IOSR Journal Of Pharmacywww.iosrphr.org
(e)-ISSN: 2250-3013, (p)-ISSN: 2319-4219
Volume 7, Issue 9 Version. 1 (September 2017), PP. 43-45

Virtual Docking Analysis of Zeorin With Fungal Glucan Transglycosylase

[*]Ashutosh Pathak
(Department of Botany, SSKGDC, University of Allahabad, Allahabad, U.P., India 211003)
Corresponding Author: Ashutosh Pathak

Abstract : *Lichen thallus, a consortium of mycobiont and photobiont, produces numerous secondary metabolites and zeorin is one of them. The antifungal activity of zeorin producing lichen extracts have provided the evidence for the current study. The present study was focused on the binding affinity and virtual docking of glucan transglycosylase (Gas2p). The structure of protein was downloaded from RSCB whereas the ligand file was downloaded from PubChem compound database. The docking was performed using AutoDock Vina and visualized by Chimera 1.11.2 whereas the active binding sites were evaluated by MetaPocket 2.0. The successful docked results of Gas2p with zeorin exhibited the potential of zeorin in the inhibition of glucan chain elongation of fungal cell wall via disturbing the hydrolysis and transglycosylation activity of glucan transglycosylase and proves its potential as candidate for future antifungal drug.*

Keywords: *Docking, fungal cell wall, Glucan transglycosylase, Lichen, zeorin*

Date of Submission: 04-09-2017 Date of acceptance: 16-09-2017

I. INTRODUCTION

Lichen thallus is a controlled mini ecosystem consists of a mycobiont (fungus) and photobiont (algae or cyanobacteria) [1]. Lichens are known for their biological activities such as antibacterial, antifungal, antiviral, antioxidant etc [2]. *Myelochroa aurulenta*, *Lecanora frustulosa* and *Parmeliopsis hyperopta* exhibited antifungal and antimicrobial property [3,4]. Zeorin, produced within the thallus of all aforementioned lichens, is a compound common compound [4,5]. In present study the binding affinity of zeorin towards the fungal surface proteins was evaluated for the future prospects of zeorin as an antifungal drug. Fungal surface protein was selected as glucan transglycosylase (RCSB PDB ID: 2W61) [6].

II. MATERIAL AND METHODS

II.I Accession of Target Protein Protein 3D structures were downloaded from RSCB 1 Glucan transglycolase: Gas2p (PDB ID: 2W61) [7].

II.II Ligand Selection Zeorin canonical smiles was copied from PubChem compound database [8]. Three dimensional structure was prepared using CADD Group Chemoinformatics Tools and User Services [9]. Structure energy was minimized and hydrogen's were added and charges were assigned using Gasteiger [10].

II.III Analysis of target active binding sites The active binding sites of aforementioned protein were analyzed via Metapocket 2.0 [11].

II.IV Molecular Docking Analysis Ligand-Protein docking was used to analyzed the binding affinity of zeorin with the 'aforementioned protein's structure. Docking was performed via AutoDock Vina [12]. Grid was assigned to each binding sites and the energy of interaction was evaluated at each step. All the remaining parameters were set as default. The docked files were visualized via UCSF Chimera 1.11.2 developed by Resource for Biocomputing, Visualization, and Informatics (RBVI) [13].

III. RESULTS AND DISCUSSION

The docking results evaluated in terms of binding energy exhibited that the target protein i.e. glucan transglycosylase protein Gas2p was successfully docked with zeorin. The docking results of three binding sites were listed in TABLE 1. The RMSD value equals to 0 was obtained in three steps and the docked results with hydrogen bonding provides the more strength to the docked ligand-protein structure. The most significant binding on the basis of hydrogen bonding was presented in Fig. 1. Glucan transferase Gas2p was isolated from Saccharomyces cerevisiae and it hels in the beta(1-3) glucan chain elongation in the yeast cell wall [6]. The previously reported results of zeorin containing extracts of lichens exhibited extract's efficacy towards fungal cell [3,4]. In present study the successful docking of zeorin on fungal glucan transglycosylase provides a new insight that the zeorin might inhibited the hydrolysis and transglycosylation activity of glucan transglycosylase which resulted into the stopping of glucan chains elongation of fungal cell wall. The disturbance in the normal physiological function of glucan

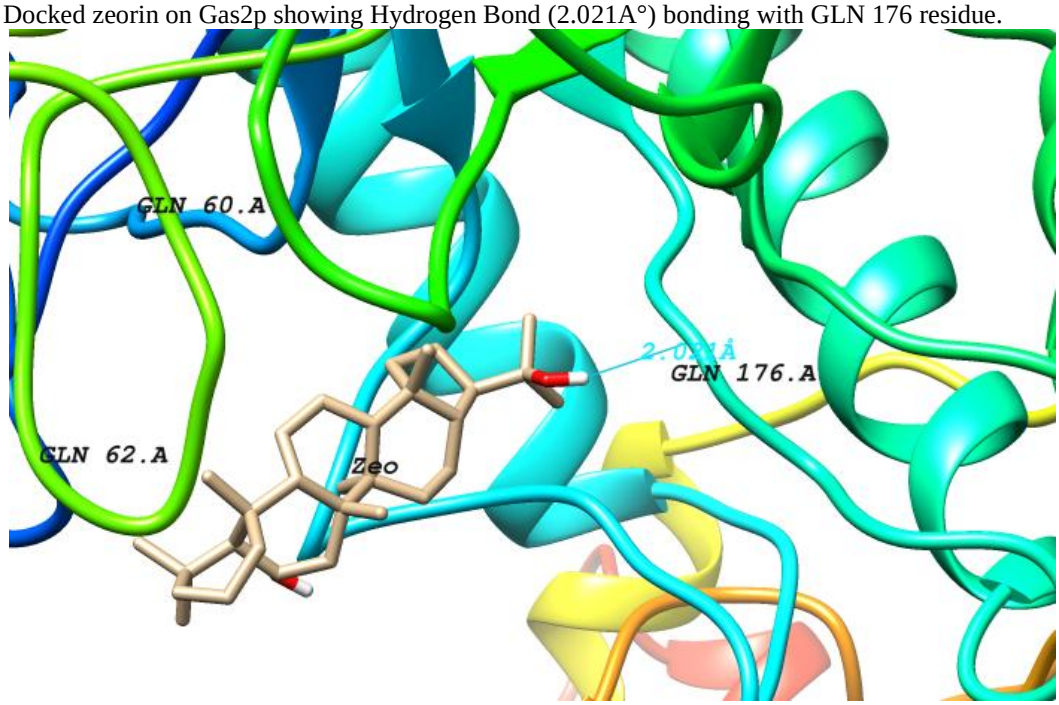
transglycosylase resulted into the depletion of fungal cell wall which resulted into the inhibition of fungal cell growth.

IV. FIGURE AND TABLE

TABLE 1: Docking results of glucan transglycosylase protein Gas2p with Zeorin.

Binding Site	State	Score	RMSD l.b.	RMSD u.b.	HBonds (all)	HBond Ligand Atom	HBond Receptor Atom
1	Viable	5.2	0.0	0.0	0	0	0
2	Viable	-2.5	0.0	0.0	1	1	1
2	Viable	-1.6	3.116	4.896	0	0	0
2	Viable	-0.8	3.09	6.834	0	0	0
3	Viable	79.8	0.0	0.0	0	0	0

Fig.1: Docked zeorin on Gas2p showing Hydrogen Bond (2.021A°) bonding with GLN 176 residue.



V. CONCLUSION

Docking study of the target protein glucan transglycosylase (Gas2p) with zeorin exhibited that the zeorin is a good ligand which docks well with glucan transglycosylase. Thus, played the important role in inhibiting the glucan chain elongation in the fungal cell wall.

ACKNOWLEDGEMENTS

The author is thankful to Head, Department of Botany and Principal of SS Khanna Girls' Degree College, Allahabad for their support and facility.

REFERENCES

[1] A. Pathak, R.K. Mishra, S.K. Shukla, R. Kumar, A. Pandey, M. Pandey, and A. Dikshit, *Flavoaparmelia caperata*, a host for *Beauveria* sp. in subalpine forest of Chakrata district, Uttarakhand, India, and Natural selection in *B. bassiana*, *Asian Journal of Microbiology, Biotechnology and Environmental Sciences, 18(4),* 2016, 983-990.

[2] K. Molnar, and E. Farkas, Current results on biological activities of lichen secondary metabolites: A Review, *Zeitschrift fur Naturforschung C, 65,* 2010, 157-173.

[3] A. Pathak, R.K. Mishra, S.K. Shukla, R. Kumar, M. Pandey, M. Pandey, A. Qidwai, and A. Dikshit, *In vitro* evaluation of antidermatophytic activity of five lichens, *Cogent Biology*, *2*, 2016, 1197472.

[4] K. Marijana, R. Branislav, and S. Slobodadn, Antimicrobial activity of the lichen *Lecanora frustulosa* and *Parmeliopsis hyperopta* and their divaricatic acid and zeorin constituents, *African Journal of Microbiology Research*, *4(9)*, 2010, 885-890.

[5] K.P. Singh, and G.P. Sinha, *Indian lichens: an annotated checklist* (Kolkata: Botanical Survey of India, 2010).
[6] R. Hurtado-Guerrero, A.W. Schuttelkopf, I. Mouyna, A.F.M. Ibrahim, S. Shepherd, T. Fontaine, J. Latge, and D.M.F. van Aalten, Molecular mechanisms of yeast cell wall Glucan Remodeling, *The Journal of Biological Chemistry, 284(13)*, 2009, 8461-8469.
[7] RSCB. [Last accessed on 2017 Aug 09]. Available from http://www.rcsb.org/pdb/home/home.do.
[8] NCBI, (National Center for Biotechnology Information). PubChem Compound Database; CID=159931, https://pubchem.ncbi.nlm.nih.gov/compound/159931 (accessed Aug. 9, 2017).
[9] https://cactus.nci.nih.gov
[10] J. Wang, W. Wang, P.A. Kollman, and D.A. Case, Automatic atom type and bond type perception in molecular mechanical calculations. *Journal of Molecular Graphics and Modelling, 25*, 2006, 247-260.
[11] Z. Zhang, Y. Li, B. Lin, M. Schroeder, and B. Huang, Identification of cavities on protein surface using multiple computational approaches for drug binding site prediction. *Bioinformatics, 27(15)*, 2011, 2083-2088.
[12] O. Trott, and A.J. Olson, AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading. *Journal of Computational Chemistry, 31*, 2010, 455-461.
[13] https://www.cgl.ucsf.edu/chimera/

Ashutosh Pathak. "Virtual Docking Analysis of Zeorin With Fungal Glucan Transglycosylase." IOSR Journal of Pharmacy (IOSR-PHR), vol. 7, no. 9, 2017, pp. 43–45.