Virol-mycol 2016, 5:1 (Suppl)
http://dx.doi.org/10.4172/2161-0517.C1.009

First report of *Begomovirus* causing yellow mosaic disease of ridge gourd in Saudi Arabia

Sayed Sartaj Sohrab[1], **Muhammad Yasir**[1], **Sherif Ali El-Kafrawy**[1], **Magdi Ali Ahmed Mousa**[1, 2] and **Ahmed A Bakhashwain**[1]
[1]King Abdulaziz University, KSA
[2]Assiut University, Egypt

Ridge gourd (*Luffa acutangula*) is an important vegetable crop; widely used for vegetables at early stage in central and eastern Asia to South Eastern Asia. Yellow mosaic disease limits the production of ridge gourd which is caused by *Begomovirus* belonging to the family Geminiviridae. In this study, naturally infected leaf samples of ridge gourd exhibiting characteristic yellow mosaic were collected during field survey from Hadasham, Jeddah, Saudi Arabia. The causative agent was identified by PCR using *Begomovirus* specific primers and transmitted by whiteflies to healthy ridge gourd seedlings. The full-length viral genome was amplified by rolling circle amplification and beta satellites were amplified by PCR using universal primers. Sequencing of full genome (~2.7 kb) and beta satellites (~1.4 kb) were performed bidirectionally. The complete viral genome sequences had 2788 nucleotides (KU248482) and showed highest (99.8% nucleotides) similarity with *Tomato yellow leaf curl virus* Jeddah isolate followed by 99.4-93.0% nucleotides similarity with an isolate of Tomato yellow leaf curl virus identified from Jizan and Al-Qasim, Saudi Arabia. The beta satellite had 1363 nucleotides (KU248483) and showed 99.6% nucleotides similarity with Tomato yellow leaf curl beta satellites Jeddah isolate. The identified virus from ridge gourd formed the closest cluster with *Tomato yellow leaf curl virus* isolates from Jeddah, Jizan and Al Qasim, Saudi Arabia. On the basis of results obtained from PCR detection, sequence analysis and phylogenetic relationship; it is concluded that the virus causing yellow mosaic disease in ridge gourd could be a variant of *Tomato yellow leaf curl virus* isolate circulating in the Kingdom. This is the first report about the association of *Begomovirus* causing yellow mosaic disease of ridge gourd in Saudi Arabia.

ssohrab@kau.edu.sa

Computational mutagenesis, molecular docking and simulation study on NS3 protein of *Flavivirus* encephalitis to identify the antiviral compounds

Sunil Kumar Gupta
Bioinformatics Centre, India

Flavivirus encephalitis is an acute central nervous system inflammatory disease generally causes by the Japanese Encephalitis Virus (JEV), *West Nile virus* (WNV) St. Louis encephalitis virus (STEV), Murray Valley encephalitis virus (MVEV) and Tick-borne encephalitis virus (TBEV) belonging to genus *Flavivirus* (family Flaviviridae). Over 100 countries throughout the world, more than 2.5 billion people are at risk of infection and around 20 million infections are annually reported. In the present study, NS3 protein of *Flavivirus* encephalitis has been preferred as probable molecular target for drug development. *Flavivirus* encephalitis NS3 protein is a large multifunctional protein plays an essential role in the *Flavivirus* life cycle. The NS3 N-terminal protease (NS3pro) simultaneously with its critical cofactor NS2B is involved in proteolytic processing of the viral poly protein, whereas the C-terminal NTPase/helicase is responsible for RNA replication. The three dimensional (3D) structure of all NS3 proteins of *Flavivirus* encephalitis were designed and validated using modeler 9.12 and PROCHECK tool, respectively and also optimized using molecular dynamics simulation. Mutation analysis and amino acid residues associated in active pocket have been analyzed. About 17588 lead molecules were used for computational virtual screening against NS3 protein and finally 361 lead molecules were found appropriate for docking study. Five top ranked lead molecules with strong binding affinity to all NS3 proteins were identified based on minimum binding energy. Molecular dynamic simulation was also performed for protein-ligand complex which have minimum binding energy, to study the mobility of complex at various time intervals. Drug likeliness, comparative bioactivity and other biochemical properties of lead molecules were recognized using OSIRIS Property Explorer. As result of the study 4-Epi Minocycline (CID 54687237) was found suitable as viral replication inhibitor therapeutic molecule for *Flavivirus* Encephalitis, which may be considered as a potential ligand for treatment of *Flavivirus* Encephalitis. Such studies may contribute to new approaches to antiviral drug development against Encephalitis.

skgupta.bi@gmail.com