Insilco Gene Expression Profiling and Comparative Analysis of Legionellosis

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INTRODUCTION

Legionellosis is potentially a fatal infectious disease caused by gram-negative, aerobic bacteria belonging to the genus Legionella.1,2 Over 90% of legionellosis cases are caused by Legionella pneumophila, a ubiquitous aquatic organism that thrives in temperatures between 25 and 45 °C (77 and 113 °F), with an optimum temperature of 35 °C (95 °F).3 Legionellosis takes two distinct forms:

- **Legionnaires’ disease**, also known as “Legion Fever”,4 is the more severe form of the infection and produces high fever and pneumonia.5,6

- **Pontiac fever** is caused by the same bacteria but produces a milder respiratory illness without pneumonia that resembles acute influenza.5 Pontiac fever also has a spontaneous resolution.

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. On January 18, 1977 the causative agent was identified as a previously unknown strain of bacteria, subsequently named Legionella. Some people can be infected with the Legionella bacteria and have only mild symptoms or no illness at all.

Outbreaks of Legionnaires’ disease receive significant media attention. However, this disease usually occurs as single, isolated cases not associated with any recognized outbreak. When outbreaks do occur, they are usually in the summer and early autumn, though cases may occur at any time of year. The fatality rate of Legionnaires’ disease has ranged from 5% to 30% during various outbreaks and approaches 50% for nosocomial infections, especially when treatment with antibiotics is delayed.7 Most infections occur in those who are middle-age or older.8

RESEARCH METHODOLOGY

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. 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.
RESULT AND DISCUSSION

**Figure: 1** PATHWAY IDENTIFICATION - KEGG

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

**HTPB – Protein**

>gi|149690|gb|AAA25298.1| 58-kDa common antigen [Legionella pneumophila]
MAKELRGDDARLQMAGALADAVQVTMGPRGRNVLEKSYGAPTVTGVSVAKEIEFEHRFNMNGA
QMVKEVASKTSNTAGDDTTATVLARSILVEGKAAYGACMNPMDLKRIDKAVLAVTKKLQAMSKPCKDS
KIAAQVGTSANSDEAIAGIALBESMEVKGKEVITVEDGNGLENSVVEGMLIAVHSPYFINNQNMS
CELEHPFILLVDDKVSIREMLSLVEVAKSNGPLIAEDVEGEALATLVNMMGIVKCAVAKPGFG
DRRKAQLQDIALTQGQVISEEGKSLEGATLEDGSRAKVIVKENTTIIIDGEKATEINARITQRAQ
MEETSDYDREKLRQERVAKLVAVGIAVNEKKEKKAARVEDALHRAAVVEEIVVAGGGVALIRA
QKALDSLKDNNDOQMNINLRAIESPMQIVTNAYEASVVMVNVKVAEHKDYNGFNAATGEYDMVEMG
ILDPTKVTRMALQNAASVSLMLTTECMVADLPKKEEGVGAGDMGGMGMGGMGMG

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

**Figure: 2** GENE EXPRESSION ANALYSIS - JCAT

**Codon Adaptation Tool**

U/informatic tools from our team:

- **PRODORIC**
- **JmGel**
The above result shows the CAI-value of the improved sequence is 1.0 and GC-content is 32.36%. Sequence before adaptation, after adaptation and their relative adaptiveness is 1.05-500. The codons of the GC-content of legionella pneumophila (strain paris): 38.373% and the translation is 50-500.

COMPARATIVE ANALYSIS - BIOCYC

Comparative analysis (Biocyc Tool) 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.

<table>
<thead>
<tr>
<th>Reaction Type</th>
<th>L. pneumophila 2300/99 Alcoy</th>
<th>M. fermentans JER</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactions in which all substrates are small molecules</td>
<td>916</td>
<td>296</td>
</tr>
<tr>
<td>Reactions of proteins with small molecules</td>
<td>231</td>
<td>28</td>
</tr>
<tr>
<td>Reactions in which all substrates are proteins</td>
<td>10</td>
<td>2</td>
</tr>
<tr>
<td>Reactions in which one substrate is a tRNA</td>
<td>46</td>
<td>40</td>
</tr>
<tr>
<td>Transport reactions</td>
<td>88</td>
<td>21</td>
</tr>
<tr>
<td>Other reactions</td>
<td>52</td>
<td>33</td>
</tr>
</tbody>
</table>
This result shows the structure of DNA sequence and indicated the nucleotides in the different colours.

Molecular Function Terms

<table>
<thead>
<tr>
<th>Probability</th>
<th>Term</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>100%</td>
<td>GO:0005488</td>
<td>binding</td>
</tr>
<tr>
<td>100%</td>
<td>GO:0017076</td>
<td>purine nucleotide binding</td>
</tr>
<tr>
<td>100%</td>
<td>GO:0005515</td>
<td>protein binding</td>
</tr>
<tr>
<td>98%</td>
<td>GO:000166</td>
<td>nucleotide binding</td>
</tr>
<tr>
<td>98%</td>
<td>GO:0051082</td>
<td>unfolded protein binding</td>
</tr>
<tr>
<td>95%</td>
<td>GO:0005524</td>
<td>ATP binding</td>
</tr>
<tr>
<td>66%</td>
<td>GO:0005554</td>
<td>adenyl nucleotide binding</td>
</tr>
</tbody>
</table>

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

*Legionella pneumophila* is a thin, aerobic, 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.

REFERENCE

6. [Clinical Microbiology by Mark Gladwin, MD & Bill Trattler, MD]
7. MedlinePlus Encyclopedia *Legionnaire’s disease*