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Micro RNA-Gene Docking in the Strains of Oryza Sativa

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Abstract:- Micro RNA is a small non coding conserved ssRNA, which helps in regulating gene expression. miRNA are being used in the pathogenesis of various human diseases like cancer, neurological disorders, and in other infectious diseases. miRNA are typically short of 17-25 nucleotides which are known to affect the messenger RNA, affecting the translation thereby regulating the gene.

In plants, the mature miRNA enters an RNA induced Silencing Complex called RISC, negatively regulating the gene expression. Nowadays these miRNA are being used to silence the genes which are not essential for the survival of plants, so that the other beneficial genes like the drought resistance, salt tolerance, immunity and vitamin inducing genes can be regulated.

In the present, research we tried to get the mi RNA of the already sequenced plant strain using miRNA database, comparison was done to find the similarities amongst the two strains and then miRNA-protein docking was done. It was found that MAP KINASE gene and Osa-MIR1862a an mi RNA can be docked. subject to experimental verification.

I. INTRODUCTION

Rice is the major cereal as a staple food in many countries, hence produced over half of the World. Almost 95% of the rice production is done in Asian countries with 17 countries in Asia and the Pacific, 9 countries in North and South America and 8 countries in Africa worldwide. In India, the rice production is done in a total area of about 43,388,000 hectares which contributes to 780 and 689 kcal/capita/day of the food supply. Scientifically Rice is Oryza sativa grown in excess of water and has different subspecies, two major subspecies are Indica, the long-grain rice and the Japonica, the round-grain rice. Japonica rice is mostly found in countries like China, Taiwan, Korea, Europe and USA. Indica rice varieties are grown widely in Asia [1] and also consist of the fragrant ones which are premium. INDICA RICE VARIETIES are used and its accession number is (AAD2917.10).

A. miRNA

A microRNA is a single-stranded non-coding RNA molecule (containing about 22 nucleotides) found in all organisms, whose function includes RNA silencing and in post-transcriptional regulation of gene expression. Micro-RNAs are partially complementary to one or more messenger RNA (mRNA) molecules, showing its functionality in slowing the gene expression in a variety of manner including translational repression, mRNA cleavage, and deadenylation. [2]

The regulation of gene expression is by mature miRNAs being incorporated into RNA-induced silencing complexes (RISCs) and guide RISCs to specific targets through Watson–Crick base-pairing. A large portion of miRNAs were discovered in plants during the regulation of transcription factors ; few of them are highly conserved and play an important role in plant development, stress adaptation , and hormone signaling. The sequence evolution studies on miRNAs and their target sites have been extensively explored in a variety of plant species . For example, rapid sequence evolution of the miR482/2118 gene family has promoted the evolution of resistance genes in the Solanaceae[3].

II. MATERIALS AND METHODOLOGY

For the present analysis we used miRNA of the Indica rice variety and the bioinformatics tools are used. They are

- Mir-base
- Rap-db
- Docking tools

- **Mir-base**: MIR base is a biological database that acts as an archive of micro RNA sequences and their annotations. It contains information about 15,172 micro RNA'S.

  The miRBase provides the miRNA gene with a unique name and is available at https://www.mirbase.org/ [4].

- **Rap-db**: The Rice Annotation Project Database (RAP-DB, http://rapdb.dna.affrc.go.jp/) has provided a comprehensive source of information for the genomes of plant varieties This database provides plant researchers with highly reliable and complete data on rice gene annotations, it has all manually curated data, and with 1,626 loci currently available in the database, which includes gene names or gene symbols.[5]
- **Docking tool- H-dock**: The HDOCK server (http://hdock.phys.hust.edu.cn/) is a highly integrated suite for homology search, template-based modeling, structure prediction, macromolecular docking, biological information incorporation and job management for robust and fast protein-protein docking. The server checks for the similar docking molecules from similar docked molecules in the server, otherwise the amino acids as input and a hybrid docking strategy in which experimental information about the protein–protein binding site is incorporated during the docking and post-docking processes. Using HDOCK one can perform protein–RNA/DNA docking with an intrinsic scoring function.

The server delivers both template- and docking-based binding models of two molecules and allows for download and interactive visualization.[8]

Initially the miRNA for the rice variety Indica was downloaded from the MIRBase and then comparison amongst the 2 varieties was done to find out the identities then the rice genome was browsed using RAPDb to find the genes which are playing a role in the survival of the plant and saved for the next step.

Amongst all the types of genes from the database the 6 genes named below have been taken for the present study.

RICE GENE NAME	ACCESSION NUMBER
Ascorbate peroxidase	BAA0864.1
Glutaredoxin family	CAA54397.1
RC12 homologs	PO511C01
WRKY Gene Family	AP002484.1
Cysteine rich peptide	BAA28867.1
MAP Kinase	CAD31224.1

Table1: Few Rice Genes

This table1 shows the important rice genes from the Indica variety ,which are further used for the docking. It is docked against receptors.

Then docking was done between the above said genes and the saved miRNA.

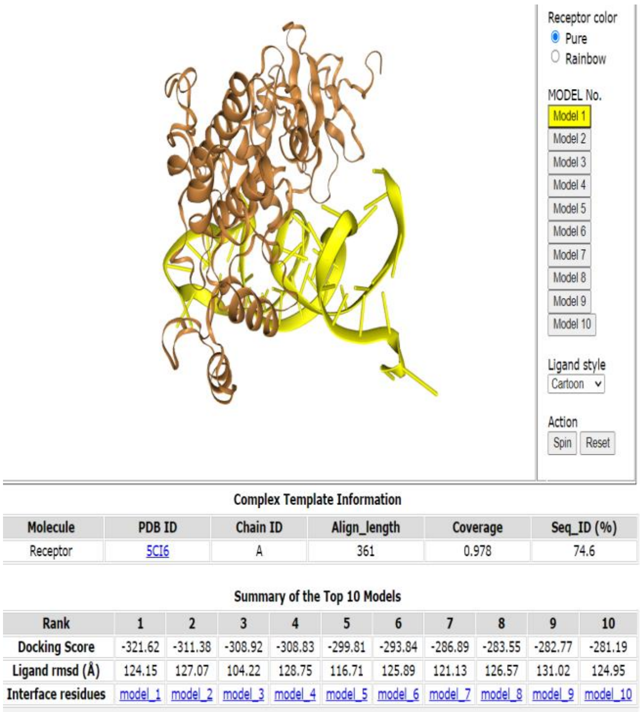
III. RESULTS

GENE	RECEPTOR 1	RECEPTOR 2	RECEPTOR 3	RECEPTOR 4	RECEPTOR 5	RECEPTOR 6
Ascorbate peroxidase	-214.88	-253.00	-240.60	-249.55	-213.68	-258.90
Glutaredoxin family	-224.93	-218.16	-212.50	-261.87	-202.87	-269.35
RC12 homology	-277.49	-282.78	-290.12	-286.66	-266.13	-280.40
WRKY gene family	-266.13	-260.92	-287.65	-234.65	-254.98	-365.89
Cysteine rich peptide	-301.81	-274.14	-268.72	-263.85	-244.43	-252.51
MAP Kinase	-291.49	-321.62	-243.67	-276.87	-211.34	-267.91

Table 2: Energy values

Receptor 1- Osa-MIR1862e- CUAGAUUUGUUUAUUUUGGGACGG
Receptor 2-Osa-MIR1441 -ACCGGAUGUCGGAAAAGGUUU
Receptor 3- Osa-MIR162a - UCGAUAAACCUCUGCAUCCAG
Receptor 4-Osa-MIR1861c- CGAUCUUGUAGCAAGAACUGAG
Receptor 5-Osa-MIR395b-GUGAAGUGUUUGGGGGAACUC

From the above table it can be inferred that protein MAP KINASE (Mitogen activated protein kinase) when docked with MI-RNA Osa-MIR 861a found to have lowest docking score hence it requires minimum energy to dock.



Complex Template Information

Molecule	PDB ID	Chain ID	Align_length	Coverage	Seq_ID (%)
Receptor	5CI6	A	361	0.978	74.6

Summary of the Top 10 Models

Rank	1	2	3	4	5	6	7	8	9	10
Docking Score	-321.62	-311.38	-308.92	-308.83	-299.81	-293.84	-286.89	-283.55	-282.77	-281.19
Ligand rmsd (Å)	124.15	127.07	104.22	128.75	116.71	125.89	121.13	126.57	131.02	124.95
Interface residues	model_1	model_2	model_3	model_4	model_5	model_6	model_7	model_8	model_9	model_10

Fig. 1: Docking between MAP Kinase and Osa-MIRI1862a

IV. CONCLUSION AND DISCUSSION

Bioinformatics is playing a vital role in the current research works. An unprecedented wealth of biological data has been generated by the human genome project and sequencing projects in other organisms. The huge demand for analysis and interpretation of these data is being managed by the evolving science of bioinformatics. Bioinformatics is defined as the application of tools of computation and analysis to the capture and interpretation of biological data. It is an interdisciplinary field, which harnesses computer science, mathematics, physics,and different types of bioinformatics tools to study the comparative analysis of mi-rna in rice variety and to find its evolutionary relationship.

Hdock is more used in research where the h-dock docking is done between the protein-protein or protein-DNA/RNA based on their hybridisation, by using this docking tool we docked between protein-mirna. By this we came to know about the energy values between the essential rice gene varieties (Ascorbate peroxidase, glutaredoxin family, RC12homolgy, WRKY Gene family, cysteine rice peptide, MAP Kinase) and mirna(Osa-MIR1862e,Osa-MIR1441,Osa-MIR162a,Osa MIR1861c,Osa-MIR395b).Docking was done using the tool Hdock and it was found that the gene MAP KINASE and the receptor Osa-MIR1862a was found to have the lowest docking score hence it requires minimum energy to dock. And hence this MAP KINASE gene can be docked with the receptor Osa-MIR1862a so that the plant growth can be enhanced. This has to be experimentally verified.

Genes which are not having a vital role in plant metabolism which is seen after docking and thus gene activity can be blocked so that other gene activity can be enhanced**.**so that it cannot harm the plant.

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