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In silco gene expression profiling and comparative analysis of legionellosis

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ABSTRACT

Legionellosis is the major problem in the world but the treatment of the disease is very difficult. The disease caused gene is Legionella and the bacterium is Legionella pneumophila. Kegg is used for the Legionellosis pathway identification. From the MGDB database list of genes present in the Legionella pneumophila are identified. The target gene for Legionellosis had been identified in NCBI. The expression of the target HtpB is viewed through Jcat. Comparative analysis of the target HtpB were done through Biocyc tool. Structural characterization of HtpB nucleotide and protein were carried out through tools like Protein colour,Yaspin,Ronn….etc. Biophysical Characterization of HtpB Protein were done using Dipole moment server.

Key Words: *Legionellosis, Legionella pneumophila,* HtpB, Comparative analysis, Structural characterization.

INTRODUCTION

Legionellosis is a potentially fatal infectious disease caused by Gram negative, aerobic bacteria belonging to the genus *Legionella.* Over 90% of *legionellosis* cases are caused by Legionella pneumophila. *legionellosis* takes two distinct forms, ***Legionnaires'* disease**, also known as "***Legion* Fever**", is the more severe form of the infection and produces high fever and pneumonia. Pontiac **fever** is caused by the same bacteria but produces a milder respiratory illness without pneumonia that resembles acute influenza. *Legionnaires'* disease acquired its name in July 1976 when an outbreak of pneumonia occurred among people attending a convention of the American Legion at the Bellevue-Stratford Hotel in Philadelphia. Patients with *Legionnaires'* disease usually have fever, tiredness, loss of appetite, loss of coordination (ataxia), and occasionally diarrhea and vomiting. Confusion and low or low normal heart rate despite the presence of a fever. Laboratory tests may show those patients' renal functions, liver functions. Chest X-rays. Wound and skin infections. Intestinal infections may only occur as part of respiratory infections, and where gastrointestinal symptoms have on occasion been described. Infection normally occurs after inhaling an aerosol (fine air born particles) containing *Legionella* bacteria. Such particles could originate from any infected water source. People of any age may suffer from *Legionnaires'* disease, particularly those who smoke cigarettes or have chronic lung disease. The treatment is antibiotics used. Sera have been used both for slide agglutination studies as well as for direct detection of bacteria in tissues using fluorescent-labelled antibody. Specific antibody in patients by the indirect fluorescent antibody test. ELISA and microagglutination tests have also been successfully applied.

MATERIALS AND METHODOS

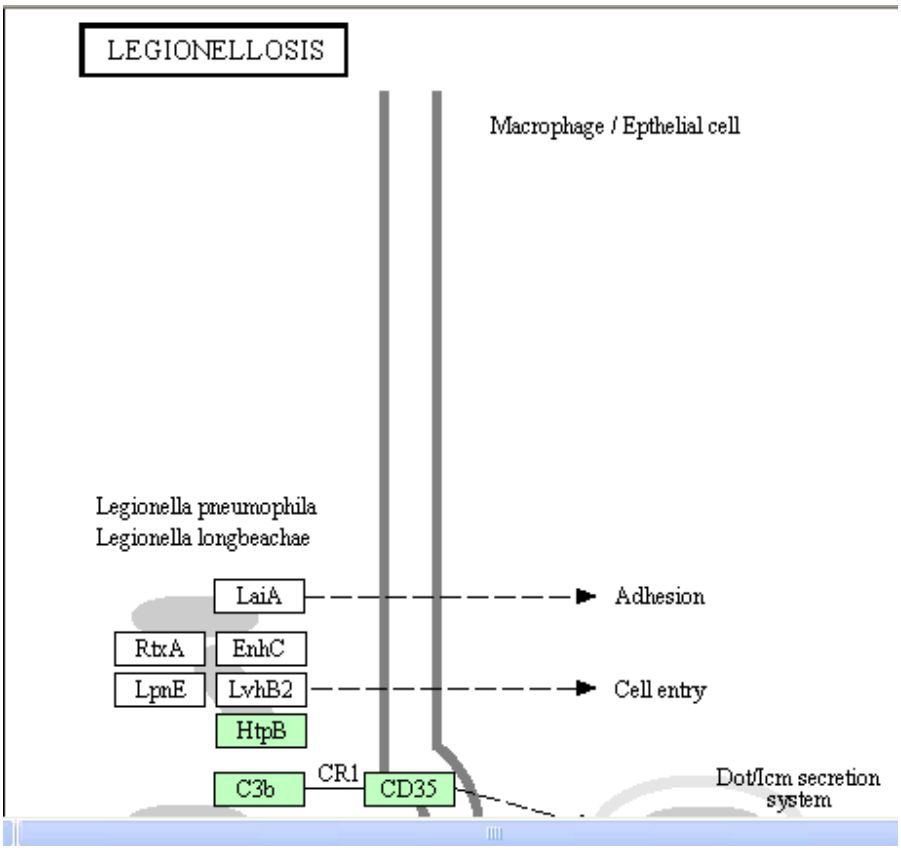
- The metabolic pathways of *legionellosis* are obtained from kegg.
- The target gene for *Legionellosis* had been identified in NCBI.

- Gene identification in the species is obtained by using mbgd.
- The expression of the target HtpB is viewed through Jcat.
- Comparative analysis of the target HtpB were done through Biocyc tool.
- Domain region of HtpB identified using domain linker prediction – short vector machine.
- Structural characterization of HtpB nucleotide and protein were carried out through tools like Protein colour,Yaspin,Ronn….etc.
- The sequence submitted to PFP for protein function studies.
- Biophysical Characterization of HtpB Protein were done using Dipole moment server.

RESULTS AND DISCUSSION

1. PATHWAY IDENTIFICATION

KEGG



The above result shows the metabolic pathways of *legionellosis Disease.*

2. SEQUENCE RETRIEVAL

NCBI

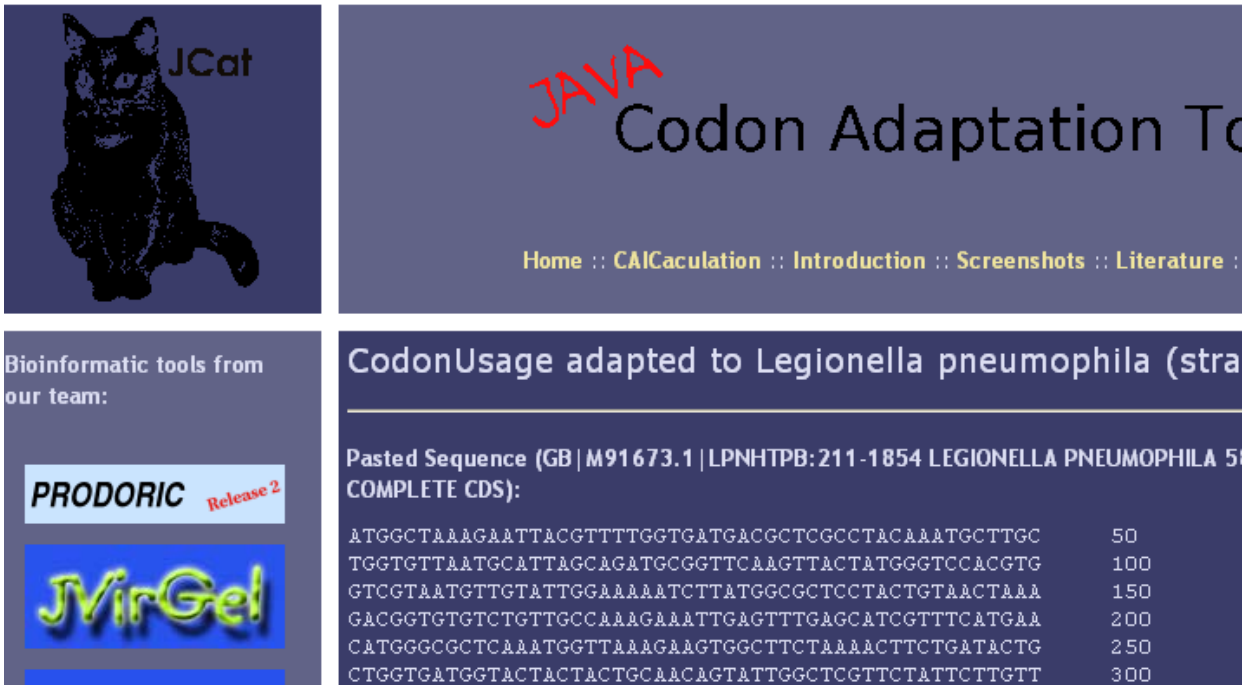
1. HtpB – Protein

>gi|149690|gb|AAA25298.1| 58-kDa common antigen [Legionella pneumophila]
MAKELRFGDDARLQMLAGVNALADAVQVTMGPRGRNVVLEKSYGAPTVTKDGVSVAKEIEFEHRFMNM
GA
QMVKEVASKTSDTAGDGTTTATVLARSILVEGHKAVAAGMNPMDLKRGIDKAVLAVTKKLQAMSKPCK
DS
KAIAQVGTISANSDEAIGAIIAEAMEKVGKEGVITVEDGNGLENELSVVEGMQLIAVHSPYFINNQQNMS
CELEHPFILLVDKKVSSIREMLSVLEGVAKSGRPLLIIAEDVEGEALATLVVNNMRGIVKVCAVKAPGFG
DRRKAMLQDIAILTKGQVISEEIGKSLEGATLEDLGSAKRIVVTKENTTIIDGEGKATEINARITQIRAQ

MEETTSDYDREKLQERVAKLAGGVAVIKVGAATEVEMKEKKARVEDALHATRAAVEEGIVAGGGVALIR
A
QKALDSLKGDNDDQNMGINILRRAIESPMRQIVTNAGYEASVVVNKVAEHKDNYGFNAATGEYGDMVE
MG
ILDPTKVTRMALQNAASVASLMLTTECMVADLPKKEEGVGAGDMGGMGGMGGMGGMM

The above results show the Fasta format sequence of HtpB target.

3. GENE IDENTIFICATION
MGDB
GENE EXPRESSION ANALYSIS
JCAT



The above result shows the CAI-value of the improved sequence is 1.0 and GC- content is 32.360097323600975.Sequence before adaptation, after adaptation and their relative adaptiveness is 1.05-500.The codons of the GC-content of *legionella pneumophila*(strain paris):38.3731082861924 and the translation is 50-500.

5. COMPARATIVE ANALYSIS

BIOCYC

Comparative analysis and statistics were computed for the following organism databases:

- *Legionella pneumophila 2300/99 Alcoy*
- *Mycoplasma fermentans JER*

Breakdown of Reactions by Type

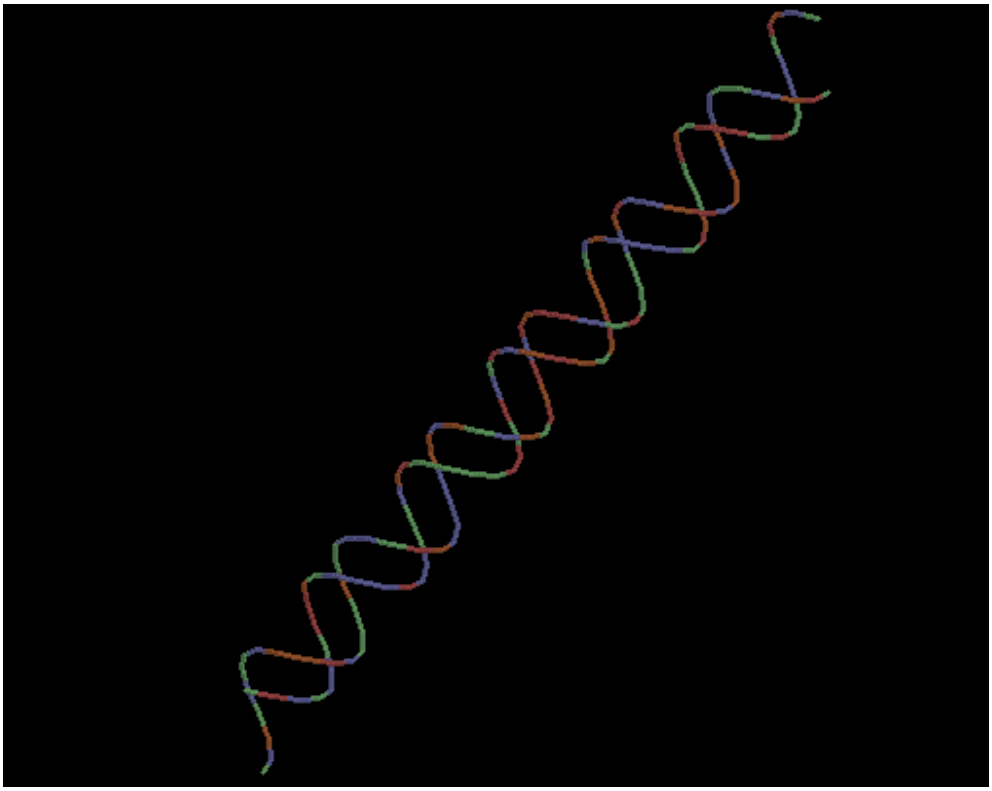
This table counts reactions based on the types of their substrates. Clicking on any row, column or cell will show the complete list of reactions included in that category.

Reaction Type	*L. pneumophila* 2300/99 Alcoy	*M. fermentans* JER
Reactions in which all substrates are small molecules	916	296
Reactions of proteins with small molecules	231	28
Reactions in which all substrates are proteins	10	2
Reactions in which one substrate is a tRNA	46	40
Transport reactions	88	21
Other reactions	52	33

6. STRUCTURE ANALYSIS

A) NUCLEOTIDE STRUCTURE ANALYSIS

i) DNA SEQUENCE TO STRUCTURE



This result shows the structure of dna sequence and indicated the nucleotides in the different colours.

b) PROTEIN FUNCTION PREDICTION
i) PFP: AUTOMATED PROTEIN FUNCTION PREDICTION SERVER

PFP Job Results

PFP Parameters

Protein Sequence:

```
MAKELRFGDDARLQMLAGVNALADAVQVTMGPRGRNVVLEKSYGAPTVTKDGVSVAKEIEFEHRF
MNMGAQMVKEVASKTSDTAGDGTTTATVLARSILVEGHKAVAAGMNPMDLKRGIDKAVLAVTKKL
QAMSKPCKDSKAIAQVGTISANSDEAIGAIIAEAMEKVGKEGVITVEDGNGLENELSVVEGMQLI
AVHSPYFINNQQNMSCELEHPFILLVDKKVSSIREMLSVLEGVAKSGRPLLIIAEDVEGEALATL
VVNNMRGIVKVCAVKAPGFGDRRKAMLQDIAILTKGQVISEEIGKSLEGATLEDLGSAKRIVVTK
ENTTIIDGEGKATEINARITQIRAQMEETTSDYDREKLQERVAKLAGGVAVIKVGAATEVEMKEK
KARVEDALHATRAAVEEGIVAGGGVALIRAQKALDSLKGDNDDQNMGINILRRAIESPMRQIVTN
AGYEASVVVNKVAEHKDNYGFNAATGEYGDMVEMGILDPTKVTRMALQNAASVASLMLTTECMVA
DLPKKEEGVGAGDMGGMGGMGGMGGMM
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Molecular Function Terms

Probability	Term	Description
100%	GO:0005488	binding
100%	GO:0017076	purine nucleotide binding
100%	GO:0005515	protein binding
98%	GO:0000166	nucleotide binding
98%	GO:0051082	unfolded protein binding
95%	GO:0005524	ATP binding
66%	GO:0030554	adenyl nucleotide binding
7 Predictions		

The above result shows the functional similarities between the target protein sequences. The target HtpB protein shows the binding value is 100 %.

7. PROTEIN BIOPHYSICAL CHARACTERISATION

Dipole vector (in atomic units): -123.68 -32.90 1.56
Mass Moments vector: 704.25 805.58 1491.56

The above results show the Electrostatic properties of HtpB protein.

CONCLUSION

Legionella pneumophila is a thin, ærobic, pleomorphic, flagellated, non-spore forming, Gram-negative bacterium of the genus *Legionella. L.pneumophila* is the primary human pathogenic bacterium in this group and is the causative agent of *legionellosis* or *Legionnaires'* disease. *Legionellosis* disease is serious and can be life-threatening. However, most people recover with antibiotic treatment. The target sequence collected using NCBI database. Highly expressed gene identification was done using Jcat tool. Domain region of HtpB identified using domain linker prediction – short vector machine and hydrophobicity region of HtpB identification done using protein colourer. The sequence submitted to PFP for protein function studies. Finally the electrostatic properties of HtpB were analyzed through using Dipole moment server. In future the testing of wet lab protocol will lead in designing novel therapeutics.

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