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Novel insight into the molecular interaction of catalase and sucrose: A combination of *in silico* and *in planta assays* study

Sunil Kumar[a,*], Khurshid Ahmad[a], Gitanjali Tandon[b], Udai B. Singh[a], Yachana Jha[c], Dipak T. Nagrale[a,d], Mahender Kumar Singh[e], Khyati Girdhar[f], Prosenjit Mondal[f,*]

[a] *ICAR-NBAIM, Kushmaur, Mau, UP 275103, India*
[b] *SHUATS, Allahabad, India*
[c] *N. V Patel College of Pure and Applied Sciences, V.V Nagar, Anand, Gujarat 388120, India*
[d] *ICAR-CICR, Nagpur, India*
[e] *NBRC, Maneser, India*
[f] *IIT Mandi, Mandi, HP 175001, India*

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ABSTRACT

Osmolytes are known to be an important factor for the stabilization and proficient functioning of proteins. However, the stabilization mechanism of proteins by the interaction of osmolytes is still not well explored. Here, we performed *in silico* 3D structure modelling of rice catalase-A (CatA) protein and its molecular interaction with sucrose. Further, *in planta* was conducted to see the effects of sucrose on catalase activity in rice grown in saline sodic soil at different time intervals. The molecular docking experiments results showed that sucrose can be ligated with CatA, protein forming hydrogen bond with precise amino acid residues like, R49, R89, P309, F311, Y335 and T338. The interaction also comprises the contribution of hydrophobic amino acid residues like V50, V51, H52, L123, A310, Q339 and R342. The *planta in vitro* catalase activity assay showed that plants treated with sucrose significantly affect the catalase activity in rice. Results revealed that maximum catalase activity was recorded in plants treated with 150 and 200 ppm of sucrose after 15 days of sucrose application. However, minimum activity was recorded in control plants. We believe that our study will provides an advanced understanding of catalase activity in plants exposed to osmotic stress.

1. Introduction

In living organisms, the interaction of carbohydrates with protein play key role in a wide range of biochemical processes that remain linked to hormones, enzyme, antibodies etc. having importance in the field of immunology, bio-synthesis, pharmacology and medicine (Metzler, 2003). These interactions also hold importance in plant response to biotic and abiotic stress, salt-stress in particular.

Salinity in the form of both hyper-osmotic and hyper-ionic stresses imparts a major threat toward crop productivity. Extensive research has been conducted to investigate the molecular mechanism for control of this stress factor (Arora et al., 2002; Foyer and Noctor, 2000; Mittler, 2002). It has been proven that salt can induce oxidative stress (Scandalios, 2005) leading to accumulation of Hydrogen peroxide (H_2O_2) in the cell organelles. H_2O_2, relatively a stable oxy-molecule if remain un-scavenged can also become deleterious to plant metabolic activity as the peroxide can undergo chemical modification producing other highly reactive oxy-radicals that can react with cellular constituents like lipids, proteins, nucleic acids etc. (Foyer and Noctor, 2003). In order to overcome the deleterious effect of H_2O_2, plants in coordination with several non-enzymatic scavengers (ascorbate, tocopherol, carotenoids etc.) also employs a group of enzymatic scavengers like catalase, peroxidase and other substrate specific peroxidases (ascorbate peroxidase, glutathione peroxidase etc.) to scavenge H_2O_2 in order to maintain the cellular concentration of peroxide to a level having its physiological significance (Willekens et al., 1997).

Among the various H_2O_2 scavenging enzymes, catalase having a low affinity for its substrate (high *Km*) but with significantly high processing rate (conversion of H_2O_2 to H_2O and O_2) plays a central protective role against oxidative stress developed by salt-induced accumulation of H_2O_2. However, literature reports suggest that catalase is highly susceptible to salt-stress where its activity is down regulated (Cavalcanti et al., 2004; Lee et al., 2001; Nishikawa et al., 2004; Shim et al., 2003; Valluru and Van den Ende, 2008). As expected Sahu et al. (2010) have shown a declined rice leaf catalase activity under elevated salt-treatment, however, surprisingly, supplementation of sucrose significantly

* Corresponding authors at: IIT Mandi, HP 175001, India (P. Mondal). ICAR-NBAIM, Kushmaur, Mau, UP 275103, India (S. Kumar).
E-mail addresses: skybiotech@gmail.com (S. Kumar), Prosenjit@iitmandi.ac.in (P. Mondal).

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rescues salt mediated decay in catalase activity. The investigation also evidenced that catalase in rice leaf interacts with sucrose under *in vivo* condition and renders a protective role in maintaining high enzymatic activity thus acting as the principal enzymatic source for scavenging the stress induced production of H_2O_2 (Sahu et al., 2010).

Although, the exact mechanism of interaction of sucrose with enzyme protein(s) is yet to be deciphered, it has been conclusively shown that sucrose can substantially protect the inactivation of enzymatic activity of many proteins during stress insult to organisms (García et al., 2007). In order to get some further insight into the interaction of sucrose with catalase an attempt has been made here to develop a 3D *in silico* model of rice Cat-A and the study has been extended to examine the interaction of sucrose with the enzyme protein. The best validated model was further subjected to molecular dynamics simulation to study dynamic behavior of the proteins. Further, effects of sucrose on CatA activity were evaluated in rice under saline sodic soil.

2. Material & method

2.1. Domain architecture of catalase-A (Cat-A)

The protein sequence of CatA was reported earlier, and retrieved from the NCBI (ID: ABN71233) for the present investigation. The functional domains of Cat-A protein were inferred using Conserved Domain Search Service (CD Search) (Marchler-Bauer et al., 2016), Pfam database (Finn et al., 2016) and Simple Modular Architecture Reseach Tool (SMART) (Letunic et al., 2014). ProtParam predicted various physio-chemical properties of Cat-A.

2.2. 3D structure Generation, refinement and validation

It was verified that the three-dimensional (3D) structure of the CatA protein has not yet reported in the protein data bank (PDB). Therefore, we developed the 3D model of CatA protein. BLASTP (Altschull et al., 1990) search was performed against PDB (Berman et al., 2006) to find the appropriate homologous templates for structure modelling. CatF (PDB code: 1m7s) was showing best homology with target sequence. The sequence identity was found to be 43 per cent between the template (1m7s) and (CatA) target sequence. The ClustalW (http://www.ebi.ac.uk/clustalw) (Thompson et al., 1994) program was applied for sequence alignment between CatA and 1m7s.

MODELLER (http//:www.salilab.org/MODELLER) (Šali and Blundell, 1993) was used for the development of 3D structure. The MODELLER utilizes 'probability density functions' as the spatial restraints (Sali et al., 1993; Šali and Overington, 1994). In MODELLER, python script with automodel class was used for constructing the models (Eswar et al., 2006). Total twenty models of 3D structure were generated and later discrete optimized protein energy (DOPE) scores were calculated for each model using normalized DOPE assessment method available in MODELLER. DOPE score allots a score for each model by scrutinizing the positions of all non-hydrogen atoms, with lower scores predicting more accurate models. We also calculated Ramachandran plot for all the 20 models and based on maximum residues in the favored region and less in disallowed region were selected for further course of action. Finally, CatA models with lowest DOPE value were validated by PROCHECK (Laskowski et al., 1993) and VERIFY3D (Eisenberg et al., 1997) and ERRAT was further subjected to energy minimization using CHARMm (Brooks et al., 1983) force field. The energy-optimized models of CatA were verified for stereo-chemical quality using SAVeS server (http://nihserver.mbi.ucla.edu/SAVES/). ProSA-web (Wiederstein and Sippl, 2007) was used to calculate the energy potential of the model. This model was further used for docking studies with Sucrose using GOLD docking program.

2.3. Molecular dynamics simulations

To study the dynamic properties, MD simulation for the protein–ligand complex (catalase-sucrose) was carried out with the GROMACS 4.6.4 (Hess et al., 1997) package using the GROMOS96 54a7 (Oostenbrink et al., 2004) force field. The conformation with lowest binding energy was used as the initial conformation for MD simulations. First the topology of the protein was created by using the Gromacs program while for creating sucrose topology was created using PRODRG (http://davapc1.bioch.dundee.ac.uk/cgi-bin/prodrg). The complex was immersed in dodecahedron box of simple point charge (SPC) water molecules. The solvated system was neutralized by adding counter-ions. Energy Minimization of the solvated structures was done using steepest descent and conjugate gradient algorithm till maximum force reached below 100KJ/mol/nm. To equilibrate, the system was subsequently subjected to the position-restrained dynamics simulation (NVT and NPT) at 300 K for 100 ps. Finally, this system was subjected to MD production run for 100 ps at 300 K temperature and 1 bar pressure as our previous work (Tandon et al., 2015).

For trajectory analysis, various parameters were computed using GROMACS. These included Root Mean Square Deviation (RMSD), Root Mean Square Fluctuation (RMSF) and Potential energy. Principal Component Analysis (PCA) was also performed to explore the global motion of the coordinates of atoms of the Catalase-Sucrose complex during MD Simulations. PCA can characterize the cumulative and overall motion of the system. PCA calculations were examined by using g_covar and g_aneig functions of GROMACS. Our analysis was restricted to Cα atoms, as it is less disturbed by statistical noise.

2.4. Study of protein – ligand interaction

The structure of sucrose molecule was fetched from pubchem (PubChem CID:5988) (http://pubchem.ncbi.nlm.nih.gov) in 2D-strucuture data file (SDF) format and converted into 3D-Mol2 file with the program CORINA2.6 (Hagler et al., 1974; Tetko et al., 2005). Energy minimization and ligand preparation was further performed using Discovery studio suit. Ten pockets were recognized on the modelled 3D structure of CatA protein using Q Site-Finder tool. Molecular docking study was executed using GOLD (Genetic Optimization Ligand Docking) Software. The docking parameters were set with reference to earlier studies (Afiqah et al., 2016; Fazil et al., 2012). GOLD uses a genetic algorithm (GA) to explore the full range of ligand flexibility of conformation with partial flexibility of the protein (Jones et al., 1997). The binding affinity was also estimated by using the consensus scoring function X-Score V2.1 (Wang et al., 2002). LIGPLOT (Wallace et al., 1995) was used to show 2d binding of protein ligand complex. GETNEARES tool (available with the program DOCK) was applied to double-check the hydrogen bond interactions (Ewing et al., 2001).

2.5. In planta assay

2.5.1. Planting material, growth conditions and experimental design

Rice seeds (*cv.* Pusa Basmati 1) were obtained from Farm Section, ICAR-Indian Institute of Seed Science, Kushmaur, Maunath Bhanjan, U.P., India. Seeds were planted in pots under nethouse conditions. Each pot containing 5 kg of experimental soil (pre-sterilized). The basic property of soil is saline sodic with pH 8.2 and EC 1.82. Experiments were conducted during August - September with relative humidity of 90% and average mean temperature of 31.25 °C.

The experimental design consisted of five different treatments where plants were treated with different concentration of sucrose (50, 100, 150 and 200 ppm) and absolute control (untreated). Ten seeds were sown in each pot. The moisture content in the pots was kept at field capacity (60%) by sprinkling with sterilized water on every alternate day. After thirty days of sowing, plants were treated with different concentration of sucrose solution at 5 ml per plant in the evening

hour (16:00 hrs).

2.6. Estimation of catalase activity

The effects of different concentration of sucrose were evaluated in terms of changes in the accumulation and activity of catalase in plant leaves. The catalase activity was measured following the methods of Sadasivam and Manickam (1996) with slight modification (Sharma and Dubey, 2007) at 7, 15, 30 and 45 days after sucrose application (DASA). The rate of H_2O_2 decomposition was measured at 240 nm (extinction coefficient of 0.036 mM^{-1} cm^{-1}) and enzyme specific activity was expressed as µmol H_2O_2 oxidized min^{-1} mg^{-1} protein.

2.7. Statistical analysis

Nethouse experiments were carried out in randomized block design (RBD) and the experimental data were subjected to analysis of variance (ANOVA) or Duncan's Multiple Range Test (DMRT) using Statistical Package for Social Sciences Version 16.0 (SPSS 16.0) programme. Data were compared with DMRT at $p \leq 0.05$.

3. Results & discussion

3.1. Domain organization of Cat-A

To understand the domain architecture of Cat-A, the primary amino acid sequence was subjected to various domain prediction servers. The pfam database and CD search classified Cat-A into the Catalase family. This family signifies a tiny conserved region within catalase enzymes (EC: 1.11.1.6). Catalase are known to decompose hydrogen peroxide (H_2O_2) into water and oxygen, helping to protect the cells from its toxic effects (Bai and Cederbaum, 2001). This domain is having the immune-responsive amphipathic octa-peptide, recognized by T cells (Guy et al., 2005).

3.2. Modelling and refinement

The 3D structure of the CatA protein in rice has not been determined yet experimentally nor by X-ray crystallography nor via NMR. Thus, we built a 3D model using homology modelling approach. BLASTP search against PDB resulted CatF (PDB ID: 1M7S) (Carpena et al., 2003) as the template for homology modelling. It exhibits 43% identities and 95% query coverage. Sequence alignment between CatA and 1m7s was done using ClustalW program (supplementary Fig. 1). The alignment is characterized by a number of insertions and deletions in the loop regions of protein. Since the first 13 residues from the N-terminal end did not have matching regions in 1m7s, the modelling was performed from the 14th to 479th residues, followed by a thorough refinement of the generated models by means of energy minimization using CHARMm (Brooks et al., 1983) force field. Based on the target-template alignment, Modeller facilitated in the development of three dimensional protein models, among which the best model (with lowest DOPE score) was refined and subsequently considered for model validation by using several model validation tools. The PROCHECK was employed to assess the quality of the protein stereochemistry i.e distribution of dihedral angles (φ and ψ) of each amino acid through Ramachandran plot. Ramachandran plot of the predicted model showed good stereo chemical properties with 90.1% residues in most favoured and 8.9% allowed regions with overall G-factor of -0.11. The final stable structure of catA contains 13 helices and 10 sheets. The VERIFY 3D environment profile was satisfactory. The energy profile analysis performed by ProsA showed Z-score of -5.92, which were in agreement with that of the experimental PDB structures of similar size. The overall ERRAT value was 65.11 above cut-off value of 50. The structural superimposition of C^{α} trace of the model over 1m7s was done using CE Program (http://cl.sdsc.edu) resulting in a small root mean square deviation (RMSD) of 2.13 Å shown, in which indicate a valid structure of the model and could be employed for the further docking study. The amino acid sequence alignment between the template and final model of CatA were generated using CLUSTALW program. The secondary structures were analyzed and compared by the JOY (Mizuguchi et al., 1998) server (protein sequence-structure representation and analysis) and it was found that the secondary structures of template and final catA are highly conserved, which showed that final model is highly reliable as shown in Fig. 1. Overall keeping stereo-chemical qualities, energy profile and other parameters into consideration, the projected model was found to be of good quality.

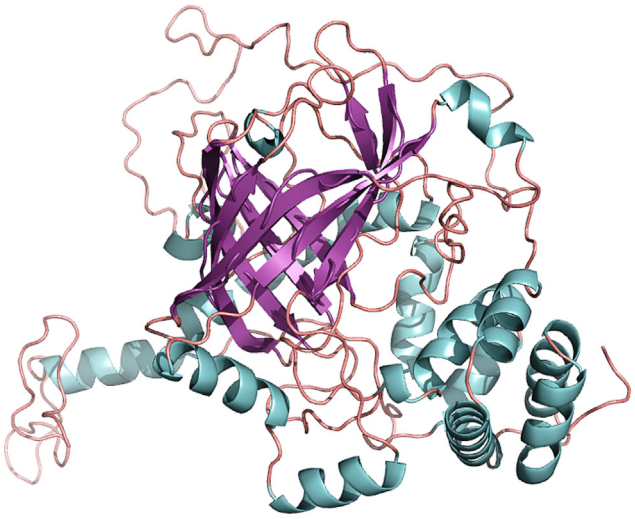

Fig. 1. 3D structure of CatA protein (Cartoon view).

3.3. Molecular dynamics simulation

We carried out the MD simulations for ligand-bound protein complex (catalase-sucrose complex) using GROMACS package through GROMOS force field parameters. To explore the dynamics and stability of the system, RMSD profile, Cα-RMSF and energy were analyzed from the resultant MD trajectories using GROMACS utility toolkits. For this, the complex was put into dodecahedron box solvated with water. To neutralizing the system, five Na^+ counter-ions were added. After completion of final simulation of 50 ns, stability patterns of the complex were studied using various functional packages of MDS analysis available in GROMACS. To access the dynamic stability of system, RMSD profile for backbone residues were generated and plotted against time scale of 50 ns (Fig. 2). Root Mean Square Deviation (RMSD) signifies the

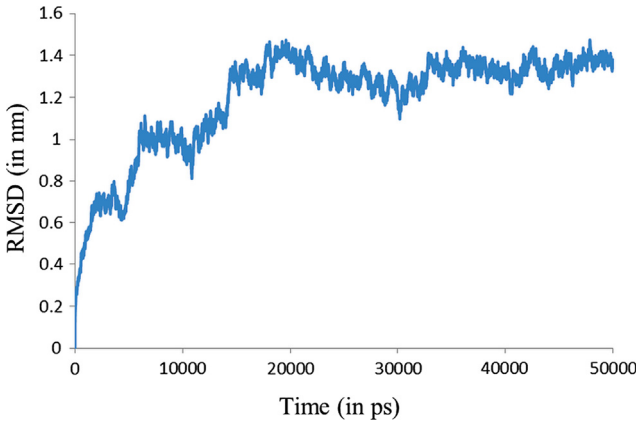

Fig. 2. Conformational stability of catalase sucrose complex at 50 ns time duration.

change in the protein structure during simulations. Larger changes indicate that protein might have undergone larger conformational change (Maiorov and Crippen, 1994). After 50 ns, the average RMSD value for Complex was 11.9 Å, which depicts that there have occurred large conformational changes during simulation of this complex. The backbone RMSD of the complex followed a stable deviation up to 20 ns and afterward it was stable. From RMSD profile, it can be observed that the system was well equilibrated and portrays a minimal deviation with RMSD which highlights the stable nature of the complex.

Another parameter Root Mean Square Fluctuation (RMSF) was calculated to study the deviation between the positions of the atoms. It basically provides a trajectory for each residue in the protein (Fuglebakk et al., 2012). It showed that the maximum peaks in the graph possess a value of 0.325 nm. The result indicates that the ligand-bound protein complex was stable throughout MD simulations and thus ligands possess the ability to stably bind to the protein. The average trajectories of all the atoms were observed as 0.325 nm while the detail wise trajectory is given in the Fig. 3. One more important parameter that was considered is the potential energy. Change in potential energy was studied from the time at t = 0 ns till time at t = 50 ns. At time t = 0 ns potential energy of Complex was -2306646.00 KJ/mol which changed to -2317395.75 KJ/mol when time changed to 50 ns (Fig. 4).

The activity of atoms of complex was correlated with essential dynamics calculations that greatly influence the overall motion of the complex. Structural rearrangements are important for proper signalling (Maisuradze et al., 2009). Dynamic cross-correlation conducted to study the motion of residues is shown in Fig. 5. The value of correlation lies between −1.17 ([1]blue) to 2.98 (red) which represents negative and positive correlation respectively (As shown in Fig. 5). This figure represents the matrix showing covariance between Cα atoms. Red means two atoms move together so that they lie mostly on the diagonal while blue means they move in opposite directions.

3.4. Docking simulation

Docking with sucrose was performed on the binding site of CatA in rice using GOLD software using default parameters with fifty GA runs. The GOLD fitness function includes four components: (a) protein-ligand hydrogen bond energy (external H-bond); (b) protein-ligand vanderwals (vdw) energy (external vdw); (c) ligand internal vdw energy (internal vdw); (d) ligand torsional strain energy (internal torsion). To validate the estimations computed by the GOLD program, we used X-Score, a consensus scoring program. The scoring function used in X-Score computes a binding score for input protein-ligand complex structure, and this binding score correlates to experimental binding constants. The sucrose-CatA complex has best GOLD fitness value of 16.09 from fifty genetic algorithm runs. The predicted binding energy for the docked complex is −6.51 kcal/mol and predicted average −log Kd is 4.77 using X-Score program. Ligplot (Fig. 6) shows hydrogen bonding (R49, R89, P309, F311, Y335 and T338) and hydrophobic interacting residues (V50, V51, H52, L123, A310, Q339 and R342) with the sucrose ligand in the binding site of CatA protein in rice.

3.5. Estimation of catalase activity

Plants treated with different concentrations of sucrose under salt stress condition induces metabolic pathways and induced systemic responses that reprogrammed the whole/partial catabolic and metabolic cascade related to salt tolerance and signalling (Kumar et al., 2013; Sahu et al., 2010). It was found that plants treated with sucrose activated stress related cascade and caused manifold increase in the activation of catalase activities (Fig. 7). Quantitative estimation of catalase activity varied significantly in plants treated with different concentrations of sucrose as compared to control (untreated) at different time intervals in glasshouse experiments. Maximum activity was recorded in

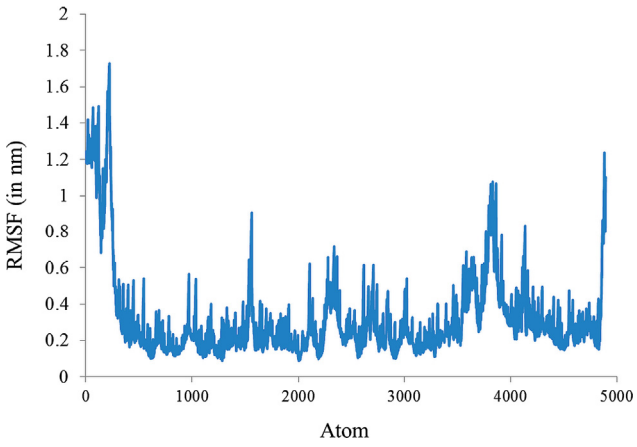

Fig. 3. Cα RMSF profile of catalase sucrose complex during 50 ns MD.

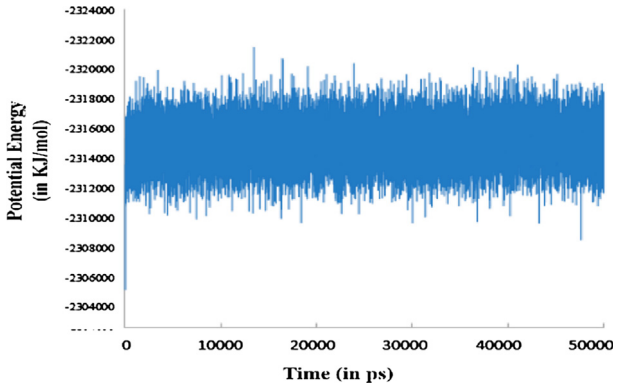

Fig. 4. Energy calculation of catalase sucrose complex.

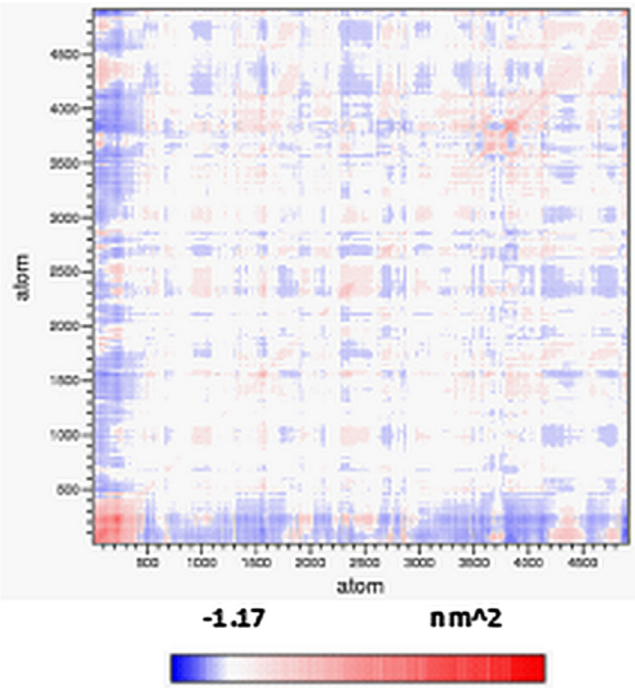

Fig. 5. Essential dynamics of catalase sucrose complex.

[1] For interpretation of color in Fig. 5, the reader is referred to the web version of this article.

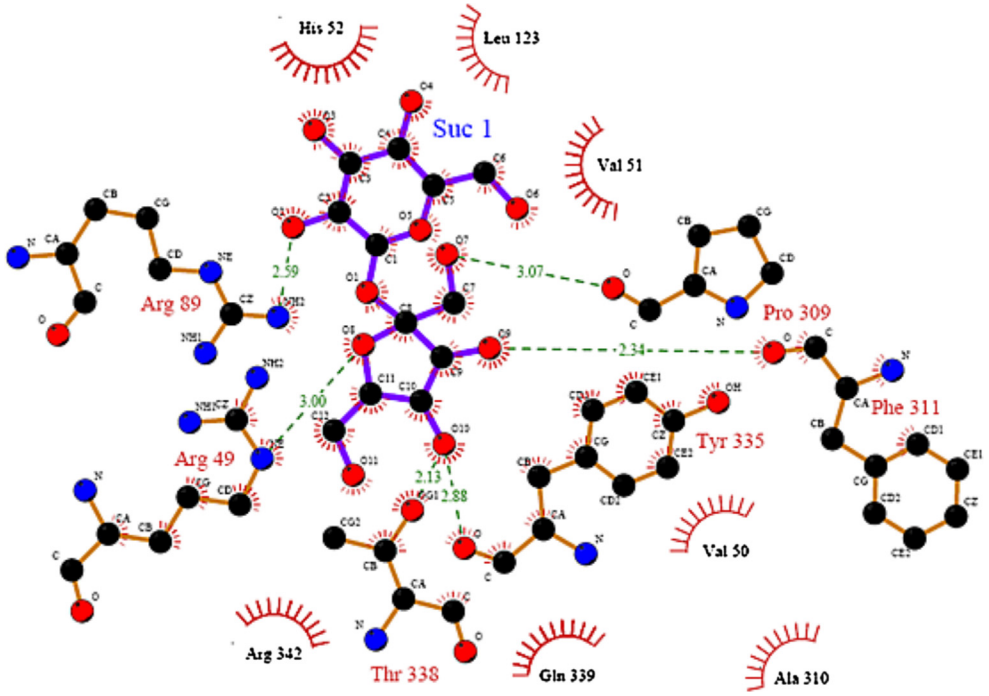

Fig. 6. Molecular interaction between catalase and sucrose.

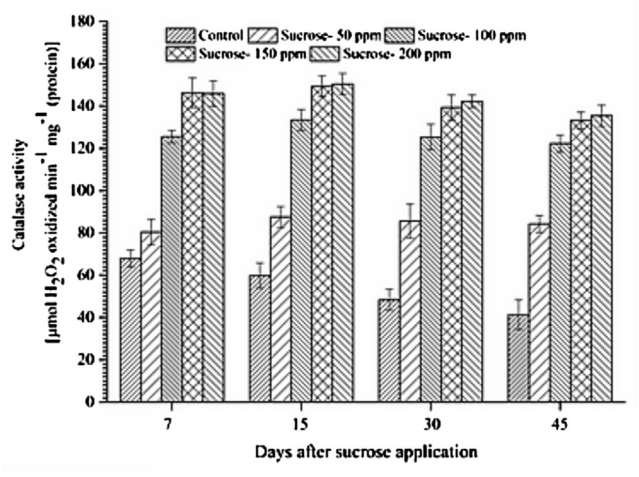

Fig. 7. Quantitative estimation of catalase activity.

the plants treated with 200 ppm of sucrose solution (150.45 µmol H_2O_2 oxidized min^{-1} mg^{-1} protein) followed by 150 ppm (150 µmol H_2O_2 oxidized min^{-1} mg^{-1} protein) at 15 DASA. However, minimum activity of catalase was recorded in the control plants as compared to treated one. Interestingly, it was found that catalase activity showing more or less similar pattern upto 45 DASA, whereas, in control plants the activity was drastically decreasing with the time interval. From the results, it was depicted that sucrose playing an important role in the expression and accumulation of catalase genes in the rice plants under saline conditions. Our results are in consonance with the findings of Kumar et al., 2013, who showed that application of osmolytes induced cascades relating to salt stress and up-regulation of enzymes over a period of time. Also, to respond and adopt to the environmental conditions, plants rely on a diverse array of cell-surface protein-receptors and secondary metabolites (Maisuradze et al., 2009; Sharma and Dubey, 2007). The enzyme components associated with salt tolerance against ROS include SOD, catalase, peroxidase and enzymes of ascorbate_/glutathione cycle. Catalase has been identified as enzymatic protectors against peroxidation reactions (Li et al., 2017).

4. Conclusion

The introduction of sugars and polyhydric alcohols into the solvent medium has been shown to stabilize enzyme molecules in solution by preventing the loss of enzymatic activity by arresting its aggregation and above all by elevating the thermal transition temperature. Sucrose, a dimeric carbohydrate is no exception to this. It is also postulated that the carbohydrate-induced stability to protein molecule is achieved by more than one mechanisms like through its direct bonding interactions, action through effects on structure and properties of the solvent or by the combination of these two mechanisms. Our *in silico* modelling of CatA studies also indicate that the interaction of sucrose with CatA includes both hydrogen bonding with specific amino acid residues in the protein molecule and also hydrophobic interaction with specific amino acid residues which stabilized the protein structure under salt stress conditions. Further, *in planta* evaluation also depicted the same as results achieved *in silico* analysis. Nethouse results showed that maximum enzyme activity was recorded in plants treated with sucrose and the activity remains maintained over period of time under saline sodic soil. These results clearly indicated that sucrose play an important role in stabilization of catalase under salt stress condition in rice. This study opens avenues for researchers to explore the mechanisms and role of sucrose under salt stress.

Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.compag.2018.06.005.

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