International Journal of Scientific Research in Science and Technology
Print ISSN: 2395-6011 | Online ISSN: 2395-602X (www.ijsrst.com)
doi : https://doi.org/10.32628/IJSRST229627

In-silico Characterization of Target Protein in Dengue Infection

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Article Info
Volume 9, Issue 6
Page Number : 215-218

Publication Issue
November-December-2022

Article History
Accepted : 10 Nov 2022
Published : 22 Nov 2022

ABSTRACT

Infection of humans with the virus is primarily mediated by the Aedes mosquito. The virus grows in the mosquito gut and migrates to aq 1 the salivary glands.. Dengue virus (DENV), which includes four serotypes (DENV1–4), is transmitted to humans by Aedes mosquitos and is the etiological agent of dengue fever and dengue hemorrhagic fever. DENV causes an estimated 50–100 million cases of dengue fever, 500,000 cases of severe dengue (dengue hemorrhagic fever/dengue shock syndrome (DHF/DSS)), and more than 20,000 deaths each year in tropical and subtropical regions, representing a considerable public health threat in over 100 countries worldwide. However, there are still no specific antiviral drugs or licensed vaccines against DENV infection. Dengue virus primarily propagates in skin dendritic cells, and subsequently virus proliferation is thought to occur in target cells such as those of the monocyte/macrophage lineage. Second, carbohydrate binding proteins, termed lectins, expressed on dendritic cells (DCs) and macrophages under the human skin are involved in initial contact of DENV introduced by mosquito bite. Among these lectins, dendritic cell-specific intercellular adhesion molecule-3-grabbing non integrin (DCSIGN) has been best characterized in virus-DC interaction.

Keywords: Dengue Infection, Viral fever, DC-SIGN, Host protein, DENV.

I. INTRODUCTION

Dengue has become a global problem since the Second World War and is common in more than 110 countries, mainly in Asia and South America (1) .Each year between 50 and 528 million people are infected and approximately 10,000 to 20,000 die (5) .The earliest descriptions of an outbreak date from 1779. Its viral cause and spread were understood by the early 20th century (4). Apart from eliminating the mosquitoes, work is ongoing for medication targeted directly at the virus it is classified as a neglected tropical disease.

The dengue virus belongs to genus Flavivirus (family Flaviviridae) that includes about 70 distinct viruses, all of which are serologically related and in majority of cases, (3) maintained in nature by transmission

from hematophagous arthropod vectors (mosquito or ticks) to vertebrate hosts. More than 50% of the flaviviruses have been associated with human diseases, and of these the most important in terms of disease incidence are dengue (DEN) virus (types 1 to 4), and yellow fever (YF) virus(4). DEN virus is present in tropical and subtropical areas around the world, as these provide the ecological conditions required for maintaining the natural cycles of the virus (10). There are four dengue virus serotypes: DEN-I, DEN-2, DEN-3 and DEN-4(12). DC-SIGN is a C-type lectin and has a high affinity for the ICAM3 molecule. It binds various microorganisms by recognizing high-mannose-containing glycoprotein's on their envelopes and especially functions as receptor for several viruses such as Dengue, HIV and Hepatitis C (11). Binding to DC-SIGN can promote Dengue, HIV and Hepatitis C virus to infect T-cell from dendritic cells (3). Thus binding to DC-SIGN is an essential process for Dengue infection (6). Dendritic Cell-Specific Intercellular adhesion molecule-3-Grabbing Non-integrin also known as CD209 (Cluster of Differentiation 209) is a protein which in humans is encoded by the CD209 gene. When an infected mosquito feeds on a healthy person, the virus is inoculated subcutaneously Epidemic dengue/dengue hemorrhagic fever as a public health, social and economic problem in the 21st century.

II. METHODS AND MATERIAL

- **Retrieval of protein sequence information of DC-SIGN protein:**
  - The protein sequences of DC-SIGN were retrieved from the major protein sequence database like UniprotKB and NCBI protein database.
- **Analysis of physicochemical parameters of DC-SIGN protein:**
  - The analyses of physicochemical properties of DC-SIGN protein was done by using protein prediction tool Protparam.
- **Secondary structure prediction of DC-SIGN protein:**
  - The secondary structure predicted of DC-SIGN protein was carried out by using online secondary structure prediction tool SOPMA, It was employed for calculating the secondary structure features of the selected sequence.
- **Tertiary structure prediction of DC-SIGN protein:**
  - The tertiary structures of DC-SIGN were obtained by using SWISS Model tool by selecting the template with maximum homology and optimized parameters.
- **Visualization of tertiary structure of DC-SIGN protein:**
  - The predicted tertiary structures of DC-SIGN were visualized by using structure visualization tool Rasmol.
- **Domain analysis of DC-SIGN protein:**
  - The domains of DC-SIGN protein were predicted by using Pfam database.

III. RESULTS AND DISCUSSION

- **Retrieval of protein sequence information of DC-SIGN protein:**
  - The protein sequences of DC-SIGN were retrieved from the major protein sequence database like UniprotKB and NCBI protein database. The sequences obtained were stored in FASTA format with its accession numbers as shown in table 01.
- **Analysis of physicochemical parameters of DC-SIGN protein:**
  - The analyses of physicochemical properties of DC-SIGN protein was done by using protein prediction tool Protparam which gives a detailed information of protein like Moleclar Wt. , theoretical PI, extension coefficient, instability index, Aliphatic index, GRAVITY, etc, were predicted, calculated and tabulated as shown in table 02.
- **Secondary structure prediction of DC-SIGN protein:**
  - The secondary structure predicted of DC-SIGN protein was carried out by using online secondary structure prediction tool SOPMA, which gives the information of Alpha helix, beta sheets, extended

strands and random coils were predict as shown in table 03.

- **Tertiary structure prediction of DC-SIGN protein:**
  - The tertiary structures of DC-SIGN were obtained by using SWISS Model tool by electing the template with maximum homology with optimized parameters. The obtained were stored in PDB format for visualization.
- **Visualization of tertiary structure of DC-SIGN protein:**
  - The predicted tertiary structures of DC-SIGN were visualized by using structure visualization tool Rasmol. Visualization was done using different models and formats to understand structural features of DC-SIGN protein as shown in figure 01.
- **Domain analysis of DC-SIGN protein:**
  - The domains were analysed from Pfam database. The domain structure was shown in figure 02.

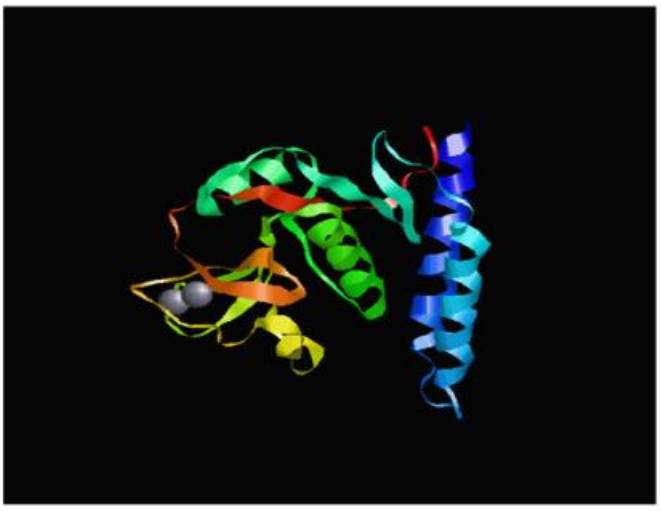

Fig. 1 Visualization of tertiary structure of DC-SIGN protein

Fig. 2 Domain analysis of DC-SIGN protein

Table.No.01. Sequence of DC-SIGN protein

Accession. No.	DC-SIGN protein sequence	No. of Amino acids
Q9NNX6	MSDSKEPRLQQLGLLEEEQLRG LGFRQTRGYKSLAGCLGHGPLV LQLLSFTLLAGLLVQVSKVPSSI SQEQSRQDAIYQNLTQLKAAVG ELSEKSKLQEIYQELTQLKAAV GELPEKSKLQEIYQELTRLKAA VGELPEKSKLQEIYQELTWLKA AVGELPEKSKMQEIYQELTRLK AAVGELPEKSKQQEIYQELTRL KAAVGELPEKSKQQEIYQELTR LKAAVGELPEKSKQQEIYQELT QLKAAVERLCHPCPWEWTFFQ GNCYFMSNSQRNWHDSITACK EVGAQLVVIKSAEEQNFLQLQS SRSNRFTWMGLSDLNQEGTWQ WVDGSPLLPSFKQYWNRGEPN NVGEEDCAEFSGNGWNDDKCN LAKFWICKKSAASCSRDEEQFL SPAPATPNPPPA	404

Table.No.02. physicochemical parameters of DC-SIGN protein.

Properties	Values
Molecular weight	45774.93
Instability	55.50
pI value	5.43
Aliphatic index	81.16
GRAVITY	-0.606

Table.No.03. Secondary structure prediction of DC-SIGN protein.

Properties	Percentage (%)
Alpha helix	57.67%
Extended strand	9.16%
Beta turn	2.48%
Random coil	30.69%

IV. CONCLUSION

Dengue fever is a mosquito-borne tropical disease caused by the dengue virus. Symptoms typically begin three to fourteen days after infection. This may include a high fever, headache, vomiting, muscle and joint pain, and a characteristic skin rash. DC-SIGN is a C-type lectin and has a high affinity for the ICAM3 molecule. It binds various microorganisms by recognizing high-mannose-containing glycoprotein's on their envelopes and especially functions as receptor for several viruses such as Dengue, HIV and Hepatitis C. Binding to DC-SIGN can promote Dengue, HIV and Hepatitis C virus to infect T-cell from dendrite cells. Thus binding to DC-SIGN is an essential process for Dengue infection. Hence the present investigation mainly deals with the understanding of detailed molecular features of DC SIGN protein to uncover its key role in the infection of Dengue by retrieving its protein sequence information, analysis of physicochemical properties, secondary structure, conserved domains and tertiary structure. The analysis reveals that the protein is highly stable with helix dominating secondary structure. This can lead to a novel approach to combat viral infections through computer aided drug designing in Bioinformatics.

V. REFERENCES

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Cite this article as :

Vinod P Sinoorkar, Umme Aiman Md. S. Kumthe, "In-silico Characterization of Target Protein in Dengue Infection", International Journal of Scientific Research in Science and Technology (IJSRST), Online ISSN : 2395-602X, Print ISSN : 2395-6011, Volume 9 Issue 6, pp. 215-218, November-December 2022. Available at doi : https://doi.org/10.32628/IJSRST229627
Journal URL : https://ijsrst.com/IJSRST229627