In silico molecular modeling and docking studies of Nano Composites compound to Regulation , inhibition and treatment leaf and stem wheat rust

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Abstract
Puccinia graminis f. sp. *tritici* (Pgt) and *P. triticina* (Pt), the causal agents of stem rust and leaf rust, respectively form new physiological races that significantly reduce growth and yield of wheat cultivars. Therefore, seeking for exploring if there an inhibition effect of the Nano Composites compound on leaf and stem rust to Regulation , inhibition and treatment leaf and stem wheat rust to continuously produce new wheat pesticides resistant to stem and leaf rust. In this study we determined the two vital proteins in stem and leaf wheat rust MAP kinase 1 [Puccinia triticina] **and PGTG** *Puccinia graminis f. sp. Tritici* , then we select the natural and Nano Composites compounds to explore the effectively of them in the treatment and inhibition of the wheat rust The aim of the present study was to finding natural and Nano compounds are sheep and natural to control and treatment and Regulation of wheat rust

Keywords: Molecular docking , stem rust, leaf rust, nanoparticle.

Introduction

Wheat (Triticum aestivum) is an important source of food grain domestically and internationally. The demand for wheat particularly for developing countries will grow to 60% by 2050. (FAO, 2016). This increase in wheat demand is very serious especially in light of climate change which would lead to a 29-percent reduction in final productivity (Rosegrant et al. 1995). In addition, three rust diseases, i.e. strip, leaf and stem rust, strike wheat.. Puccinia Graminis Pers later triggered it. f. Sp. sp. tritici (Eriks. & E. henn.) is a devastating disease of wheat plants all over the world, when an outbreak is caused by a disease (Naseri and Sabeti, 20). Wheat stem rust fungus attacks wheat plants, in particular plants which have recently been planted, which block the vascular system, stun and finally cause damage of up to 100% due to grain and tillers (Boukhatem et al 2002 and Kokhmetova et al 2011). The stem rust in local wheat varieties in Egypt are 1.96 to 8.21 per cent (Ashmawy et al 2013). The stem rust disease has another explanation in the last two decades because of the latest Ug99 race. Roughly 90% of the world's weed crop can suffer destructive races (Singh et al. 2011) which lead to losses of yield of up to 70%. (Singh et al. 2006). There were up to 100% reduction in yield losses in Kenya due to stem rust (Njau et al 2010).

In Egypt, up to 95% of local commercial varieties are susceptible or highly sensitive to UG99 race, while only a few older varieties show that there has been some degree of "adult plant resistance" (Wanyera et al 2006 and Njau et al 2010). Over 15 confirmed races of Ug99 were registered recently in Africa (Singh et al., 2015), and quickly spread to other countries of Africa and the Middle East (Yemen, Iraq and Pakistan), Kenya, Ethiopia, Sudan, Tanzania, South Africa, Zimbabwe, Mozambique and Egypt) (Wanyera et al 2006, Nazari et al 2009, Pretorios et al 2010, Wolday et al 2011 and Abou-Zeid et al 2014). It is anticipated It is expected that the Ug99 could be attack cereal gown in another geographical regions around the world in the future.

Rust fungi are one of the most harmful biotrophy pathogens that infect cereal crops and are part of the Puccinia genus. This genus poses a significant threat to worldwide wheat production, which in many parts of the world is a major staple food for mankind. Three main rust pathogens, Puccinia graminis f, are host to wheat. Sp. Sp. Puccinia striiiformis f. (pgt), Pgt. Sp. Sp. The causal agents of stem roast, strip rust and rust leaf respectively are tritiz (Pst) and Puccinia triticina (Pt) (Bolton et al., 2008; Chen et al., 2014; Singh et al., 2011). Wheat leaf rust (WLR) is more commonly found among the three rust-based diseases, wherever wheat is cultivated (Kolmer, 2005). The leaf rust results in greater cumulative annual losses globally as a result of adapting to various climatic conditions and widespread occurrence (Huerta-Espino et al., 2011). Under severe epidemic conditions, Pt can inflict yield losses ranging from 10 percent to 70 percent (Herrera-Foessel et al., 2006).Fungicides are commonly used for rust disease control, but chemical inputs are associated with financial costs and negative environmental effects. Moreover, the high risk of reduced sensitivity or developing resistant pathogens is a key concern in the overuse of antimicrobial

compounds. Thus, the identification of MAP kinase 1 (leaf rust) and PGCTG puccinia grminis f pathogenic proteins. Sp. Sp. Tritici (system rust), which is the subject of leaf and stem rust, is a key research goal nowadays .The Chemical information technology Cheminformatics has evolved in a number of ways to recognize the therapeutic properties of chemical compounds contained in chemical databases or modern Nano Composites.

Materials and Methods

Database Search, Structural Modeling, and Model Validation.

The NCBI (https://www.ncbi.nlm.nih.gov) and uniprot (https://www.uniprot.org/) Protein sequences are accessible. With GenBank accession no in fasta format. Table 2. For the search of NCBI Blast server 1, (Altschul et al., 1997) with standard sequence and non redundant protein sequences, fungal proteins were selected with organism searching for all sequential orthodox and orthodox homologues. The sequences were obtained as an amino acid sequence in FASTA format and are used for the production. The SWISSMODLE server (https://swissmodel.expasy.org/) was used to build a 3D structure. The SWISSMODLE server was used to build a homology model for the fung protein. A sequence of Blast-P similarities was queried with a PDB database 14 to detect close-related structural fungal homologues14 (Berman et al., 2000). In order to classify the models in which the Blast-p annotation was first hit (PDB temple ID, identity, QMEAN). The Protein Data Bank gathered the templates' PDB file (PDB). The alignment data were found by BLAST. With the target sequence file, the alignment file, and the prototype PDB file all temple proteins were started.Model design was conducted with Fungus proteins with a QMEAN score. Furthermore, the protein model with a score below -4 was selected for final confirmation. On the basis of several qualitative backgrounds, including ERRAT and PROCHECK (PDB sum) and Verify-3D, the optimized models MAP kinase 1 (Puccinia triticina) and PGTG Puccinia graminis f. sp Tritici have been found to be adaptable. The Ramachandran plot evaluating residues that lie in favorite regions that the predicted models are nearer to the template (91%, 93%). The score of ERRAT (91.56 %, 78.43 %) and Verify-3D were good enough to demonstrate consistency in the prediction model. The predicted model has been reliable and satisfactory, since the ideal score values for the Verify-3D were 80% for a model with a good resolution and around 95 percent for the ERRAT (Colovos and Yeates, 1993).

Preparation of Protein and Ligands

The fungal protein has been chosen as a target receptor protein and imported into the3Drefine server to minimize the power of 2 proteins for pre-docking (http://sysbio.rnet.missouri.edu/3Drefine/); all molecules of water and ligands were taken off while the hydrogen atoms were applied to the target protein. The system for docking was designed using software SAMSON 2020 (https://www.samson-connect.net). And then the SAMSON imported The structures have been developed with the Autodock Vina expansion protein preparation wizard. The use of software from SAMSON 2020. A receptor grid X, Y and Z protein values in table 2 were created in order to investigate the effect of the ligands on protein best on the blind docking.The ligand (chitosan) were retrieved from the PubChem database. and the chitosan with CU are prepared and designed in chemdraw **https://www.perkinelmer.com/category/chemdraw**) in pdb format, then converted into MOL2 format by using openbable software (**http://openbabel.org/wiki/Main_Page). then** The energy minimization was done at neutral pH 7.0 ± 2.0.in SAMSON software.

Binding site prediction, Protein-ligand docking

For predicting the binding site, Discovery studio is used. It is able to identify powerful binding places using the energy interplay between the protein and a simple van der waals probe. AutoDocking Vina is used by this program to increase the accuracy of these forecasts while reducing machine time (Trott e al., 2010). The software functions on the basis of quantum mechanics. It predicts the possible affinity, molecular structure, structure geometry optimization, atom coordinate vibrations frequencies, bond length and bond angle. After the exhaustive investigation, 100 poses were analyzed to measure the ligand's binding affinity using the best scoring poses. The ligands that tightly bind to target protein with high score were selected **Table2** The proteins were docked against the compounds chitosan and cu using SAMSON software (https://www.samson-connect.net/).[15] The interaction was carried out to find the favorable binding geometries of the ligand with the proteins by using Discovery studio software to get the interaction of the Docked protein ligand complexes with high score to the predicted active site.

Protein ligand interaction using SAMSON and Discovery studio software

The ligands were docked with the target protein, and the best docking poses were identifying. Figures 3-4 shows 3D structure of the binding poses of the compounds with the interacting residues of the active site of the proteins

Results

Database Search, Structural Modelling, and Model Validation.

the homology of the query protein sequences with the target proteins from pdb . The query coverage of proteins sequences showed MAP kinase 1 [Puccinia triticina] **and PGTG** *Puccinia graminis f. sp. tritici* (84% , 12) query coverage's with (56.14 , 56.15) identity with the template proteins (2vkn.1.A , 2fa2.1.A) they used as a template proteins for homology modeling of our target proteins

Protein	GenBank/ID:	Template	Seq Identity	Coverage	QMEAN
MAP kinase 1 [Puccinia triticina]	AAY89655.1	2fa2.1.A	56.14	0.84	-1.53
PGTG *Puccinia graminis f. sp. tritici*	10532062	2vkn.1.A	56.14	0.12	-0.69

Table 1 show the proteins with their GenBanck id with the template proteins with there sequence identity with quarry coverage of the our protein with the template proteins with the validation method which is QMEAN.

Structural Modeling, in silico Characterization, and Model Validation

The SWISSMODLE server generated (25 ,35) predictive models for MAP kinase 1 [Puccinia triticina] **and PGTG** *Puccinia graminis f. sp. tritici* proteins with different (QMEAN) score values. The model with low values for QMEAN score(-1.53 and -0.69) were selected as a final model for *in silico* characterization and docking studies. The selected model was verified for their stereochemical quality assessment. Furthermore, in each case of qualitative assessment, a comparative study was done with experimentally solved crystal structures, to check the quality, reliability, accuracy, stability and compatibility of the computationally predicted protein. The Ramachandran plot obtained through The PROCHECK module of the PDBSum server revealed that the predicted model

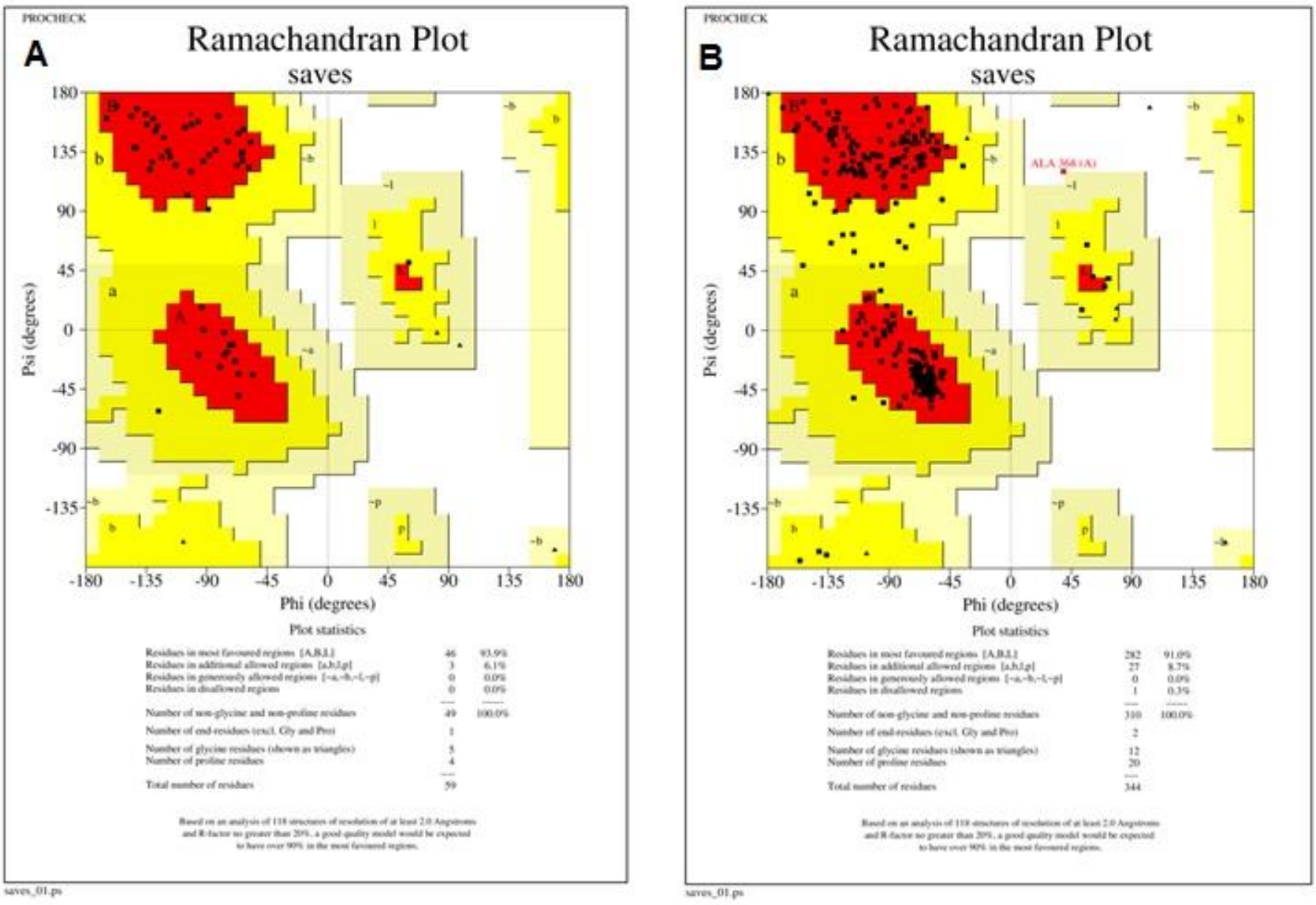

Fig .1. Ramachandran plot based on The PROCHECK module of the PDBSum server for proteins models of MAP kinase 1 [Puccinia triticina] **(A) and PGTG** *Puccinia graminis f. sp. Tritici* (B)

The PROCHECK module of the PDBSum server, further justified the stereochemical goodness of the predicted models MAP kinase 1 [Puccinia triticina] **and PGTG** *Puccinia graminis f. sp. Tritici* , with 91% , 93% residues accommodating in the most favored regions (A, B, and L) and only 8.7% , 6.1 % residues occupied in the additionally allowed regions (a, b, l, and p) representatively .This confirms the predicted models quality MAP kinase 1 [Puccinia triticina] **and PGTG** *Puccinia graminis f. sp. tritici* had good stereochemical quality and was close to the template structure. the ProQ is a neural network-based predictor based on a number of structural features predicts the quality of protein model. The ERRAT score for the modeled structure was found to be 96.22% , 78.4314 representetevely The Verify 3D evaluated that the predicted proteins MAP kinase 1 [Puccinia triticina] **and PGTG** *Puccinia graminis f. sp. tritici* have 96.22% , 81.36% of the residues have averaged 3D-1D score >= 0.2 **Pass** At least 80% of the amino acids have scored >= 0.2 in the 3D/1D profil

Binding site prediction, Protein-ligand docking

The predicted model was visualized through the visualization module of the Discovery Studio 3.0 (Figure 2). The ligand binding sites identified in the target proteins structure .

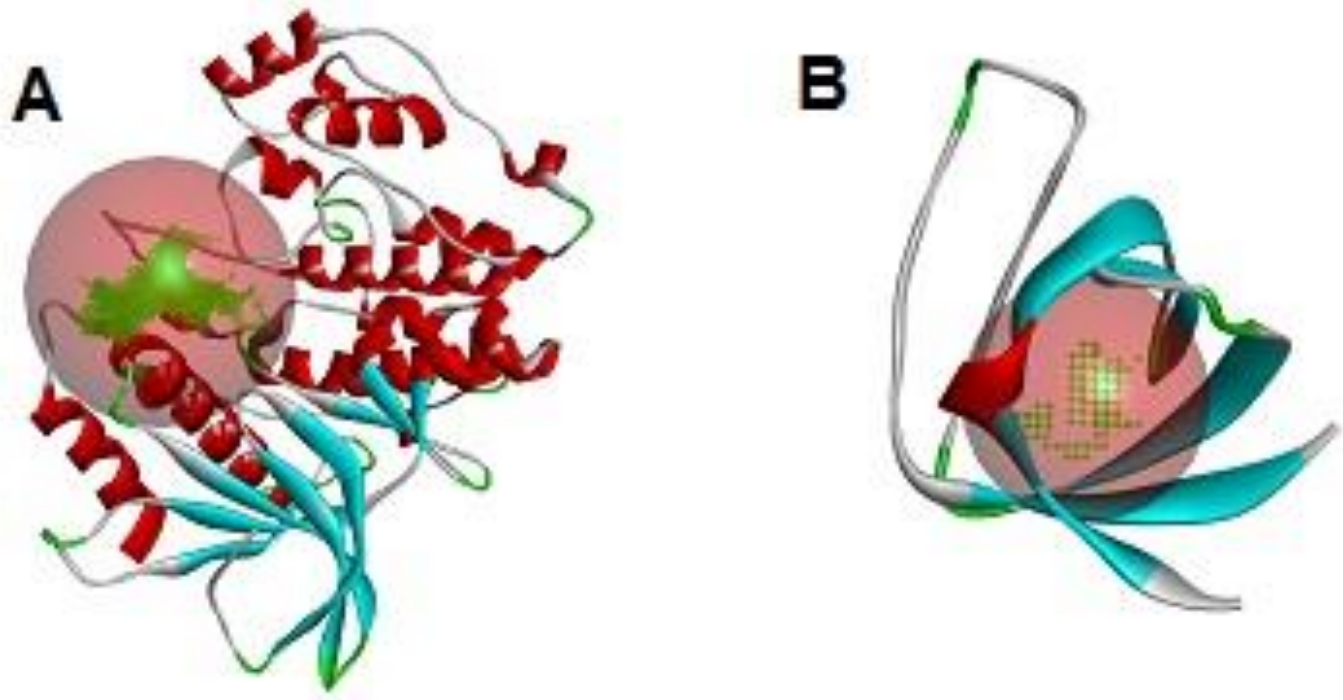

Fig 2 represent the binding site of the MAKP1 of the fungus and B its the PGTG protein The binding sites inside the proteins, the protein with red balls showing active sites

Active Site Prediction and Protein–Fungicide Interaction

Discovery studio software identified the supposed ligand binding sites (major and minor) for the predicted protein. With all the chitosan and chitosan cu mode the modeled proteins MAPK1 and PGAT were combined to provide their binding mode to refine the optimum position by changing conformationally the MAPC1 and PGAT systems.Our study software has assessed the interaction of protein fungicides. The result of the tool has been shown to be discrepant in the predictions for precise posing between the various supposed docking positions, which can lead to the conclusion that the docking scores are accurate to show the protein binding affinity (Suenaga et al., 2012).

Target	Ligands	Binding energy	X,Y , Z value
MAP kinase 1 [Puccinia triticina]	Chitosan	-6.6	center_x = 8.6875 center_y = 7.9130 center_z = 26.0847
	cu-chitosan	-6.9	
PGTG *Puccinia graminis f. sp. tritici*	Chitosan	-4.6	center_x = 11.3055 center_y =22.877 center_z = 1.3282
	cu-chitosan	-5.6	

Table 2 Docking score and molecular properties of bioactive and Nano Composites compounds

The MPAK1 its bind to chitosan with ΔG_{bind} and docking score are -6.9 kcal/mol with the interactive binding site residues (ARG106 , ASP192 , GLU210 , GLY212 , LEU213 , GLU223 , THR224 , GLY225 , MET227 , VAL231 , ALA232 and ARG234) , for the MPAK1 with chitosan -CU the ΔG_{bind} are -6.6 kcal/mol with the interactive binding site residues (ARG106, LYS194, GLU223, MET227, GLU229, VAL231, ALA232, GLN247 and GLY273) . then the PGAT its bind to chitosan with ΔG_{bind} -4.6 kcal/mol with the interactive binding site residues (TYR441 , PRO448 , ASN449 , SER483,SER478,GLN470,LYS467) , and the PGAT its bind to chitosan- CU the ΔG_{bind} are -5.6 kcal/mol with the interactive binding site residues (ALA443 , PRO448 , ASN449 , GLY452 , PHE453 , GLN470 , ARG472 , GLY476 , GLU477 , SER478)

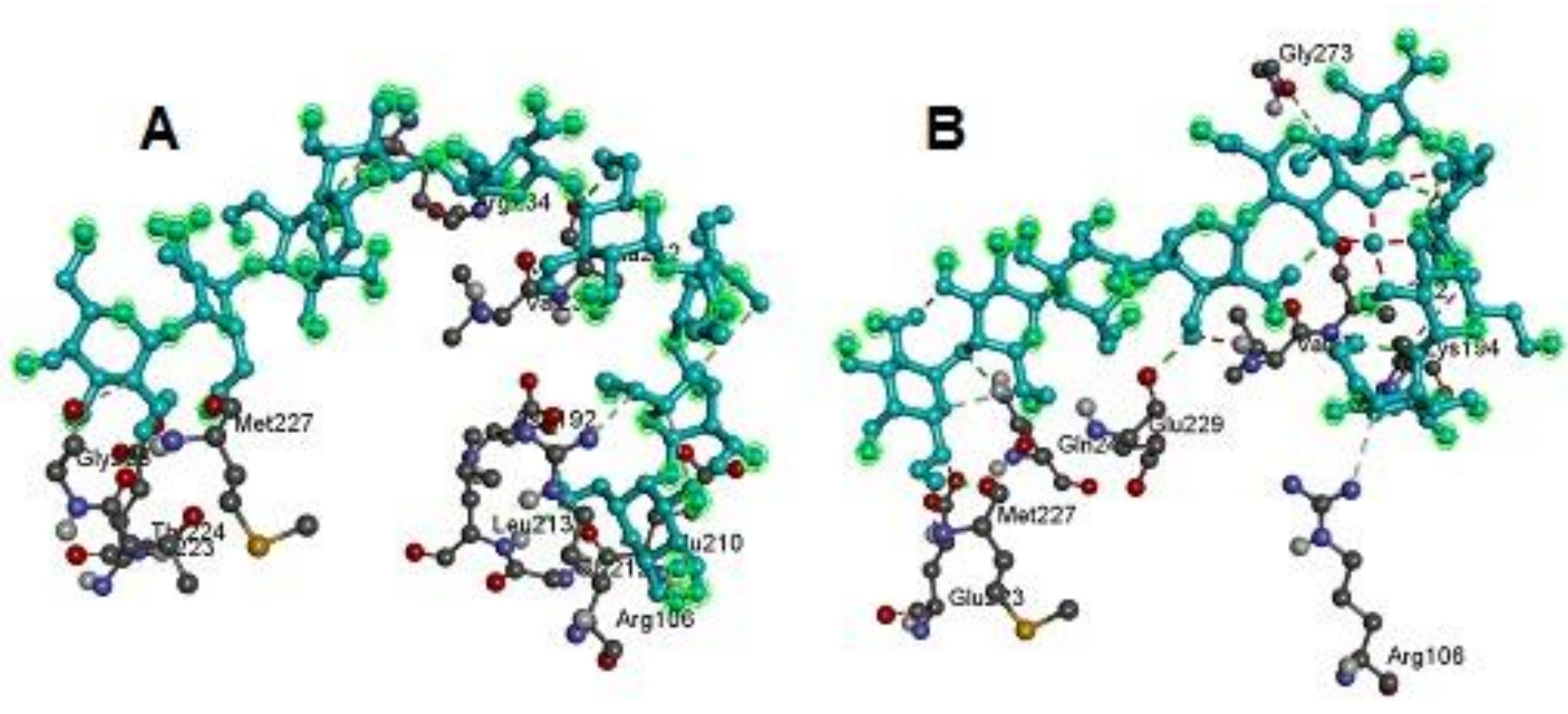

FIGURE 3. (A) The 3D surface view of MAPK1 modeled protein with chitosan reveals only the interactive residues on the binding site of a protein. (B) chitosan MAPK1 –Cu was the interactive residue of binding sites of the protein binding sites (active sites).

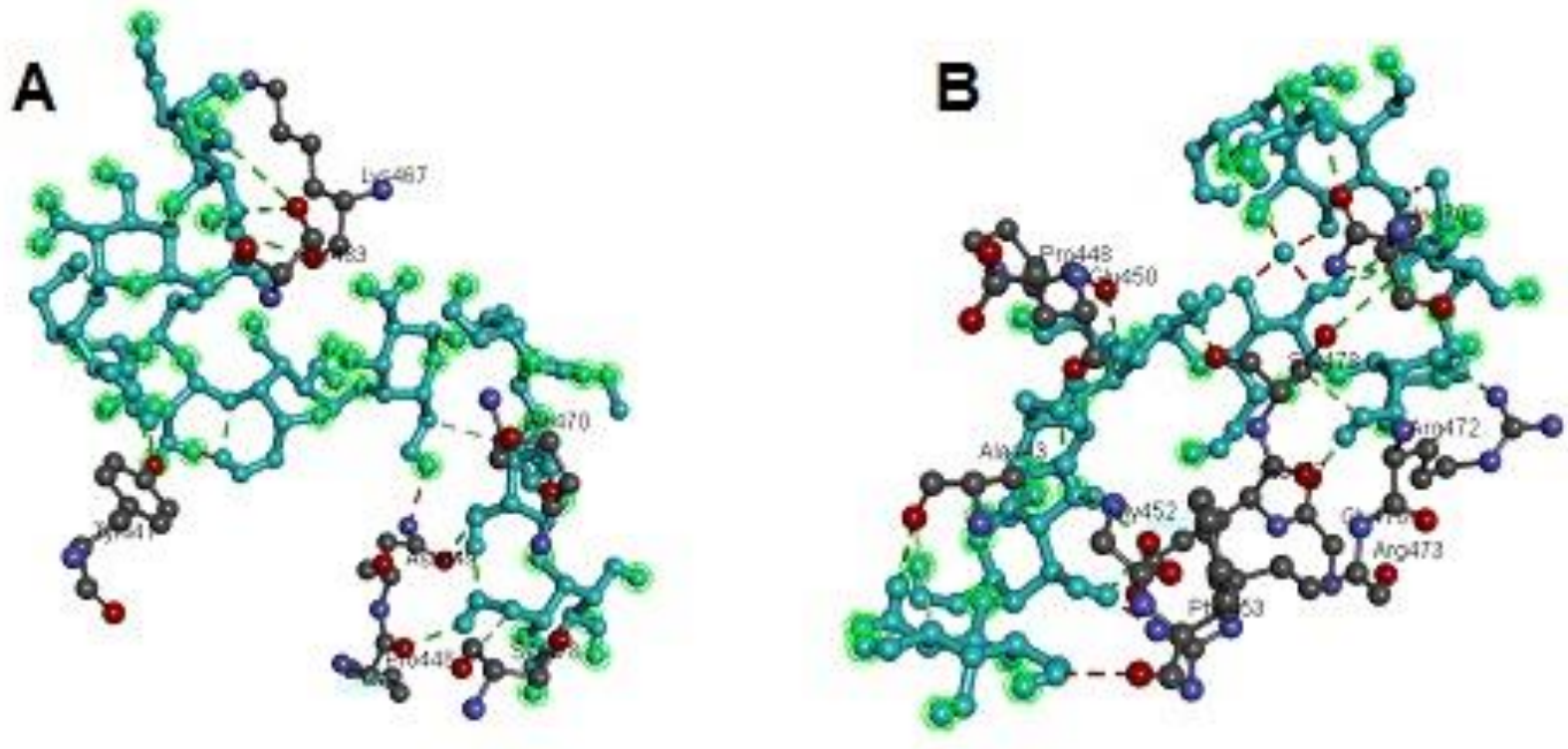

FIGURE 4 (A) The 3D surface view of PGAT modeled protein with chitosan reveals only the interactive residues on the binding site of a protein. (B) PGAT chitosan –Cu was the interactive residue of binding sites of the protein binding sites (active sites).

Discussion

This best docking poses shows how the ligand molecule fits into the binding region of the target protein. Intermolecular flexible docking simulations were performed and energy values were calculated from the docked conformations of the MAPK1 and PGAT proteins–inhibitor complexes. all of the ligands (chitosan and chitosan –Cu) had a greater binding affinity with the target proteins MAPK1 and PGAT proteins. Inhibition was measured by the binding energy of the best ligand pose measured in kcal/mol. The binding pose and their energy are listed in Table 2.

Conclusion

A gain in wheat lines tolerance to stem rust from P. graminis sp. tritici and leaf rust from P. triticina is urgent as the resistance of genes against the destructive diseases caused by global wheat is rare. Therefore, new inhibitor tools must be identified by the planet. The Egyptian chitosan and chicosan-cu can also be used as a new source of treatment for rust to obtain and produce a new inhibitor of wheat rust. Egypt is also able to reduce wheat rust. Chitosan NPs has previously been reported in tea and finger millet plants as an immune modulator due to the induction of antioxidant/defense enzymes. Silk analysis suppresses and inhibits the activities of MAP kinase 1 [Puccinia triticina] and PGTG Puccinia graminis f. sp. tritiz This work is carried out by the Chitosan and Chitosan Cu, which have been selected for the study. MAPK1 and PGAT proteins interacted in the compounds The bioactive compounds interacting with the objective can therefore be used as a powerful inhibitor to block the action of our proteins

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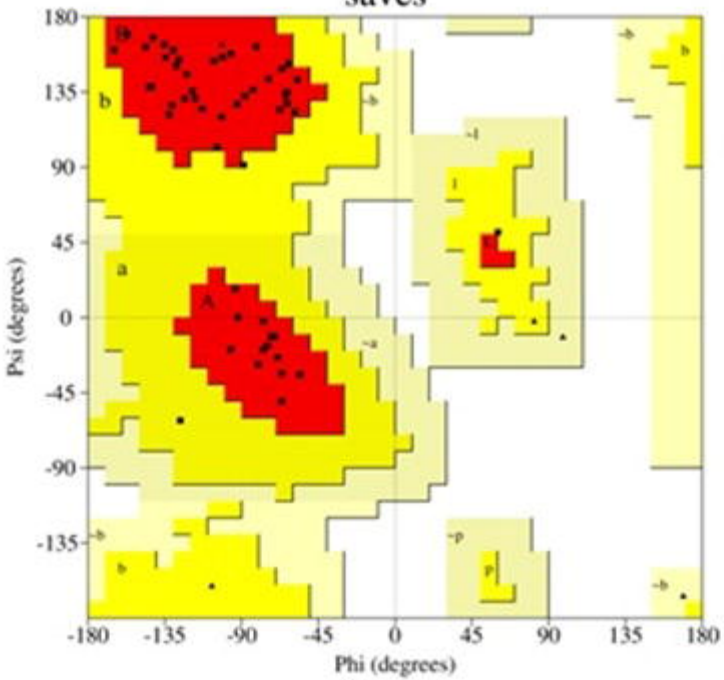
PROCHECK

A

Ramachandran Plot

saves



Plot statistics

Residues in most favoured regions [A,B,L]	46	93.9%
Residues in additional allowed regions [a,b,l,p]	3	6.1%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%
Residues in disallowed regions	0	0.0%
Number of non-glycine and non-proline residues	49	100.0%
Number of end-residues (excl. Gly and Pro)	1	
Number of glycine residues (shown as triangles)	5	
Number of proline residues	4	
Total number of residues	59	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

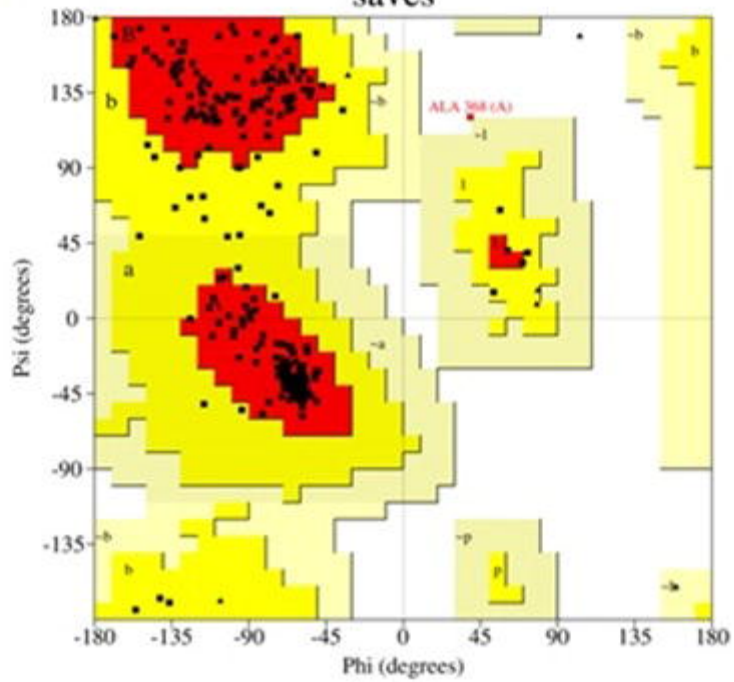
saves_01.ps

PROCHECK

B

Ramachandran Plot

saves

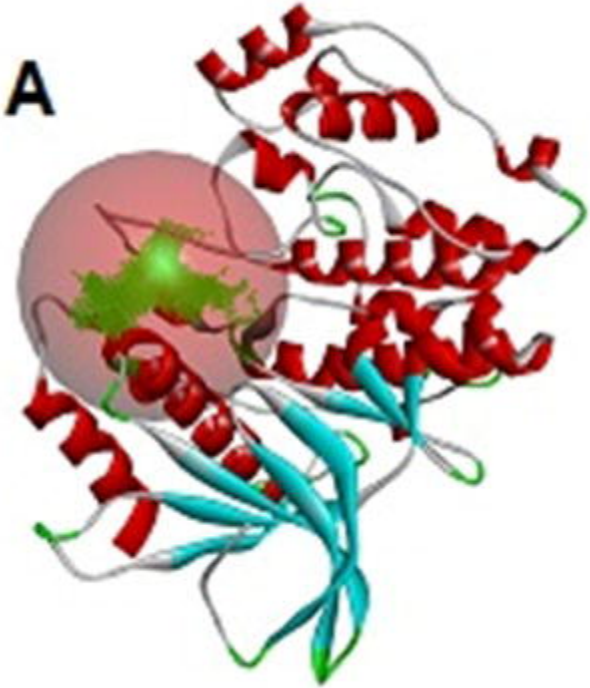


Plot statistics

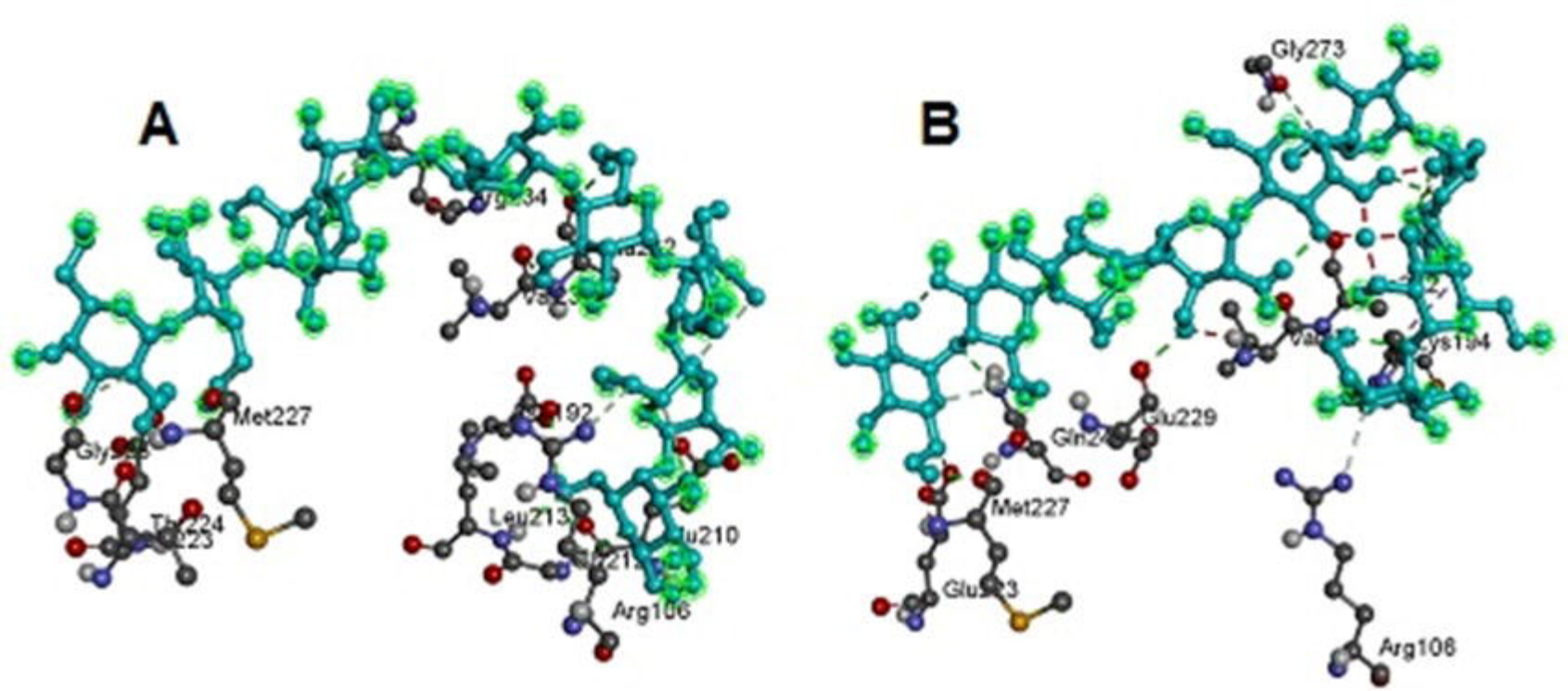
Residues in most favoured regions [A,B,L]	282	91.0%
Residues in additional allowed regions [a,b,l,p]	27	8.7%
Residues in generously allowed regions [~a,~b,~l,~p]	0	0.0%
Residues in disallowed regions	1	0.3%
Number of non-glycine and non-proline residues	310	100.0%
Number of end-residues (excl. Gly and Pro)	2	
Number of glycine residues (shown as triangles)	12	
Number of proline residues	20	
Total number of residues	344	

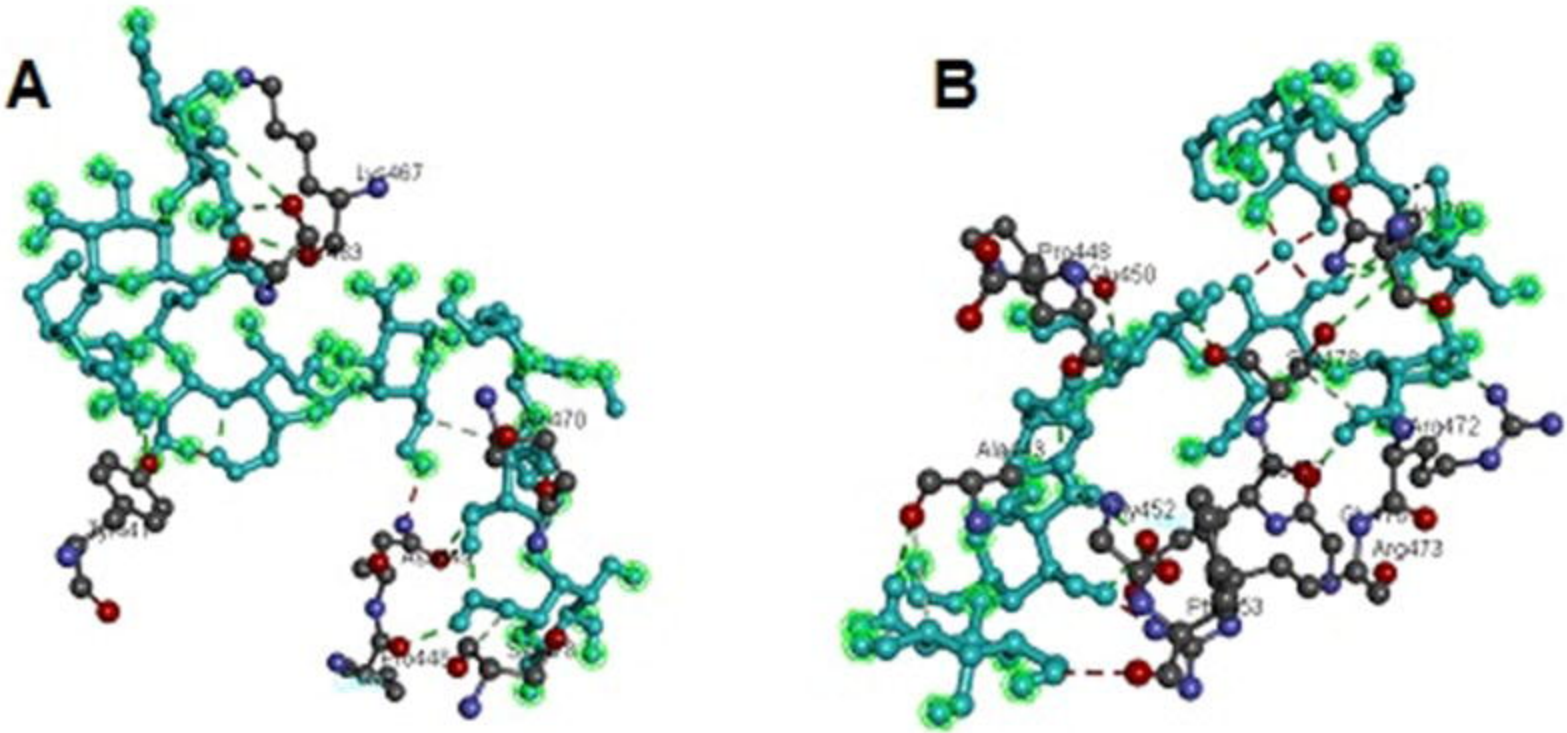
Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

saves_01.ps


A

B


A
Met227
Leu213
Arg106
B
Gly273
Glu229
Met227
Arg106


A
B
Pro448
Glu450
Arg472
Arg473