ISSN (online): 2319-6599
ISSN (Print): 2319-6580

Modeling studies and interaction of pathogenesis related protein (PR5) of *Hordeum vulgare* and candidates for secreted effector proteins (CSEP0064) of *Blumeria graminis*

Somya Sharma[1*], Vijendra K. Sharma[2]

[1]*M.S.J. Government PG College, Bharatpur-321001 (Rajasthan), India*
[2]*Government PG College, Karauli-322241 (Rajasthan), India*
somya1902@gmail.com, sharmavijenk@gmail.com

Abstract

Background / Objective: Barley has its own immunity but not sufficiently effective. Pathogenesis Related protein (PR5) of barley has anti-fungal properties which releases in result of virulence factor Candidate for Secreted Effector Proteins (CSEP0064) of *B. graminis*. The objective of this study is to generate molecular models of PR5 and CSEP0064 and to dock them for understanding the role PR5 in immunity of barley against CSEP0064 released during powdery mildew infection.
Methods/Statistical analysis: PR5 and CSEP0064 molecular interaction gives insight in the immunity of barley. In this study, we generate the molecular models of PR5 and CSEP0064 through Easy Modeller 4.0, further refinement of model from SAVES server, RAMPAGE, 3D refine srver and HexDocking Server was used for their mutual interaction study nd generation of PR5-CSEP0064 complex.
Findings: The interaction between PR5 and CSEP0064 molecular models were studied for the first time proving the role of PR5 and CSEP0064 in barley immunity. This study shows the complex formed between PR5 and CSEP0064 through bioinformatics tools. The complex is formed with 619.9 kCal/mol e-value which represents the requirement of very high energy for breaking the bond between two molecules.
Application/Improvements: Various factors affect crop quality and yield of barley. Various CSEPs are released during and after haustoria formation in barley. *Blumeria graminis* affects the barley as it causes powdery mildew disease. Therefore, biologists are continuously working towards the plant immunity and control of diseases.
***Keywords*:** *Hordeum vulgare*, *Blumeria graminis*, CSEP0064, Modeling, PR5.

1. Introduction

A variety of crops is grown under diverse climatic situations in different cropping systems. Agriculture is not only important but it also provides a base for development. Agriculture has been related with production of essential food crops. With increase in economic development, many fields allied to farming came to be recognized as a part of agriculture. Barley genome was sequenced in 2012 [1].

There are multiple factors for the crop damage and loss of yield both biotic and abiotic factors. Fungi are plant pathogens that require living plant tissue to survive and complete their life cycle. They represent some of the most destructive plant parasites as huge economic losses and threatening global food security are caused by them [2]. The degree of disease susceptibility in barley leaves is directly proportional to the distance between the cells of leaves and primary compatible haustorium; the induced susceptibility is generally localized; in powdery mildews, the information required for cellular conditionings does not transfer to long distance [3].

PRs accumulate under certain abiotic (wounding) and biotic stress conditions such as pathogen attack by virus, viroids, bacteria, fungi, nematodes, insects and herbivores [4]. PRs are low molecular weight proteins (10-40 kDa). Their biochemical properties help them to survive in harsh environments. They are localized in the vacuole, cell wall and the intercellular space; remain soluble and stable at low pH where most other plant proteins are denaturized; they are resistant against proteolytic cleavage; also they have extreme isoelectric points (pI) [5].

PR from different plant species with same family designation does not necessarily mean that they are identical proteins. The families are numbered in the order in which they were discovered and new PRs identified in different

ISSN (online): 2319-6599
ISSN (Print): 2319-6580

species are assigned to the existing recognized families and, if there is no similarity exists, a new family is created. The PR-5 family proteins are also known as thaumatin-like (TL) proteins because they show sequence similarities to the sweet-tasting plant protein thaumatin [6]. The first leaf of transgenic barley plants in which basic PR-5 is fused with a pathogen-inducible epidermis specific promoter revealed enhanced resistance against *B. graminis*, *Rynchosporium secalis* and *Drechslera teres*, while there is no disease reduction was observed on infection with *Puccinia hordei* [7]. The stable overexpression of a cDNA coding for a 13-LOX (lipoxygenase) in transgenic barley plants which for the first time indicate a link between the occurrence of LOX-100 protein and senescence [8].

A large number of CSEPs have been identified in powdery mildew fungi. Two CSEPs, CSEP0105 and CSEP0162 which are important for pathogen success as they are required during and after haustoria formation, interact with barley small heat shock proteins Hsp16.9 and Hsp17.5 and silencing of either one can significantly reduce the fungal haustoria formation rate [9]. Small heat shock proteins stabilize a number of intracellular proteins by their chaperone activity and defense related signaling components are one of them.

Here, we are investigating about the interaction between PR5 of *H. vulgare* and CSEP0064 of *B. graminis*. Anti-fungal activities are assigned to PR5, it accumulates in barley leaves after powdery mildew infection and some also possess 1,3-β-Dglucan binding activity [10].

Homology modeling allows constructing an unknown atomic-resolution model of the protein from its amino acid sequence and an experimental 3D structure of a related homologous protein. It is a big challenge to generate accurate models through computational structure prediction methods but they provide a cost-effective alternative in the absence of experimental structures. Model for the target protein can be generated on the basis of an experimentally established protein structure (template) that shares the template significant sequence (30% or more) or structural similarity [11]. With the help of computational methods we can safely use *in silico* models of proteins for structure based drug design, analysis of protein function, interactions, antigenic behavior, and rational design of proteins with increased stability or novel functions where experimental structures provides a solid reasoning [12].

We are constructing their models using bioinformatics tools and further with docking studies we analyze their interaction and study the immunity of barley against powdery mildew. There is a lot of study is going on in terms of plant immunity for example to increase the tolerance in plants against various pathogen attacks and to increase the crop yield and quality. Here, we studied the barley immunity against *Blumeria graminis* to protect plant from powdery mildew disease. As we can observe, the immunity of barley was predicted or studied through various methods and studies. In this study, we generate the molecular models of PR5 and CSEP0064 which was not present earlier and through HexDocking Server their mutual interaction was studied. The PR5 and CSEP0064 interaction was suggested [13]; their molecular models and interaction were generated and indicating the role of PR5 with CSEP0064.

2. Methods

2.1. Template selection and homology analysis

a) The primary structures of PR5 and CSEP0064 were obtained from UNIPROT and downloaded in FASTA format.
b) BLASTp was performed for every target and ligand to consider the similar proteins with similarity from 25% to 55%.

2.2. Homology modeling

The PDB structure obtained from BLASTp was run in Easy Modeller 4.0 [14] (offline software available with easy graphical user interface from MODELLER).

2.3. Model optimization

a) The model was analyzed using PyMOL software
b) Various refinements were used: (1) Structural Analysis and Verification Server (SAVES), (2) 3D refine server and (3) RAMPAGE.

2.4. Docking studies

Protein docking was done by using HexServer [15].

ISSN (online): 2319-6599
ISSN (Print): 2319-6580

3. Results

3.1. Template selection and homology analysis

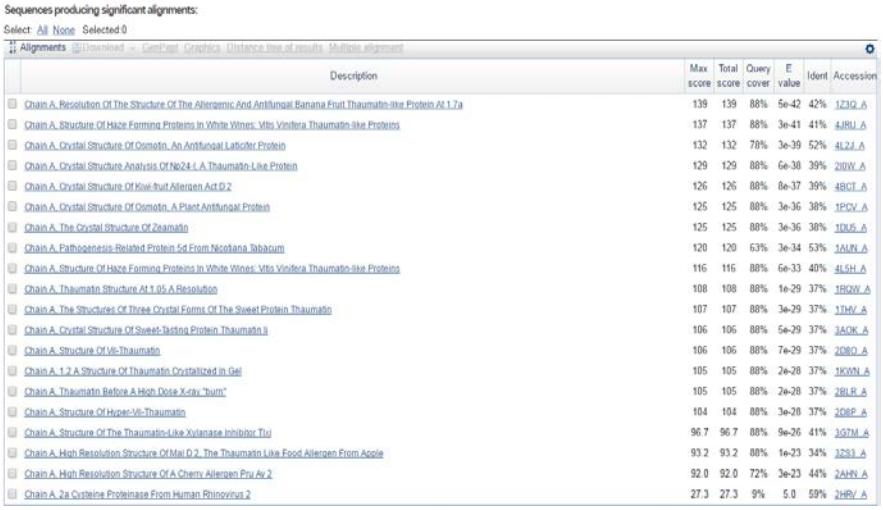
PR5 - accession number: Q5MBN5 [16]

CSEP0064 - accession number: N1JJ94 [17]

Sequence analysis and alignment of PR5 against PDB database revealed the close relation of PR5 with thaumatin like proteins out of 20 hits to query sequence as shown in figure 1. Likewise, comparative sequence alignment of CSEP0064 shows only single hit in query sequence which shows 47% identity to outer membrane decaheme cytochrome Mtrc of *Shewanella oneidensis* as shown in figure 2.

In case of PR5, out of 20 hits five were selected on the basis of their query coverage, e-value and percent identity.

Figure 1. Protein with significant alignments (20 hits) obtained from BLASTP result for PR5


Sequences producing significant alignments:

Select: All None Selected 0

Alignments Download GenPept Graphics Distance tree of results Multiple alignment

Description	Max score	Total score	Query cover	E value	Ident	Accession
Chain A, Resolution Of The Structure Of The Allergenic And Antifungal Banana Fruit Thaumatin-like Protein At 1.7a	139	139	88%	5e-42	42%	1Z3Q_A
Chain A, Structure Of Haze Forming Proteins In White Wines: Vitis Vinifera Thaumatin-like Proteins	137	137	88%	3e-41	41%	4JRU_A
Chain A, Crystal Structure Of Osmotin, An Antifungal Laticifer Protein	132	132	78%	3e-39	52%	4L2J_A
Chain A, Crystal Structure Analysis Of Np24-I, A Thaumatin-Like Protein	129	129	88%	6e-38	39%	2I0W_A
Chain A, Crystal Structure Of Kiwi-fruit Allergen Act D 2	126	126	88%	8e-37	39%	4BCT_A
Chain A, Crystal Structure Of Osmotin, A Plant Antifungal Protein	125	125	88%	3e-36	38%	1PCV_A
Chain A, The Crystal Structure Of Zeamatin	125	125	88%	3e-36	38%	1DUS_A
Chain A, Pathogenesis-Related Protein 5d From Nicotiana Tabacum	120	120	63%	3e-34	53%	1AUN_A
Chain A, Structure Of Haze Forming Proteins In White Wines: Vitis Vinifera Thaumatin-like Proteins	116	116	88%	6e-33	40%	4L5H_A
Chain A, Thaumatin Structure At 1.05 A Resolution	108	108	88%	1e-29	37%	1RQW_A
Chain A, The Structures Of Three Crystal Forms Of The Sweet Protein Thaumatin	107	107	88%	3e-29	37%	1THV_A
Chain A, Crystal Structure Of Sweet-Tasting Protein Thaumatin Ii	106	106	88%	5e-29	37%	3AOK_A
Chain A, Structure Of Vit-Thaumatin	106	106	88%	7e-29	37%	2D8O_A
Chain A, 1.2 A Structure Of Thaumatin Crystallized In Gel	105	105	88%	2e-28	37%	1KWN_A
Chain A, Thaumatin Before A High Dose X-ray "burn"	105	105	88%	2e-28	37%	2BLR_A
Chain A, Structure Of Hyper-Vit-Thaumatin	104	104	88%	3e-28	37%	2D8P_A
Chain A, Structure Of The Thaumatin-Like Xylanase Inhibitor Tlxi	96.7	96.7	88%	9e-26	41%	3G7M_A
Chain A, High Resolution Structure Of Mal D 2, The Thaumatin Like Food Allergen From Apple	93.2	93.2	88%	1e-23	34%	3ZS3_A
Chain A, High Resolution Structure Of A Cherry Allergen Pru Av 2	92.0	92.0	72%	3e-23	44%	2AHN_A
Chain A, 2a Cysteine Proteinase From Human Rhinovirus 2	27.3	27.3	9%	5.0	59%	2HRV_A

Figure 2. Protein with significant alignment (single hit) obtained from BLASTP result for CSEP0064


Sequences producing significant alignments:

Select: All None Selected 0

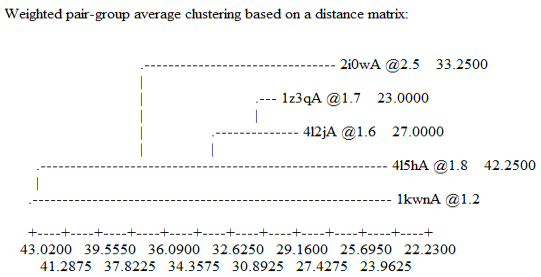
Alignments Download GenPept Graphics Distance tree of results Multiple alignment

Description	Max score	Total score	Query cover	E value	Ident	Accession
Chain A, Crystal Structure Of The Outer Membrane Decaheme Cytochrome Mtrc	26.9	26.9	26%	6.4	47%	4LM8_A

3.2. Homology modeling

The clustal dendrogram of selected sequences of PR5 shown in figure 3 was generated from pair wise distance matrix in EasyModeller 4.0.

Figure 3. Dendrogram from pairwise distance matrix (PR5)



1z3q-A has a better crystallographic resolution in comparison to 4l2j which has highest sequence identity with 52% (1.7A^0 versus 1.6A^0). Considering the major group with 2i0w-A, 1z3q-A, 4l2j-A and 415h-A; 2i0w has highest

ISSN (online): 2319-6599
ISSN (Print): 2319-6580

crystallographic resolution but less similarity with template. 4l5h has 1.8 A^0 resolutions with 40% sequence similarity. In total five models of PR5 were generated.

Only one template 4lm8-A is present for CSEP0064 homology modeling with 47% sequence similarity and e-value are 6.4. Therefore, three models of CSEP0064 were generated after aligning single template with query sequence.

3.3. Model optimization

Generally speaking, the errat method is sensitive to smaller errors than 3-D Profile analysis, but is more forgiving than Procheck. The best model for PR5 is PR5-D as deduced on the basis of molpdf, DOPE score and Errat factor data obtained from SAVES server and Easymodeler 4.0 shown in table 1 and similarly for CSEP0064 is CSEP0064-B; data described in table 2. DOPE score profiles of best selected model with reference to the templates are showing various high and low energy points for PR5-D in figure 4 and for CSEP0064-B in figure 5.

Table 1. Summary of successfully produced PR5 models by multiple template models

S.No.	Protein model	Procheck (Ramachandran Plot score)	Errat (Overall quality factor)	Molpdf score	DOPE score	Final rank
1	PR5-A	90.1	59.74	5563.70	-13816.42	2
2	PR5-B	90.1	55.26	5498.06	-13377.86	4
3	PR5-C	90.1	50.63	5640.14	-13426.95	5
4	PR5-D	89.5	64.67	5535.17	-13436.11	1
5	PR5-E	91.8	55.63	5666.36	-13783.06	3

Table 2. Summary of successfully produced CSEP0064 models by multiple template models

S.No.	Protein model	Procheck (Ramachandran Plot score)	Errat (Overall quality factor)	Molpdf score	DOPE score	Final rank
1	CSEP0064-A	91.4	21.277	738.43	-6326.95	2
2	CSEP0064-B	90.5	58.889	754.50	-6332.14	1
3	CSEP0064-C	88.8	32.323	746.01	-6238.49	3

Figure 4. DOPE score for PR5-D (query B99990004.pdb) and templates

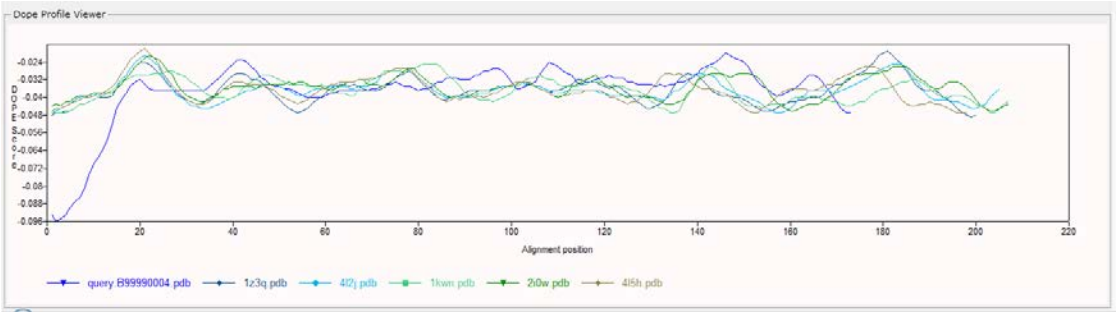
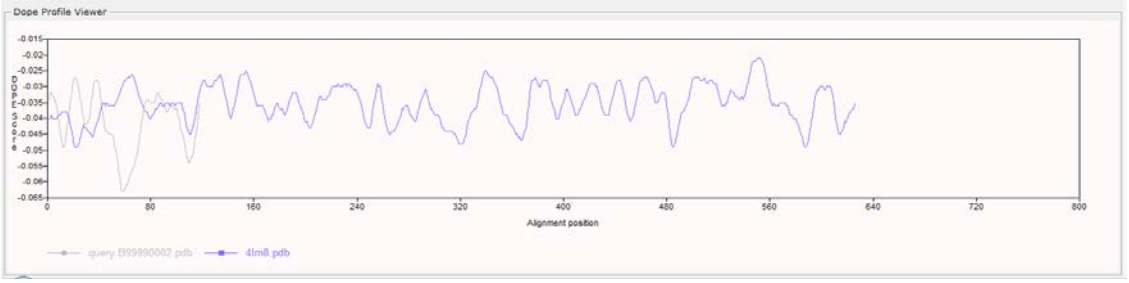


Figure 5. DOPE score for CSEP0064-B (query B99990002.pdb) and template



ISSN (online): 2319-6599
ISSN (Print): 2319-6580

3D refinement server (3D refine) was used for generation of more refined models from the selected best models. The final result for molecular modeling of PR5 gives RF5 and for CSEP0064 gives RF5 as best models on the basis of 3Drefine scores, RMSD and RWPlus; data shown in table 3 for PR5 and table 4 for CSEP0064. The final modeled structure of refined PR5-RF5 is shown in figure 6 and CSEP0064 is shown in figure 7 were obtained from 3D refine and visualized by PyMol.

Table 3. Results of PR5-D refined models with 3D refine server

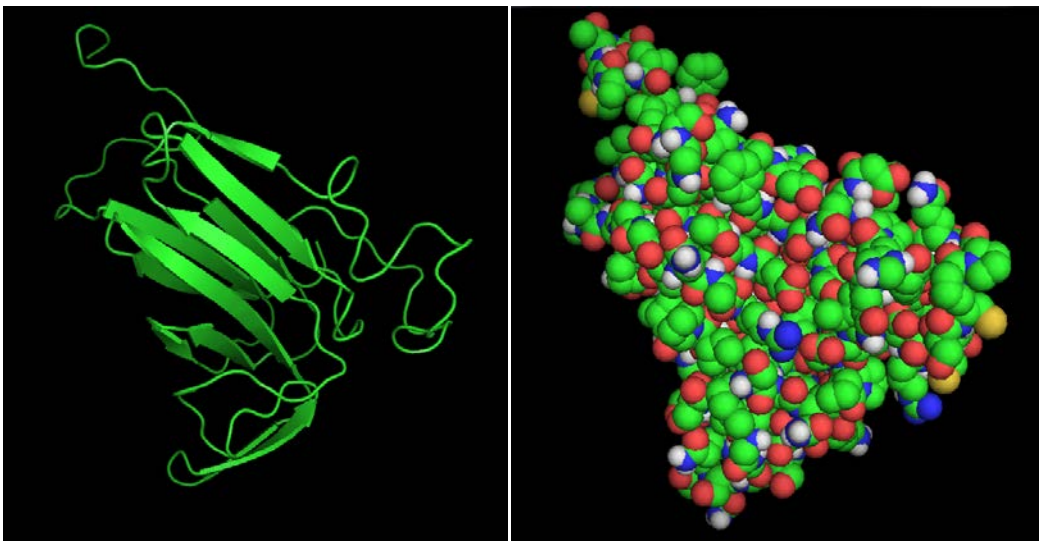
Model #	$3D^{refine}$ Score	GDT-TS	GDT-HA	RMSD (Å)	MolProbity	RWPlus ▾	Ranking
RF5	8356.21	1.0000	0.9942	0.272	2.624	-26689.59	1
RF4	8427.29	1.0000	0.9957	0.253	2.581	-26649.14	2
RF3	8547.71	1.0000	0.9971	0.233	2.537	-26624.26	3
RF2	8781.35	1.0000	1.0000	0.202	2.488	-26594.12	4
RF1	10508.5	1.0000	1.0000	0.153	2.583	-26578.73	5

Table 4. Results of CSEP0064-B refined models with 3D refine server

Model #	$3D^{refine}$ Score	GDT-TS	GDT-HA	RMSD (Å)	MolProbity	RWPlus ▾	Ranking
RF5	10027.8	1.0000	0.9958	0.280	2.995	-12031.44	1
RF4	10127.0	1.0000	0.9979	0.254	2.958	-11995.12	3
RF3	10259.2	1.0000	1.0000	0.230	2.824	-12016.99	2
RF2	10498.2	1.0000	1.0000	0.196	2.714	-11961.64	4
RF1	11514.7	1.0000	1.0000	0.145	2.681	-11927.59	5

Ramachandran Plot gives 94.2% of total energy for PR5 as shown in figure 8a and 91.4% for CSEP0064 in figure 8b through RAMPAGE server. Errat Overall quality factor for PR5 is 64.242 and for CSEP0064 is 54.717.

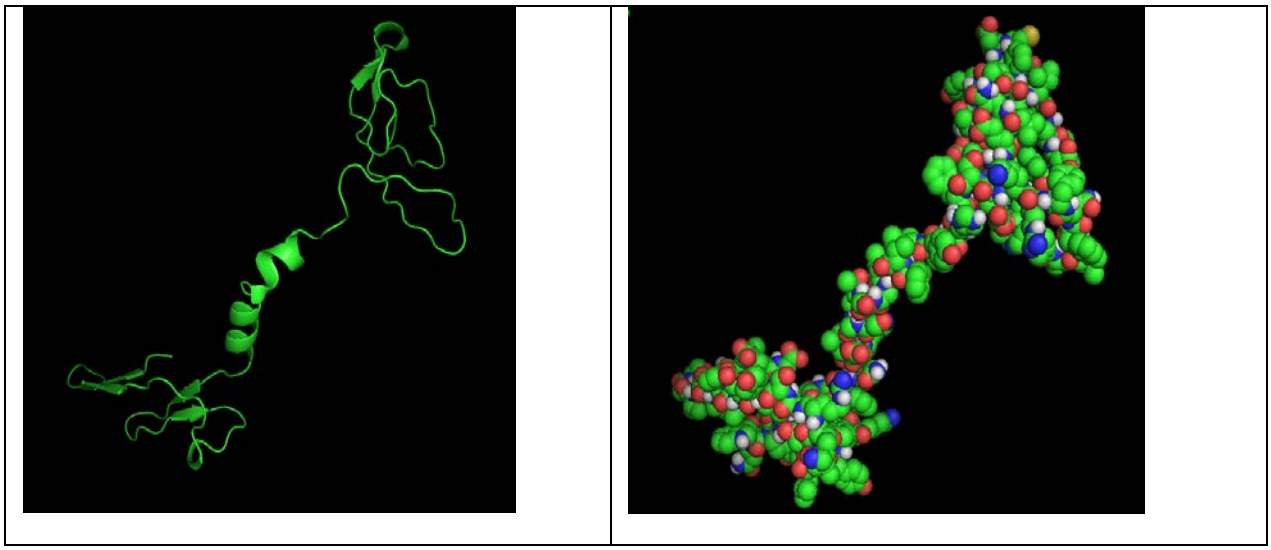
Figure 6. Visualized 3D structure of PR5-RF5 through PyMol



(a) Ribbon Structure (b) Surface Structure

ISSN (online): 2319-6599
ISSN (Print): 2319-6580

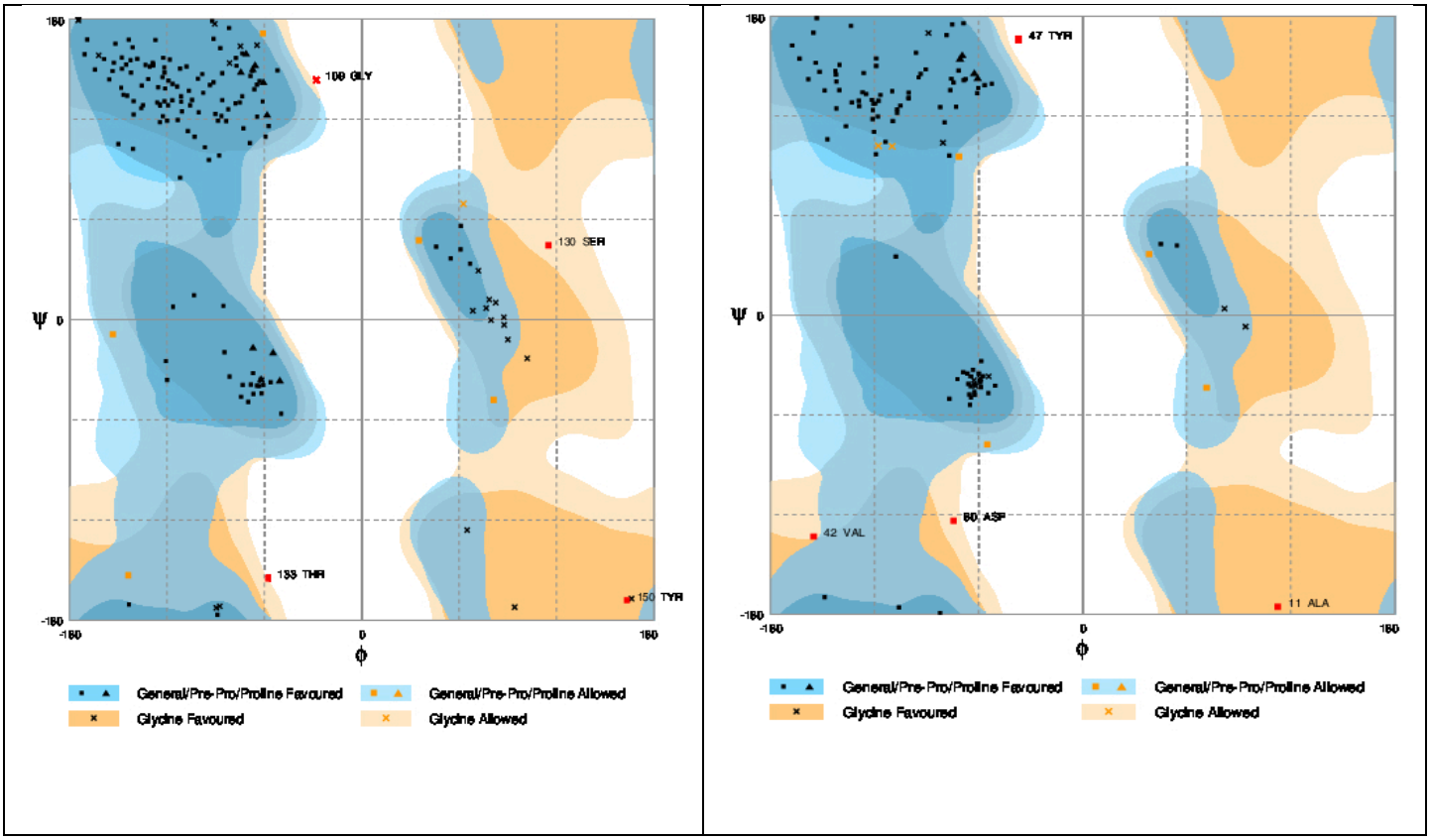
Figure 7. Visualized 3D structure of CSEP0064-RF5 through PyMol



(a) Ribbon Structure (b) Surface Structure

Figure 8a. Ramachandran Plot (PR5)

Figure 8b. Ramachandran Plot (CSEP0064)

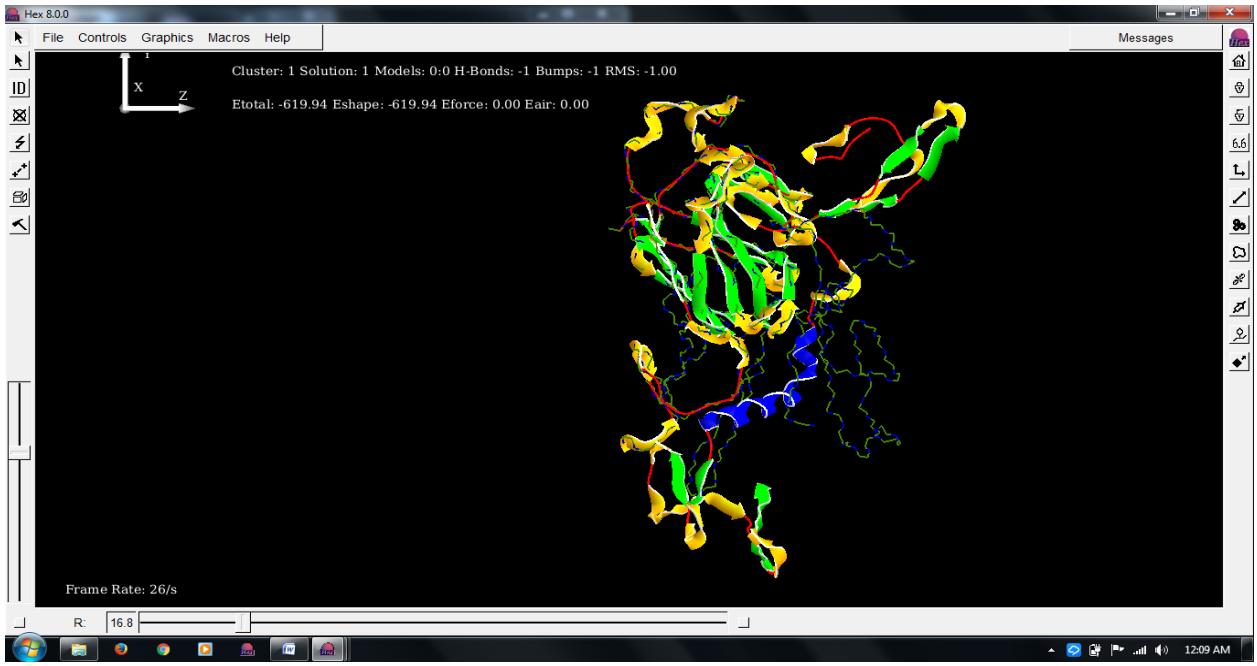


3.4. Docking Studies

In total 2000 formations were generated from Hex docking server, the best formation of PR5 and CSEP0064 is shown in figure 9 which have minimum energy value of -619.9 kCal/mol and around 500 clusters have energy value between -619.9 to -452.5. The strong bond is implied between PR5 and CSEP0064 and a strong cluster shows the interaction between both at the molecular level in barley. It also gives evidence for plant immunity against barley powdery mildew disease.

ISSN (online): 2319-6599
ISSN (Print): 2319-6580

Figure 9. Best Formation (e-value -619.9)



4. Discussion

The present study was first attempt on the modeling and docking studies of PR5 and CSEP0064. However, Pennington et al showed that the CSEP0064 interacted with various molecules of barely and it was proved by two orthogonal approaches to determine the protein−protein interactions [18]. The PR5 and CSEP0064 templates were taken from Uniprot and their molecular models were generated through similar sequences obtained from BLASTp and EasyModeller. Homology modeling is the most common structure prediction method. Nawaz et al uses PSI BLAST as similarity sequence search programs against a PDB database [19] while here we used p-BLAST against PDB database for finding a best matching template.

Five models were generated from EasyModeller; the best model was selected on the basis of various factors like DOPE score, molpdf, ramachandram score and errat value. The structural validation and quality assessment for the selection of best model was carried out with PROCHEK, RAMPAGE, Errat, Verify3D and RMSD and Z-score [20]. The best selected model after 3D refine server is the generated molecular model of the respective template.

These models were used in the Hex Docking Server to study whether they interact or not. The Hex Docking shows the interaction between PR5 and CSEP0064 at the molecular level but this interaction should be stable and the complex formed with the lowest e-value is the most stable one. Lowest e-value represents the requirement of high energy for breaking of bond. Complex formed through hex server shows the barley protein interaction with *B. graminis* protein to control the powdery mildew fungus. GLIDE tool of Schrodinger was used in docking of antifungal compound in case rice false smut disease which also shows that lowest e-value shows good binding energy against the receptor [21]

The research through sequence alignment, phylogenetic analysis, structure analysis by homology modeling and study of interaction by docking is showing that the PR5 interacts with CSEP0064 and form a strong bond that control the fungal activity in barley. Now, these results further can be used for the study of plant pathological interaction in barley, to increase immunity in barley against powdery mildew fungus and study of protein-protein interaction for the crop quality and its yield.

5. Conclusions

The interaction between PR5 and CSEP0064 can be seen through these results, as they are forming a complex with -619.9 kCal/mol e-value. This value interprets for a strong bond between both the molecules. The above

interaction between PR5 and CSEP0064 was carried out *in silico* and now it can be further used for the *in vivo* study of barley immunity.

This result implies the role of PR5 with CSEP0064 in context of barley defense system and their interaction is proved. PR5, the pathogenesis related protein in barley which has anti-fungal properties act (Candidates for Secreted Effector Proteins from *Blumeria graminis*) which release after and during hausatoria formation to loosen the barley defense.

The use of bioinformatics tools for this study proves to be very crucial. The study carried out here will help in understanding of barley immunity and its actions against powdery mildew disease. Barley powdery mildew disease is one of the main reason for crop loss and yield loss due to fungal attack. So, here considering the results, we can further control the disease with PR5 studies and improve the yield.

6. References

1. K.F.X. Mayer, R. Waugh, P. Langridge, T.J. Close, R.P. Wise, A. Graner, T. Matsumoto, K. Sato. A physical, genetic and functional sequence assembly of the barley genome. *Nature*. 2012; 491(7426), 711-716.
2. Markus Koeck, Adrienne R. Hardham, Peter N. Dodds. The role of effectors of biotrophic and hemibiotrophic fungi in infection. *Cell Microbiology*. 2011; 13(12), 1849-1857.
3. Seiji Ouchi, Hachiro Oku, Chihya Hibino. Localization of induced resistance and susceptibility in barley leaves inoculated with the powdery mildew fungus. *Phytopathology.* 1976; 66, 901-905.
4. L.C. van Loon, M. Rep, C.M.J. Pieterse. Significance of Inducible Defense-related Proteins in Infected Plants. *Annual Review of Phytopathology*. 2006; 44, 135-162.
5. A. Stintzi, T. Heitz, V. Prasad, S. Weidemann-Merdinoglu, S. Kauffmann, P. Geoffroy, M. Legrand, B. Fritig. Plant 'pathogenesis-related' proteins and their role in defense against pathogens. *Biochimie*. 1993; 75(8), 687-706.
6. H.J.M. Linthorst. Pathogenesis-related proteins of plants. *Critical Reviews in Plant Sciences*. 1991; 10, 123-150.
7. Poulsen T. Tandrup. Transgenic barley with enhanced resistance to fungal pathogens. PhD thesis. The Royal Veterinary and Agricultural University, Denmark. 2001.
8. Vijendra K Sharma, Tamas Monostori, Cornelia Göbel, Robert Hänsch, Florian Bittner, Claus Wasternack, Ivo Feussner, Ralph R. Mendel, Bettina Hause, Jutta Schulze. Transgenic barley plants overexpressing a 13-lipoxygenase to modify oxylipin signature. *Phytochemistry*. 2006; 67, 264-276.
9. Wen-Jing Zhang, Carsten Pedersen, Mark Kwaaitaal, Per L. Gregersen, Sara M. Morch, Susanne Hanisch, Astrid Kristensen, Anja T. Fuglsang, David B. Collinge, Hans Thordal-Christensen. Interaction of barley powdery mildew effector candidate CSEP0055 with the defence protein PR17c. *Molecular Plant Pathology*. 2012; 13(9), 1110-1119.
10. R.I.W. Osmond. Barley family five pathogenesis-related proteins. University of Adelaide: Glen Osmond, Australia. 2000.
11. Claudio N. Cavasotto, Shrangdhar S. Phatak. Homology modeling in drug discovery: current trends and applications. *Drug Discovery Today*. 2009; 14 (13/14), 676-683.
12. Elamer Krieger, Sander B. Nabuurs, Gert Vriend, Philip E. Bourne, Helge Weissig. Homology Modeling. Structural Bioinformatics. John Wiley & Sons. 2003.
13. Hellen G Pennington, Dana M Gheorghe, Anabelle Damerum, Clara Pliego, Pietro D. Spanu, Cramer Rainer, L.V. Blindschedler. Interactions between the powdery mildew effector BEC1054 and barley proteins identify candidate host targets. *Journal of Proteome Research*. 2016; 15(3), 826-839.
14. Bhusan K. Kuntal, Polamarasetty Aparoy, Pallu Reddanna. EasyModeller: A graphical interface to MODELLER. *BMC Research Notes*. 2010; 3, 226.
15. Gary Macindoe, Lazaros Mavridis, Viswesh Venkatraman, Marie-Dominique Devignes, David W. Ritchie. HexServer: an FFT-based protein docking server powered by graphics processors. *Nucleic Acids Research*. 2010; 38(S2), W445-W449.
16. T. Bryngelsson, B. Green. Characterization of a pathogenesis-related, thaumatin-like protein isolated from barley challenged with an incompatible race of mildew. *Physiological and Molecular Plant Pathology*. 1989; 35(1), 45-52.
17. P.D. Spanu, J.C. Abbott, J. Amselem, T.A. Burgis , D.M. Soanes, K. Stüber, E. Ver Loren van Themaat, J.K. Brown, S.A. Butcher, S.J. Gurr, M.H. Lebrun, C.J. Ridout, P. Schulze-Lefer, N.J. Talbot, N. Ahmadinejad, C. Ametz, G.R.

ISSN (online): 2319-6599
ISSN (Print): 2319-6580

Barton, M. Benjdia, P. Bidzinski, L.V. Bindschedler, M. Both, M.T. Brewer, L. Cadle-Davidson, M.M. Cadle-Davidson, J. Collemare, R. Cramer, O. Frenkel, D. Godfrey, J. Harriman, C. Hoede, B.C. King, S. Klages, J. Kleemann, D. Knoll, P.S. Koti, J. Kreplak, F.J. López-Ruiz, X. Lu, T. Maekawa, S. Mahanil, C. Micali, M.G. Milgroom, G. Montana, S. Noir, R.J. O'Connell, S. Oberhaensli, F. Parlange, C. Pedersen, H. Quesneville, R. Reinhardt, M. Rott, S. Sacristán, S.M. Schmidt, M. Schön, P. Skamnioti, H. Sommer, A. Stephens, H. Takahara, H. Thordal-Christensen, M. Vigouroux, R. Wessling, T. Wicker, R. Panstruga. Genome expansion and gene loss in powdery mildew fungi reveal tradeoffs in extreme parasitism. *Science*. 2010; 330(6010), 1543-1546.

18. G. Helen. Pennington, M. Dana. Gheorghe, Anabelle Damerum, Clara Pliego, D. Pietro. Spanu, Rainer Cramer, V. Laurence. Blindschedler. Interactions between the powdery mildew effector BEC1054 and barley proteins identify candidate host targets. *Journal of Proteome Research*. 2016; 15, 826-839.
19. Muhammed Nawaz, Naeem Iqbal, Sobia Idrees, Ihasn Ullah. *DREB1A* from *Oryza sativa* var. IR6: homology modelling and molecular docking. *Turkish Journal of Botany*. 2014; 38, 1095-1102.
20. Iti Gontia-Mishra, Vinay K. Singh, Niraj Tripathi, Shaly Sasidharan, Sharad Tiwari. Computational identification, homology modeling and docking analysis of phytase protein from *Fusarium oxysporum*. *Biologia*. 2014; 69(10), 1283-1294.
21. Mukesh Nitin, Shamshad Alam, M.S. Anantha, Yogesh Kumar, Dipankar Maiti. Comparative homology modeling and docking study of Mat 1-2-1 protein for designing bio-active molecule Effective against rice false smut (*ustilaginoidea virens)* disease. *Journal of Advanced Bioinformatics Applications and Research*. 2013; 3(4), 72-79.

The Publication fee is defrayed by Indian Society for Education and Environment (iSee). www.iseeadyar.org
Cite this article as:
Somya Sharma, Vijendra k. Sharma. Modeling studies and interaction of pathogenesis related protein (PR5) of *Hordeum vulgare* and candidates for secreted effector proteins (CSEP0064) of *Blumeria graminis. Indian Journal of Bioinformatics and Biotechnology*.Vol 4 (3), August, 2016.