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IN-SILICO ANALYSIS AND HOMOLOGY MODELING OF ANTIOXIDANT PROTEINS OF *ORYZA SATIVA SUBSP.* JAPONICA (RICE)

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ABSTRACT: Rice is much revered oriental food and the most important tropical cereal crop. It is the staple food of about half the human race and is often the main source of calories and the principal food of many millions of people. Health benefits of rice include providing fast and instant energy, stabilizing blood sugar levels and providing essential source of vitamin B1 to human body. In this study, a bioinformatics and molecular modeling approach was adopted to explore properties and structure of rice antioxidant proteins. The antioxidant proteins selected for this study are CYS PRX (P0C5C9, Q6ER94, P0C5D1) and PRDX (Q9FR35, Q7F8S5, Q9SDD6). Physico-chemical characterization interprets properties such as pI, EC, AI, GRAVY and instability index and provides data about these proteins and their properties. Prediction of motifs, patterns, disulphide bridges and secondary structure were performed for functional characterization. Three-dimensional structures for these proteins were not available as yet at PDB. Therefore, homology models for these antioxidant proteins were developed. The modeling of the three dimensional structure of these proteins shows that models generated by Modeller9.11 were more acceptable in comparison to that by Swiss Model. The models were validated using protein structure checking tools PROCHECK and WHAT IF. These structures will provide a good foundation for functional analysis of experimentally derived crystal structures.

INTRODUCTION: Rice is much revered oriental food and the most important tropical cereal crop. It is the staple food of about half the human race and is often the main source of calories and the principal food of many millions of people [1]. Health benefits of rice include providing fast and instant energy, stabilizing blood sugar levels and providing essential source of vitamin B1 to human body.

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The B-complex vitamins, especially thiamin, riboflavin and niacin offered by natural brown rice promote youthful energy and nourishment to skin and blood vessels [2].

Rice varieties such as Bora is given to the patient suffering from jaundice, 2-3 times daily for a week, Dhanwar is given to pregnant cow for safe pregnancy, healthy calf and easily removal of placenta, Karhani is useful in breathing problems and epilepsy and Gudna is useful for chronic gastric patient [3].

The protein content of the rice is lower than that of wheat, but is of superior quality and utilized better by the body than the wheat protein [4]. The ancient and modern oriental healers through traditional

medicines have always advocated the use of natural brown rice as a key to youthful health building [5]. Rice is about 98 per cent digestible. Rice starch is different from other grain starches as it contains 100 percent amylopectin, which is most completely and rapidly digested grain starch; this makes rice in ideal health food.

Rice protein, which comprises up to 8% of the grain, has a special benefit as it has eight of the essential amino acids in a delicately balanced proportion. Laboratory studies have shown that rice products may have anti-cancer properties and the potential to treat other conditions such as diabetes, kidney stones, Alzheimer's disease and heart disease [6, 7].

The oil from rice bran is unique among edible oil due to its rich source of commercially and nutritionally important phytoceuticals [8]. The oil from rice bran contains vitamin E and minerals. The vitamin E groups of compounds in rice have antioxidant properties and these compounds could explain some of the traditional medicinal uses of rice, particularly to treat cancer [9]. Antioxidants can protect against the damage induced by free radicals acting at various levels [10].

Brown rice and whole grains are said to be rich in insoluble fibre. The insoluble fibre from rice acts like a soft sponge that may be pushed through intestinal tract quickly and easily [11]. Both white rice and brown rice contain 5.2 grams of protein per every 150 grams. Rice protein is also gluten free so it's a good source of protein for those with gluten intolerance or Celiac's disease [12]. Its antioxidant activity has made rice unique among cereals.

An antioxidant is a molecule capable of inhibiting the oxidation of other molecules. Oxidation is a chemical reaction that transfers electrons or hydrogen from a substance to anti-oxidizing agent. Antioxidants are widely used in dietary supplements. They have been investigated for the prevention of diseases such as cancer, coronary heart disease and even altitude sickness [13].

Antioxidants also have many industrial uses, such as preservatives in food and cosmetics and to prevent the degradation of rubber and gasoline [14]. Rice contains some natural antioxidant proteins.

In this study, the antioxidant proteins of rice (*Oryza sativa* subsp. Japonica) have been selected for which three-dimensional structures were not available at the protein data bank (PDB). These proteins contain enzyme like peroxi-redoxins. Peroxiredoxins [15] are peroxidases that catalyze the reduction of hydrogen peroxide, organic hydroperoxides, as well as peroxynitrite. It has an essential role in tumour suppression and in cell signaling [16].

The sequences of antioxidant proteins are retrieving from Swiss-Prot. Different computational tools and softwares are used for making predictions regarding the identification and structure prediction of proteins. In this paper, the insilico analysis and homology modeling studies on antioxidant proteins of rice was reported. Three-dimensional structures for these proteins were yet not available.

Materials and Methods: Sequences of antioxidant proteins of rice were retrieved from the SWISSPROT, a public domain protein database [17]. It is a high quality annotated and non-redundant protein sequence database, which brings together experimental results, computed features and scientific conclusions. **Table 1** shows the protein sequences considered in this study. The antioxidant proteins sequences were retrieved in FASTA format and used for further analysis.

Physico-chemical characterization: For physico-chemical characterization, theoretical isoelectric point (pI), molecular weight (M. wt), total number of positive and negative residues (+R, -R), extinction coefficient (EC) [18], instability index (II) [19], aliphatic index (AI) [20] and grand average hydropathy (GRAVY) [21] were computed using the Expasy's ProtParam server [22]. The results were shown in **Table 2**. Functional Characterization: The SOSUI signal [23] server distinguishes between membrane and soluble proteins from amino-acid sequences and predicts the transmembrane region. The trans-membrane regions are rich in hydrophobic amino acids. **Table 3** represents the trans-membrane region identified for these antioxidant proteins.

Disulphide bonds are important in determining the functional linkages. Table 4 shows prediction of "SS" bonds using the primary structure (Protein sequence data) by the tool CYS_REC. It is used to

determine the cystein residues and disulphide bonds. It identifies the position of cysteins present and pattern (if present) of pairs in the protein sequence.

Prosite [24] is a database of protein families and domains and functional sites and it gives information for protein families and domains. Table 5 represents the output of Prosite database.

Secondary structure prediction: SOPMA (Self Optimized Prediction Method with Alignment) [25] was used for calculating the secondary structural features of the antioxidant protein sequences considered for this study. The results were presented in Table 6.

Model Building and evaluation: The modeling of the three dimensional structure of the proteins was performed by homology modeling programs, Swiss model [26] and Modeller 9.11 [27]. The constructed 3D models were energy minimized in GROMACS force field using steepest descent minimization Algorithms [28]. The overall stereochemical property of the protein was assessed by Ramchandran plot analysis [29]. The validation for structure models obtained from the software tools was performed by using PROCHECK [30]. The models were further checked with WHAT IF [31].The results of PROCHECK and WHAT IF analysis was shown in Table 7 and Table 8 respectively. The structures of modeled proteins were visualized by Rasmol.

Results and Discussion: Table 1 shows antioxidant proteins of rice (Oryza sativa subsp. japonica) considered in this study. These antioxidant protein sequences were retrieved from the SWISSPROT, a public domain protein database. These protein sequences were retrieved in FASTA format and used for further analysis.

TABLE 1: PROTEIN SEQUENCES CONSIDERED FOR STUDY

Antioxidant Proteins	Accession No.	Length	Description
CYS PRX	P0C5C9	220	1-Cys peroxiredoxin A Rice 1Cys-peroxiredoxin (R1C-Prx) Thioredoxin peroxidase A
	Q6ER94	261	2-Cys peroxiredoxin BAS1, chloroplastic Thiol-specific antioxidant protein
	P0C5D1	220	1-Cys peroxiredoxin B Thioredoxin peroxidase B
PRDX	Q9FR35	162	Peroxiredoxin-2C Peroxiredoxin IIC Thioredoxin reductase 2C
	Q7F8S5	225	Peroxiredoxin-2E-2, chloroplastic Peroxiredoxin IIE-2 Thioredoxin reductase 2E-2
	Q9SDD6	198	Peroxiredoxin-2F, mitochondrial Peroxiredoxin IIF Thioredoxin reductase 2F

Parameters computed using Expasy's ProtParam tool was represented in **Table 2**. Isoelectric point (pI) is the pH at which the surface of protein is covered with charge but net charge of protein is zero. At pI proteins are stable and compact. The computed pI value of all proteins except Q9SDD6 were less than 7 (pI<7) indicates that these antioxidant proteins were considered as acidic. The pI value of Q9SDD6 is greater than 7 (pI > 7) reveals that this protein is basic in character. The computed isoelectric point (pI) will be useful for developing buffer system for purification by isoelectric focusing method.

TABLE 2: PARAMETERS COMPUTED USING EXPASY'S PROTPARAM TOOL

Antioxidant Proteins	Accession No.	Length	M. wt	pI	-R	+R	EC	II	AI	GRAVY
CYS PRX	P0C5C9	220	24042.4	5.97	31	27	20002.5	33.7	80.18	-0.35
	Q6ER94	261	28096.9	5.67	30	27	21555	36.9	87.89	-0.046
	P0C5D1	220	24232.6	5.4	34	27	17085	37.07	82.91	-0.267
PRDX	Q9FR35	162	17290.8	5.59	19	16	13980	34.28	99.32	0.027
	Q7F8S5	225	23179.5	6.15	24	23	8542.5	30.38	94.67	0.231
	Q9SDD6	198	20873.6	7.76	21	22	28022.5	30.1	89.24	0.013

Extinction coefficient of all proteins (at 280 nm) is ranging from 8542.5 to 28022.5 M^{-1} cm^{-1} with respect to the concentration of Cys, Trp and Tyr. The high extinction coefficient of Q9SDD6, Q6ER94 and P0C5C9 indicates presence of high concentration of Cys, Trp and Tyr. The computed extinction coefficients help in the quantitative study of protein–protein and protein–ligand interactions in solution.

The instability index provides an estimate of the stability of protein in a test tube. A protein whose instability index is smaller than 40 is predicted as stable, a value above 40 predicts that the protein may be unstable. The instability index value for the rice antioxidant proteins were found to be ranging from 30.1 to 37.07. The result classified that all the proteins show in the Table 2 are stable.

Aliphatic index for the antioxidant protein sequences ranged from 80.18 to 99.32. The very high aliphatic index of all antioxidant protein sequences indicates that these antioxidant proteins may be stable for a wide temperature range.

The Grand Average hydropathy (GRAVY) value for a peptide or protein is calculated as the sum of hydropathy values of all the amino acids, divided by the number of residues in the sequence. GRAVY indices of rice proteins are ranging from -0.35 to 0.231. This low range of value indicates the possibility of better interaction with water.

Functional analysis of these proteins includes prediction of transmembrane region, disulphide bond and identification of important motifs. SOSUI signal server distinguishes between membrane and soluble proteins from amino acid sequences. The Transmembrane regions and their length were tabulated in **Table 3**.

The server SOSUI signal classifies CYS PRX (Q6ER94) and PRDX (Q7F8S5 and Q9SDD6) as membrane protein and other rice antioxidant proteins as soluble proteins. The transmembrane regions are rich in hydrophobic amino acids.

TABLE 3: TRANSMEMBRANE REGIONS IDENTIFIED BY SOSUI SIGNAL SERVER

Antioxidant Proteins	Accession No.	Transmembrane region	Length	Type
CYS PRX	Q6ER94	MAACCSSLATAVSSSS	16	Signal Peptide
PRDX	Q7F8S5	MAAPTAAALSTLSTASVT	18	Signal Peptide
	Q9SDD6	MASALLRKATVGGSAAA	17	Signal Peptide

As disulphide bridges play an important role in determining the thermostability of these proteins. CYS_REC was used to determine the Cysteine residues and disulphide bonds. Possible pairing and pattern with probability were presented in **Table 4**. Result shows that Q6ER94 protein contains disulphide linkages.

The functions of antioxidant proteins of rice were analyzed by submitting the amino acid sequence to Prosite server [32]. Prosite analysis suggested the functionality of these proteins with profiles and patterns identified for characteristic functionality were represented in **Table 5**.

The secondary structure of rice proteins were predicted by SOPMA (Self Optimized Prediction Method with Alignment) which correctly predicts 69.5% of amino acids for a state description of the secondary structure prediction.

The secondary structure indicates whether a given amino acid lies in a helix, strand or coil. Secondary structure features as predicted using SOPMA were represented in **Table 6**.

The results revealed that random coils dominated among secondary structure elements followed by alpha helix, extended strand and beta turns for all sequences. The secondary structure were predicted by using default parameters (Window width: 17, similarity threshold: 8 and number of states: 4).

TABLE 4: DISULPHIDE (SS) BOND PATTERN OF PAIRS PREDICTED BY CYS_REC

Antioxidant Proteins	Accession No.	CYS_REC
CYS PRX	P0C5C9	-
	Q6ER94	Cys4-Cys114
	P0C5D1	-
PRDX	Q9FR35	-
	Q7F8S5	-
	Q9SDD6	-

TABLE 5: FUNCTIONAL CHARACTERIZATION OF PROTEINS OF RICE AT PROSITE

Antioxidant Proteins	Accession No.	Motif Found	Profile	Position in the protein	Description
CYS PRX	P0C5C9	-	THIOREDOXIN_2	4 - 165	Thioredoxins are small proteins of approximately one hundred amino-acid residues which participate in various redox reactions via the reversible oxidation of an active center disulfide bond. They exist in either a reduced form or an oxidized form where the two cysteine residues are linked in an intramolecular disulfide bond. Thioredoxin is present in prokaryotes and eukaryotes and the sequence around the redox-active disulfide bond is well conserved.
	Q6ER94	-	THIOREDOXIN_2	68 - 227	
	P0C5D1	-	THIOREDOXIN_2	4 - 165	
PRDX	Q9FR35	-	THIOREDOXIN_2	4 – 162	
	Q7F8S5	-	THIOREDOXIN_2	63 – 225	
	Q9SDD6	-	THIOREDOXIN_2	34 – 198	

TABLE 6: CALCULATED SECONDARY STRUCTURE ELEMENTS BY SOPMA

Antioxidant Proteins	CYS PRX			PRDX		
Secondary structure	P0C5C9	Q6ER94	P0C5D1	Q9FR35	Q7F8S5	Q9SDD6
Alpha helix	28.64%	31.42%	25.91%	30.25%	33.33%	28.79%
310 helix	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Pi helix	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Beta bridge	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Extended strand	21.36%	16.48%	19.55%	24.07%	25.33%	23.74%
Beta turn	6.36%	6.51%	6.36%	4.32%	4.89%	6.57%
Bend region	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Random coil	43.64%	45.59%	48.18%	41.36%	36.44%	40.91%
Ambiguous states	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Other states	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%

Three dimensional structures for these proteins are not yet available in PDB databases. Three dimensional structures were modeled for all six proteins. The modeling of the three dimensional structure of the protein was performed by homology modeling programs, Swiss Model and Modeller 9.11.

The constructed three dimensional models were energy minimized in GROMACS force field using steepest descent minimization Algorithms. The psi and phi distribution of the Ramachandran Map generated by of non-glycine, non proline residues were summarized in **Table 7**. The final modeled structures were visualized by Rasmol that was shown in **Figure 1**.

TABLE 7: RAMACHANDRAN PLOT CALCULATION AND COMPARATIVE ANALYSIS OF THE MODELS FROM SWISS-MODEL AND MODELLER 9.11 COMPUTED WITH THE PROCHECK PROGRAM

Server	Antioxidant Proteins	CYS PRX			PRDX		
		P0C5C9	Q6ER94	P0C5D1	Q9FR35	Q7F8S5	Q9SDD6
Swiss Model	Residues in the most Favored Region	89.60%	86.60%	84.70%	88.10%	82.00%	79.60%
	Residues in additionally allowed Region	9.30%	12.80%	13.70%	11.90%	16.50%	16.20%
	Residues in generously allowed Region	0.50%	0.00%	1.60%	0.00%	0.70%	4.20%
	Residues in disallowed Region	0.50%	0.60%	0.00%	0.00%	0.70%	0.00%
Modeller 9.11	Residues in the most Favored Region	89.60%	90.60%	88.10%	92.60%	82.70%	86.00%
	Residues in additionally allowed Region	9.30%	8.50%	11.40%	7.40%	11.70%	8.70%
	Residues in generously allowed Region	1.10%	0.40%	0.50%	0.00%	4.10%	4.10%
	Residues in disallowed Region	0.00%	0.40%	0.00%	0.00%	1.50%	1.20%

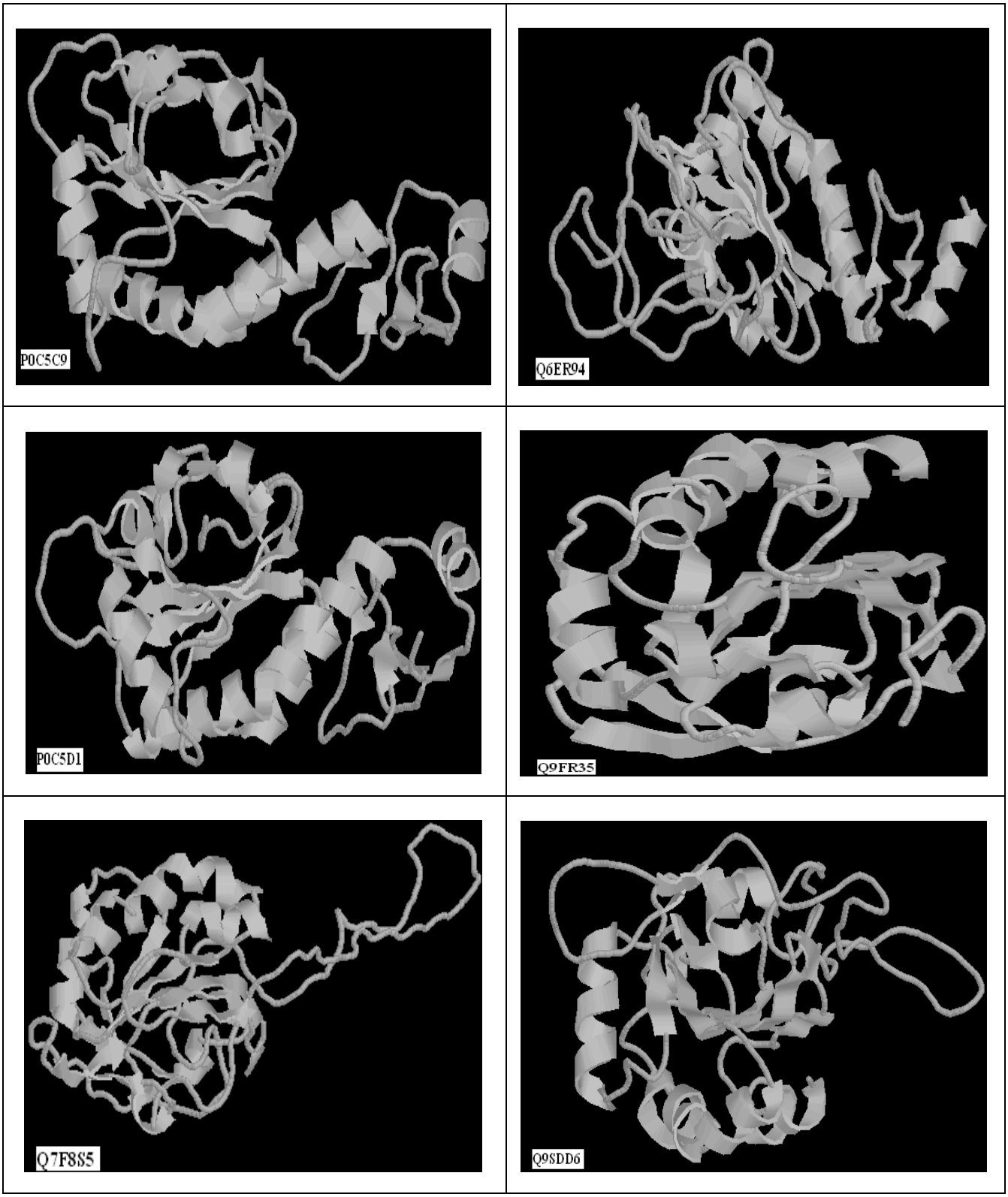

FIGURE 1: MODELED STRUCTURE OF RICE PROTEINS

The stereo chemical quality of the predicted models and accuracy of the protein model was evaluated after the refinement process using Ramachandran Map calculations computed with the PROCHECK program.

The assessment of the predicted models generated by Modeller 9.11 was shown in **Figure 2**. In the Ramachandran plot analysis, the residues were classified according to its regions in the quadrangle.

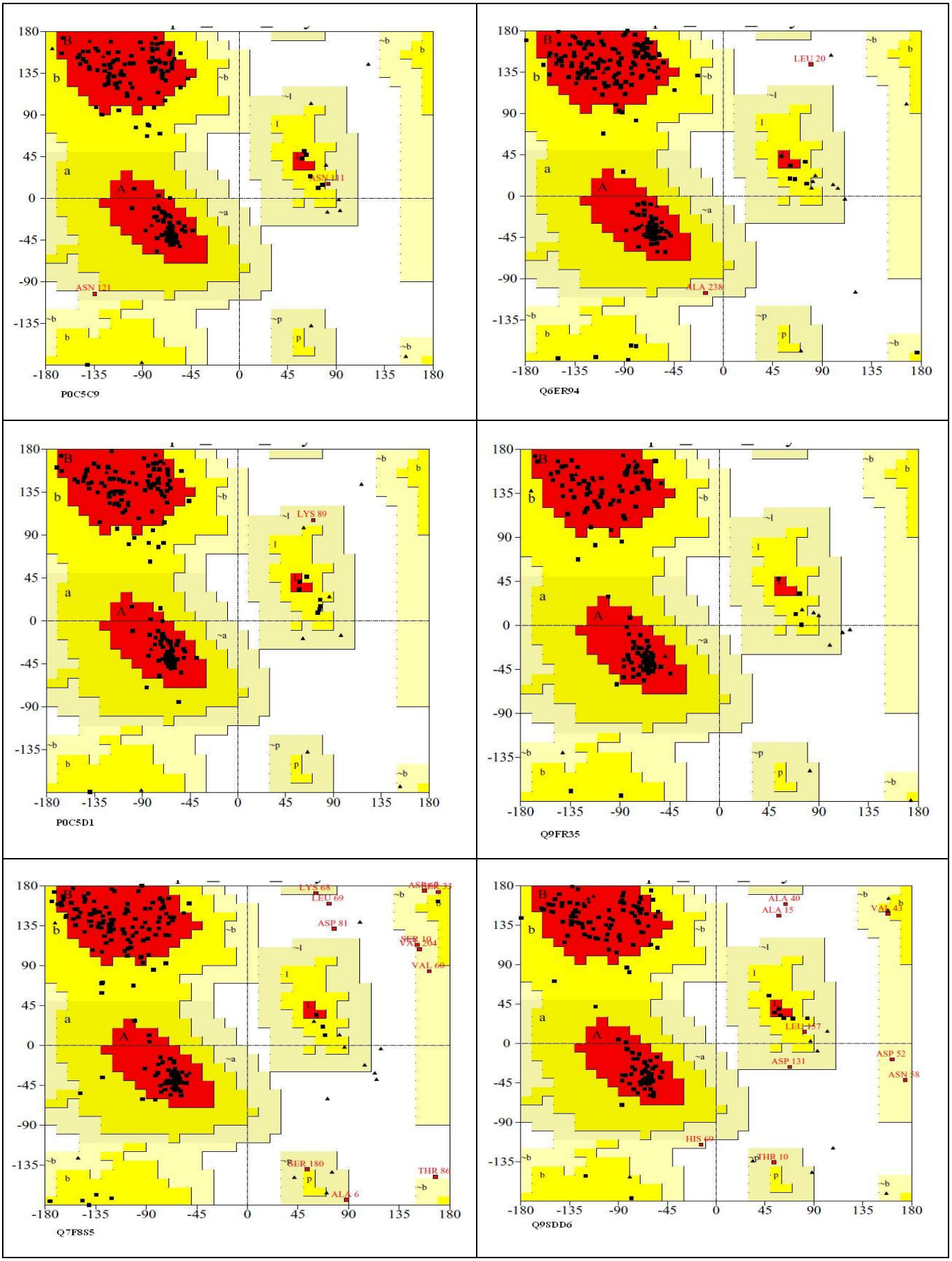

FIGURE 2: RAMACHANDRAN'S MAP OF RICE PROTEINS

The red regions in the graph indicate the most allowed regions whereas the yellow regions represent allowed regions. Glycine is represented by triangles and other residues are represented by squares. The result revealed that the modeled structure for P0C5C9, Q6ER94, P0C5D1, Q9FR35, Q7F8S5 and Q9SDD6 has 89.6%, 90.6%, 88.1%, 92.6%, 82.7% and 86.0% residue respectively in allowed region. Such figures assigned by Ramachandran plot represent a good quality of the predicted models.

The modeled structures of rice antioxidant proteins were also validated by other structure verification servers WHAT IF. Standard bond angles of the six models are determined using WHAT IF. The results were shown in **Table 8**. The analysis revealed RMS Z-scores were almost equal to 1 suggesting high model quality. The predicted structures conformed well to the stereochemistry indicating reasonably good quality.

TABLE 8: RMS Z-SCORE FOR BOND ANGLES OF MODELED PROTEIN STRUCTURE USING WHAT IF.

Antioxidant Proteins	Accession No.	RMS Z-score for bond angles
CYS PRX	P0C5C9	1.291
	Q6ER94	1.332
	P0C5D1	1.254
PRDX	Q9FR35	1.273
	Q7F8S5	1.850
	Q9SDD6	1.342

CONCLUSION: In this study, antioxidant proteins of rice (*Oryza sativa subsp. japonica*) were selected. Physico- chemical characterization were performed by computing theoretical isoelectric point (pI), molecular weight, total number of positive and negative residues, extinction coefficient, instability index, aliphatic index and grand average hydropathy (GRAVY). Functional analysis of these proteins was performed by SOSUI signal server. For these proteins disulphide linkages, motifs and profiles were predicted.

Secondary structure analysis revealed that random coils dominated among secondary structure elements followed by alpha helix, extended strand and beta turns for all sequences. The modeling of the three dimensional structure of the proteins were performed by automated homology programs, Swiss model and Modeller 9.11. The models were validated using protein structure checking tools PROCHECK and WHAT IF. These structures will provide a good foundation for functional analysis of experimentally derived crystal structures.

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