

Comparative modelling and simulation of Replication Initiation Protein in Banana Bunchy Top Virus

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Abstract: Banana Bunchy Top Disease is one of the most severe disease in banana. It is caused by Banana Bunchy Top Virus. The disease is highly prevalent in Africa and Asia. The virus is transmitted by some kind of sources. One of the main source of transmission is through banana aphid - the *Pentalonia nigronervosa*. The vector is globally distributed and transmits the virus. The virus also spreads through contaminated planting material, and it is also found that all banana cultivars were vulnerable due to a lack of known resistance sources. The symptoms of bunchy top of banana are unique and easily recognised from those produced by other banana viruses. Plants that have been infected have a 'bunchy top' look and rosette appearance. Plants that have been affected do not recover or revive. The virus has a multi-component genome made up of at least six circular DNA segments, single stranded DNA (ssDNA) components ranging in length from 1000 to 1100 nucleotides. Because the 3D structure of the proteins linked with BBTV has yet to be established by experimental approaches, we projected the protein structure using comparative modelling. The research focusses on comparative modelling and simulation of replication initiation protein in Banana Bunchy Top Virus.

Keywords : BBTD, BBTV, *Pentalonia nigronervosa*, Bunchy top, Rosette appearance and Comparative modelling.

INTRODUCTION

Banana belongs to the family Musaceae. It is one of the most important fruits cultivated and consumed. It is being cultivated for two main reasons: 1. Food, 2. Fibre for Textile industry. Each and every part of the plant has its own value and uses. The plant gets diseased and infected by various sources. One among those diseases is BBTD (Banana Bunchy Top Disease). This disease is caused by a virus named BBTV (Banana Bunchy Top Virus).

There is no control measures to control BBTV. Once after it gets infested in the field, the plant won't grow well. It will express rosette appearance (Figure 3, 4) and stunted growth. This is the epic and most unique symptom of BBTV attack. Main reason for the transmission of the virus is Banana Aphid, *Pentalonia nigronervosa*. Control of the aphids is only a preventive measure. There's no post attack management for this BBTD. So focussing on comparative modelling and simulation of replication initiation protein in Banana Bunchy Top Virus is very important because the attack of BBTV causes more economical loss to the farmer and there is no chance for the crop to get revived to normal stage after infection.

HEALTHY BANANA PLANT**Figure 1****Figure 2****ROSETTE APPEARANCE****Figure 3****Figure 4****BBTV taxonomic tree**

- Domain: Virus
- Group: "ssDNA viruses"
- Family: Nanoviridae
- Genus: Babuvirus
- Species: Banana bunchy top virus

Banana aphid taxonomic tree

- Domain: Eukaryota
- Kingdom: Metazoa
- Phylum: Arthropoda
- Subphylum: Uniramia
- Class: Insecta
- Order: Hemiptera
- Suborder: Sternorrhyncha
- Family: Aphididae
- Genus: *Pentalonia*
- Species: *Pentalonia nigronervosa*

METHODOLOGY**• Protein Modeling:**

Template-based modeling (TBM) is a structure prediction approach that uses homologous proteins as templates in this context.

Computational Screening of Leads:

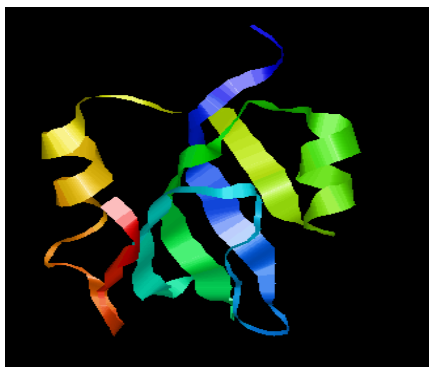
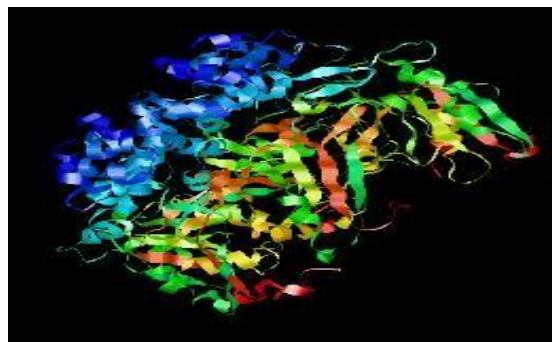
The web server MTiOpen Screen comprises two services, MTiAutoDock and MTiOpen Screen. MTiAutoDock supports docking compounds into a pre-determined or a user-defined binding site and a rigid docking with Autodock 4.2. MTiOpen Screen automates virtual screening by docking with Autodock Vina.

Process

- **Step 1:** Finding details for Banana Bunchy Top Virus in NCBI.
- **Step 2:** Search for FASTA Sequence of protein.
- **Step 3:** Copy the FASTA Sequence.
- **Step 4:** Paste the FASTA Sequence in SWISS MODEL to develop a model for the sequence identified.
- **Step 5:** Download the predicted models from SWISS MODEL.
- **Step 6:** View the downloaded structures in RasMol.
- **Step 7:** Check the quality of the structures in Ramachandran Plot.
- **Step 8:** Perform docking using MTiOpen Screen

RESULTS

The Rampage server's target protein quality provided knowledge of non-bonding interactions between the protein and the ligands (Figure - 5, 6, 7) to determine their binding free energy. This MTi automated docking research identified 7176 compounds in the drug library and the best fit of 1500 molecules. The protein had the most excellent relationship for the Mk3207 chemical, with a -11.3Kcal/mol binding energy. Because of the reduced binding energy, the ligand is more stable than another molecule. Figure 8 gives the details regarding the DNA Sequence of BBTV. Figure 9 showcases the test results made on the transmission of BBTV through Aphids.

PREDICTED STRUCTURAL ORIENTATIONS OF REPLICATION INITIATION PROTEIN**FIGURE 5****FIGURE 6****FIGURE 7**

BBTV DNA-	Primer name	Sequence	Location
1	BT1RepEx	5' GATGGCGGATATGTGG 3'	129-144
	BTRepFD	5' GAGCTCTCAGCAAGAAACCAAC 3'	989-974
2	BT2R3	5' CCTAATCTGTCAAGGA 3'	266-282
	BT2F3	5' CGTTAGTATACGTTCCG 3'	574-558
3	BT3V.Exp	5' TAGATCCATGGTCAGACAAGAA 3'	206-229
	BT3C.Exp	5' ATAAAGCTTTCAAACATGATATGT 3'	749-726
4	BT4V.V3	5' ATGGCATTAAACAACAGA 3'	279-295
	BT4C.C2	5' GAACATAGTCCAGCGT 3'	629-613
5	BT5V.Exp	5' AAGAGCCATGGAGTCTGGGAATC 3'	233-256
	BT5C.Exp	5' GATATAAGCTTAGACTTAATGTTAC 3'	734-711
6	BTP2B2.17	5' GATCTATTGAAGCTGTG 3'	426-442
	BTP2R1.17	5' CTAATCTCCATGCTCTCT 3'	666-651

FIGURE 8

No infective aphids ^a	No. plants tested (n)	No. plants infected	Mean % transmission
0	52	7	13.5
1	9	3	33.3
2	11	4	36.4
3	6	4	66.7
4	31	23	74.2
5	72	60	83.3

^a At the end of the IAP, five aphids per group were tested for BBTV. This represents the number of aphids that tested positive for BBTV.

FIGURE 9

CONCLUSION

Banana is a cash crop in tropical climate which yields more and brings good profit to the farmer who is cultivating it. If this BBTV attacks one banana plant or tree, it will quickly spread its infection to the whole field and there is no management to control the spread. So identifying the replication initiation protein structure is very important for silencing it and for future drug discovery purposes.

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