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Editorial

Prediction of Binding Site in Eight Protein Molecules of Begomovirus and its Satellite Components i.e. Betasatellite and Alphasatellite Isolated from Infected Ornamental Plant

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Abstract

Earlier reported the molecular characterization of complete genome of a begomovirus and its satellite molecules isolated from an ornamental plant Marigold i.e., Ageratum enation virus (AEV: KC589699), Ageratum leaf curl betasatellite (ALCB: KC589700) and Marigold leaf curl alphasatellite (MLCuA: KC206078). It presented and highlighted the computational approach for prediction of binding sites in protein molecules of the three begomovirus components for in depth study using two servers. Thus, in order to take a step forward to find a cure against such viruses that causes major crop loss worldwide.

Key words: Marigold, begomovirus, satellites, proteins, binding sites

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INTRODUCTION

Begomovirus are an outsized varied family of plant viruses (Mansoor *et al*., 2003) which infects an expansive assortment of plants such as ornamentals (Marwal *et al*., 2013b), weeds (Marwal *et al*., 2014) and crops and causes a noteworthy loss to Agriculture and Horticulture worldwide (Lima *et al*., 2013). Ornamental plants are extensively scattered worldwide and have high environmental adaptability (Marwal *et al*., 2013c). Ornamentals are considered as a foundation of new viruses and reservoirs of unidentified economically imperative viruses but are often neglected during diversity study (Urbino *et al*., 2013).

Many scientific reports have demonstrated that ornamental plants serve as reservoir or alternative hosts for begomovirus survival (Raj *et al*., 2007) and spread in the absence of the main crops (Ilyas *et al*., 2013). Thus, there is a pressing need for additional information on the diversity and distribution of begomovirus in ornamental plants.

Proteins constitute the backbone of cellular function by carrying out the tasks encoded in the genes expressed by a given cell type. It does, however, remain challenging to efficiently classify the operational role of the individual protein entities identified in such procedures (Bairoch, 2000). Functional properties of a protein domain, such as enzymatic activity or the ability to interact with other proteins can often be derived from the approximate spatial arrangement of its amino acid chain in the folded state (Hannum *et al*., 2009).

Knowledge of the structure of a newly discovered protein is thus highly valuable in determining the role it plays in biological processes and it can serve as an important stepping stone in generating hypotheses or suggesting experiments to further explore the protein's nature. Therefore 3DLigandSite and RaptorX are web servers for the prediction of ligand binding sites in protein molecules. In 3DLigandSite server the ligands bound to structures similar to the query are superimposed onto the model and used to predict the binding site. The web server enables users to submit either a query sequence or structure. Predictions are usually displayed via an interactive Jmol applet. 3DLigandSite is available for use (http://www .sbg.bio.ic.ac.uk/3dligandsite) (Wass *et al*., 2010).

RaptorX distinguishes itself from other servers by the quality of the alignment between a target sequence and one or multiple distantly related template proteins (especially those with sparse sequence profiles) and by a novel nonlinear scoring function and a probabilistic-consistency algorithm. Consequently, RaptorX delivers high-quality structural models for many targets with only remote templates (http://raptorx.uchicago.edu/) (Kallberg *et al*., 2012).

Earlier characterized this begomovirus and its satellite molecules (Marwal *et al*., 2013a) and submitted the viral sequence in NCBI. The FASTA sequence of all the proteins was uploaded on the protein comparative modeling server 3D-Jigsawn (http://bmm.cancerresearchuk.org//~ 3djigsaw). The 3D-Jigsawn is an automated system to build three dimensional models for proteins based on homologues of known structure. The 3D-Jigsawn sends the PDB files on the e-mail address that assigned to the modeling server (Heinrichs, 2008). In order to find the binding site of the proteins, PDB files of all the proteins were uploaded on the servers and the results were obtained.

The server provides the detail of the amino acids responsible for binding as well as the list of ligand molecules as heterogens provided by Uniprot that are unlikely to be present in protein structures as solvent and manually supplemented it with further likely to be biologically relevant. The protein and predicted binding site can be shown in cartoon, spacefill or wireframe formats. The protein can be colored to show the predicted binding site or residue conservation.

During the analysis of AC1 protein it was found that Asparagine, Glutamine and Glycine residues at 90, 92 and 93 position are responsible for binding site of AC1 protein. The heterogen/ligand present in binding site were NAG (N-Acetyl-D-Glucosamine) (Fig. 1a). Glycine at position 37 and phenylalanine at position 41 was found responsible for binding site in AC2 protein molecule. Flavin-Adenine Dinucleotide (FAD) acts as a ligand molecule/heterogen very much present in the vicinity of the protein (Fig. 1b).

Investigation of AC3 protein revealed that residues responsible for binding and their position were found to be Isoleucine at 62, Cysteine at 65, Isoleucine again at position 71, Tryptophan at 72, Methionine at 73, Threonine at 74, Threonine again at 79, Leucine at 83, Valine at 112 and again at position 116 Valine was accountable. The heterogen/ligand present in binding site were Adenosine-5'-Diphosphate (ADP) (Fig. 1c).

The binding sites exhibit chemical specificity, a measure of the types of ligand that bond and the affinity that measure strength of the chemical bond (Balakrishnan *et al*., 2010). When AC4 protein PDB file was uploaded on the server, it was establish that the residues Glutamic acid and Asparagine at position 72 and 75, respectively were in charge for binding site, whereas the ligand was found to be 4-Methylidene-5-One Peptide Derived Chromophore (MDO) (Fig. 1d). While studying the coat protein AV1, it was instituted that heterogen Calcium ion (Ca) was responsible for binding at Glycine residue in the 125th position of AV1 protein model (Fig. 1e).

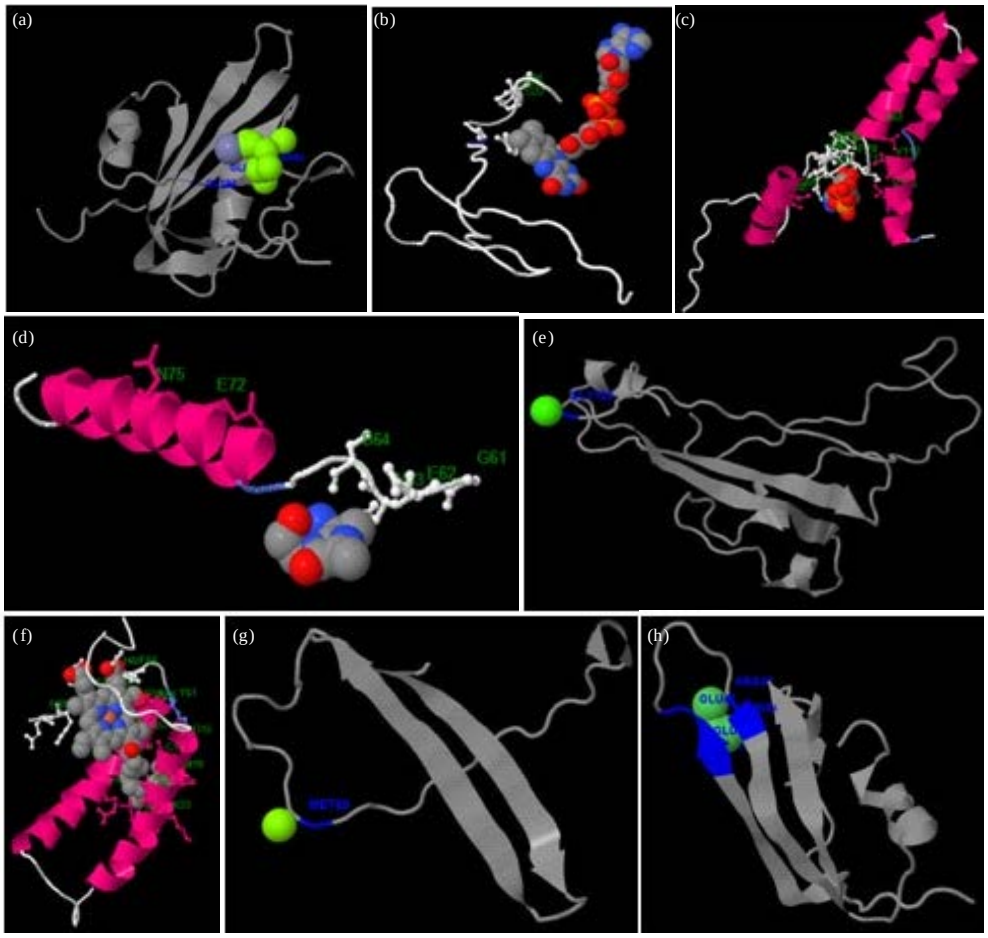

Fig. 1(a-h): 3DLigandSite and RaptorX server generated visualization of prediction for target proteins of Ageratum enation virus (a) AC1, (b) AC2, (c) AC3, (d) AC4, (e) AV1, (f) AV2), Ageratum enation betasatellite (g) βC1 and Marigold leaf curl alphasatellite (h) Rep. The Jmol applet displays the protein structure with predicted binding site colored blue. The ligands in the cluster used to make the prediction are displayed with ions in spacefill and organic molecules in wireframe formats

The AV2 protein is the most active protein in begomovirus, hence remarkable findings were observed while analyzing the AV2 protein molecule. Surprisingly 16 amino acid residues are present at the binding site of the AV2 protein molecule. It includes Glycine, Cysteine, Methionine, Alanine, Valine, Lysine, Leucine, Arginine at 15th, 18th, 19th, 21st, 22nd, 23rd, 25th and 50th position, respectively and Asparagine, Tyrosine, Valine, Glutamine, Alanine, Serine at 53rd, 54th, 55th, 56th, 57th and 59th position, further including Arginine and Tyrosine at 60th and 61st position respectively. The ligand responsible at the binding site was HEA (HEME-A) (Fig. 1f).

It was found that only one binding site was predicted in Ageratum leaf curl betasatellite C1 protein at position 69, conquered by Methionine having Magnesium ion (Mg) as the ligand molecule (Fig. 1g). Whereas in the case of Rep protein of Marigold leaf curl alphasatellite five residues are functional at the binding site, which includes Glutamine at the 39, 40 and 41st position, Arginine and Histidine at 48th and 49th position, respectively. The heterogen molecule was revealed to be NI (Nickel(II) Ion) (Fig. 1h).

Ornamental plants act as an alternate host of begomoviruses and its associated satellite molecules in the absence of main crop (Marwal *et al*., 2013b). Marigold (*Tagetes patula*) an important ornamental plant, widely cultivated in India were found infected with three begomovirus components i.e. Ageratum enation virus (AEV: KC589699), Ageratum leaf curl betasatellite (ALCB: KC589700) and Marigold leaf curl alphasatellite (MLCuA: KC206078).

Proteins often perform their function on ligands (e.g. enzyme substrates) or are regulated by them. Therefore the identification of ligand-binding sites was important. This study supported evidence that virus associated with Marigold

was studied through computational analysis. Such new approach has never been tried earlier in case of begomovirus and its satellite molecules. Our results provide much new information on these topics and will be used for the screening of inhibitors against begomovirus proteins and can be further applied in future antiviral agent designing.

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