean Beta hydrophobic moment	0.208483
Mean helix hydrophobic moment	0.122993
Number of basic amino acids	14
Number of acidic amino acids	14
Total linear charge density	0.186335
Estimated Pi for protein	7.5
Polar area of extended chain (Angs ²)	10447.3
Non polar area of extended chain (Angs ²)	166229.3
Total area of extended chain (Angs ²)	27076.6
Polar ASA of folded protein (Angs ²)	2814.4
Non Polar ASA of folded protein (Angs ²)	4990.51
Packing volume (est) (Angs ³)	20417.2
Solvent free energy of folding (kcal/mol)	-143.37

ADHESIN. It is useful for observing how the amino acids are positional in relation to one another^[8].

CONCLUSION

Uropathogenic *E.coli* cause 90% of the urinary tract infections (UTI) in anatomically-normal, unobstructed urinary tracts. Since its reported that Uropathogenic *E.coli* have developed antibiotic resistance^[7], protein analysis data of Afimbrial adhesin virulence protein will be very useful in insilico drug discovery.

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