Life Science Informatics Publications

Research Journal of Life Sciences, Bioinformatics, Pharmaceutical and Chemical Sciences

Journal Home page http://www.rjlbpcs.com/

RJLBPCS

ISSN 2454-6348

Original Research Article **DOI - 10.26479/2017.0303.15**

VIRTUAL DOCKING ANALYSIS OF ATRANORIN WITH FUNGAL CLASS I HYDROPHOBIN

Ashutosh Pathak

Department of Botany, SSKGDC, University of Allahabad, Allahabad, U.P., India 211003

ABSTRACT: Lichen thallus is an organism of composite nature i.e. consortium of photo and mycobiont. The secondary metabolites produced by the fungal partner exhibited various biological activities. In present study, one of the compounds produced by the lichens i.e., atranorin was evaluated for its binding affinity with the class I hydrophobin. Hydrophobin are present outside the cell wall and thus forming the layer of biofilms. Biofilms present outside the cell wall of the fungal pathogens might represents the first barrier for the antifungal agents. The present study investigates the binding affinity and in silico docking of Dew A (Class I Hydrophobin). The protein ligand docking was performed by the AutoDock Vina and visulaized by the Chimera. The hydrogen bonds present in the docked files presents the atranorin as a potent ligand and its potential in near future as biofilm degrading agent.

KEYWORDS: Atranorin, Biofilm, Hydrophobin, Lichens.

***Corresponding Author: Dr. Ashutosh Pathak Ph.D.**

Department of Botany, SSKGDC, University of Allahabad, Allahabad, U.P., India 211003 * Email Address: ashupathaks@rediffmail.com

1.INTRODUCTION Lichens are unique group of fungi and the thallus is formed by the consortium of photo and mycobiont forming a new entity [1]. There are around 1050 secondary metabolites have been reported so far from the lichen thallus [2]. The secondary metabolites produced by the fungal partner are well known for their biological activities. Few of the already known biological activities are antibacterial, antifungal, antiherbivore, antioxidant etc [3-6]. In present study, atranorin, one of the compound produced from lichens was investigated in silico for its binding affinity against hydrophobin class I protein. Hydrophobin class I proteins are the surface proteins forming the biofilm outside the fungal cell [7, 8].

2. MATERIAL AND METHODS

2.1 Accession of Target Protein: Protein 3D structures were downloaded from RSCB: Class I Hydrophobin DewA (PDB ID: 2LSH)[9].

Ligand Selection: Atronorin 3D structure was downloaded from PubChem compound database[10]. Three dimensional structure was prepared using CADD Group Chemoinformatics Tools and User Services[11]. Structure energy was minimized and hydrogen's were added and charges were assigned using Gasteiger[12].

Analysis of target active binding sites: The active binding sites of aforementioned protein were analyzed via Metapocket 2.0[13].

Molecular Docking Analysis

Ligand-Protein docking was used to analyzed the binding affinity of Atranorin with the aforementioned protein's structure. The PDB file was analyzed before docking solvents were deleted and hydrogens and other parameters was set[14]. Docking was performed via AutoDock Vina[15]. The docked files were visualized via UCSF Chimera 1.11.2 developed by Resource for Biocomputing, Visualization, and Informatics (RBVI)[16].

3. RESULT AND DISCUSSIONS

The investigated docking results were expressed in terms of binding affinity between class I hydrophobin DewA (2LSH) and atranorin. The docking results of three binding sites were listed in Table 1. The binding site 2 and 3 exhibited more promising results and good binding affinity with the atranorin. The hydrogen bonding and bond lengths provides sufficient evidence of the successful docked atranorin in binding site of DewA. The most significant docked results were exhibited in the Fig. 1 and 2. The class I hydrophobin Dew A protein was isolated from *Aspergillus nidulans* and is fibril forming class I hydrophobin[7]. *A. nidulans* is a rare pathogen in the patients suffering from neutrophil defects[17]. *A. nidulans* is an invasive pathogen[18]. The hdrophobins present outside the cell of *A. nidulans* may represent first barrier for antibiotics[7, 19]. The successful docking of atranorin provides the insight in the biofilm degration of *A. nidulans* and its future potential as a biofilm degrading agent.

Table 1: Virtual docking results of DewA with Atranorin.

S.No.	Binding site	State	Score	RMSD l.b.	RMSD u.b.	HBond (all)	HBond Ligand Atom	HBond Receptor Atom	Ligand	Amino acid residue	Bond Length A°
1	1	Viable	-4.7	0.0	0.0	0	0	0	-	-	-
2	1	Viable	-4.7	1.683	3.775	0	0	0	-	-	-
3	1	Viable	-4.3	2.109	3.848	0	0	0	-	-	-
4	1	Viable	-2.7	2.048	7.446	0	0	0	-	-	-

5	1	Viable	-2.7	2.679	6.865	0	0	0	-	-	-
6	1	Viable	-2.5	2.202	5.161	0	0	0	-	-	-
7	2	Viable	-4.1	0.0	0.0	1	1	1	O8	Asn110	2.478
8a	2	Viable	-3.9	1.945	3.466	2	2	2	O8	Asn 110	2.357
8b									O4	Ser 65	2.559
9	2	Viable	-3.8	2.145	6.833	0	0	0	-	-	-
10	2	Viable	-3.8	2.272	6.915	0	0	0	-	-	-
11a	2	Viable	-3.5	1.589	2.782	2	2	2	O7	Ser 65	2.310
11b									O8	Asn 110	2.531
12	2	Viable	-3.5	1.606	3.229	0	0	0	-	-	-
13	2	Viable	-3.5	2.146	3.196	0	0	0	-	-	-
14	2	Viable	-3.5	1.859	7.62	0	0	0	-	-	-
15	2	Viable	-3.4	2.575	5.623	0	0	0	-	-	-
16	3	Viable	-3.3	0.0	0.0	1	1	1	O7	Ala 6	2.019
17	3	Viable	-2.9	2.675	7.175	0	0	0	-	-	-
18	3	Viable	-2.8	2.018	7.228	1	1	1	O3	Ala 6	1.947
19	3	Viable	-2.8	2.482	5.895	1	1	1	O6	Ala 6	2.007
20	3	Viable	-2.8	2.467	6.188	0	0	0	-	-	-
21	3	Viable	-2.6	1.885	3.57	1	1	1	O2	Ala 6	1.972
22a	3	Viable	-2.6	2.114	6.399	2	2	2	O6	Ala6	2.022
22b									O8	Lys 8	2.019
23	3	Viable	-2.6	2.072	6.079	1	1	1	O8	Ala 6	2.272
24	3	Viable	-2.6	2.679	4.703	0	0	0	-	-	-
25	3	Viable	-2.5	2.792	4.992	1	1	1	O2	Lys8	2.214

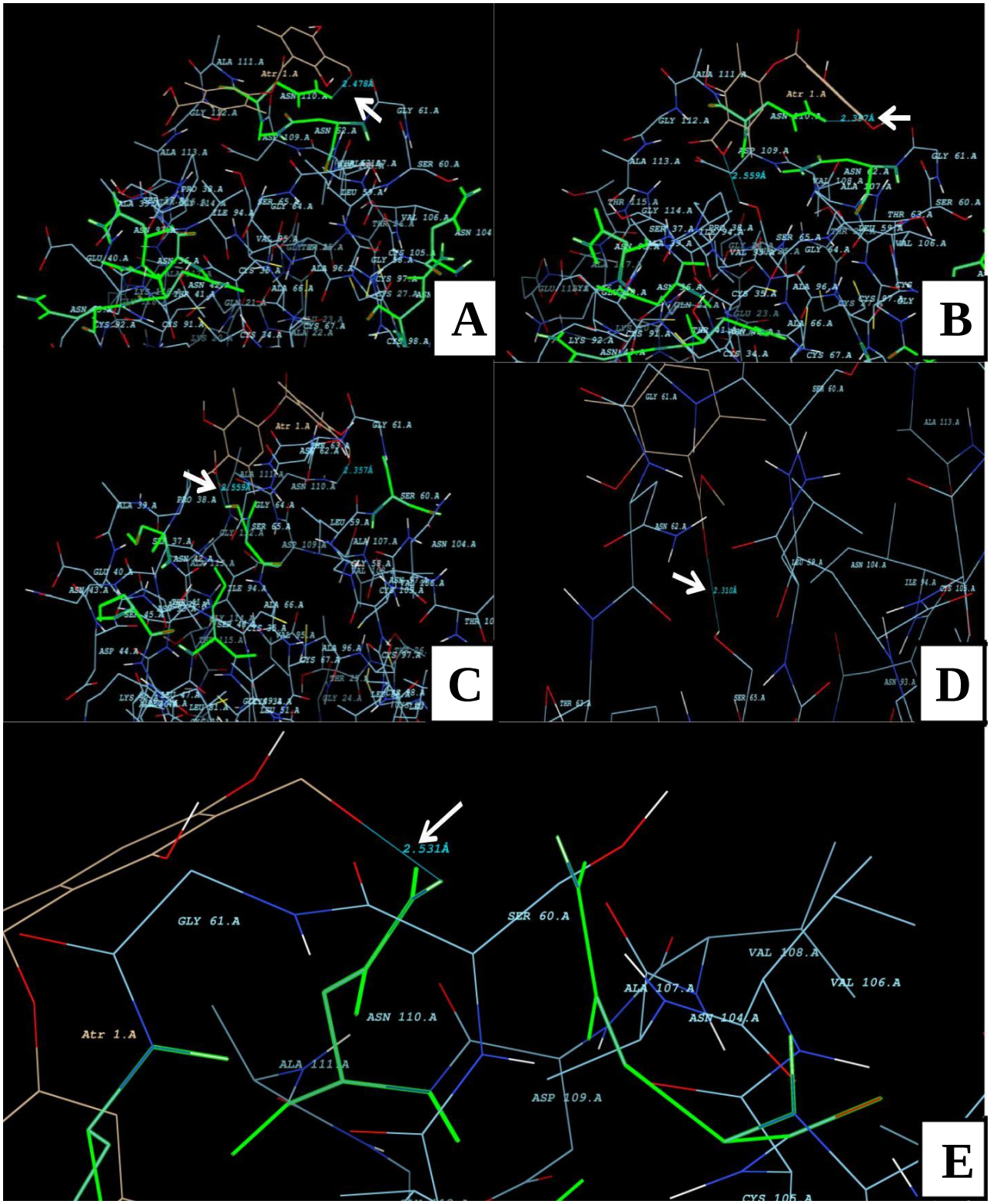

Fig. 1: Virtual docking at binding site 2 A. Hydrogen Bonding at Table 1 Sr. No. 7; B. Hydrogen Bonding at Table 1 Sr. No. 8a; C. Hydrogen Bonding at Table 1 Sr. No. 8b; D. Hydrogen Bonding at Table 1 Sr. No.11a; E. Hydrogen Bonding at Table 1 Sr. No. 11b. All the Hydrogen bonds were indicated white arrow.

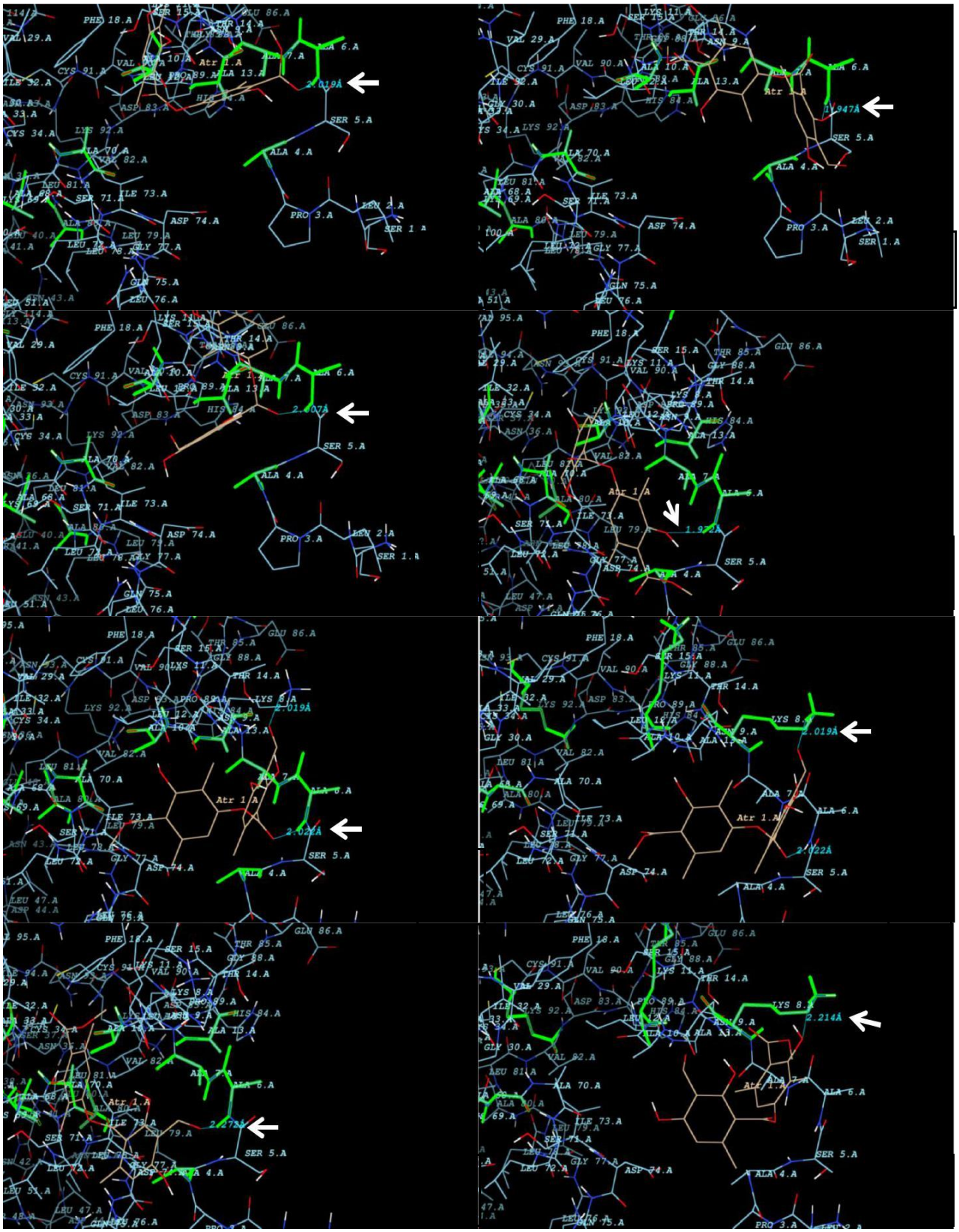

Fig. 2: Binding site 3 A. Hydrogen Bonding at Table 1 Sr. No. 16; B. Hydrogen Bonding at Table 1 Sr. No. 18; C. Hydrogen Bonding at Table 1 Sr. 19; D. Hydrogen Bonding at Table 1 Sr. No. 21; E. Hydrogen Bonding at Table 1 Sr. No. 22a; F. Hydrogen Bonding at Table 1 Sr. No. 22b; G. Hydrogen Bonding at Table 1 Sr. No. 23; H. Hydrogen Bonding at Table 1 Sr. No. 25. All the Hydrogen bonds were indicated white arrow.

4. CONCLUSION

Docking study of the targeted Dew A hydrophobin with atranorin concludes that atranorin is a good ligand which docks well within the binding sites of Dew A. Thus, it might play an important role in the fungal biofilm degradation in near future.

CONFLICT OF INTEREST

Author has no conflict of interest.

ACKNOWLEDGEMENTS

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

REFERENCES

1. Alexopoulos CJ, Mims CW. Introductory mycology 3rd edition. Wiley New york, 1979.

2. Stocker-Worgotter E. Polyketides and Pks genes in lichen-forming fungi: The impact of algal transfer metabolites (polyols and glucose) on the production of "lichen substances". Abstracts/Comparative Biochemistry and Physiology Part A, 2007; 14:S217.

3. Molnar K, Farkas E. Current results on biological activities of lichen secondary metabolites: A Review. Zeitschrift fur Naturforschung C, 2010; 65:157-173.

4. Pathak A, Shukla SK, Pandey A, Mishra RK, Kumar R, Dikshit A. *In vitro* antibacterial activity of ethno medicinally used lichens against three wound infecting genera of Enterobacteriaceae. Proc. Natl. Acad. Sci., India, Sect. B Biol. Sci., 2015; 86 (4):863-868.

5. Pathak A, Mishra RK, Shukla SK, Kumar R, Pandey M, Pandey M, Qidwai A, Dikshit A. In vitro evaluation of antidermatohytic activity of five lichens. Cogent Biology. 2016; 2: 1197472.

6. Pathak A, Upreti DK, Dikshit A. Antidermatophytic activity of fruticose lichen *Usnea orientalis*. Medicines, 2016; 3:24. doi:10.3390/medicines3030024

7. Morris VK, Kwan AH, Sunde M. Analysis of the structure and conformational states of DewA gives insight into the assembly of the fungal hydrophobins. Journal of Molecular Biology, 2012; 425(2):244-256.

8. Khalesi M, Zune Q, Telek S, Riveros-Galan D, Verachtert H, Toye D, Gebruers K, Derdelinckx G, Delvigne F. Fungal biofilm reactor improves the productivity of hydrophobin HFBII. Biochemical Engineering Journal, 2014; 88(2014): 171-178.

9. RSCB. [Last accessed on 2017 Aug 09]. Available from http://www.rcsb.org/pdb/home/home.do

10. National Center for Biotechnology Information. PubChem Compound Database; CID=68066, https://pubchem.ncbi.nlm.nih.gov/compound/68066 (accessed Aug. 9, 2017).

11. https://cactus.nci.nih.gov

12. Wang J, Wang W, Kollman PA, Case DA. Automatic atom type and bond type perception in molecular mechanical calculations. Journal of Molecular Graphics and Modelling, 2006; 25:247-260.

13. Zhang Z, Li Y, Lin B, Schroeder M, Huang B. Identification of cavities on protein surface using multiple computational approaches for drug binding site prediction. Bioinformatics, 2011; 27(15):2083-2088.

14. Dunbrack RL Jr. Rotamer libraries in the 21st century. Current Opinion in Structural Biology, 2002; 12(4):431-440.

15. Trott O, Olson AJ. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading. Journal of Computational Chemistry, 2010; 31:455-461.

16. https://www.cgl.ucsf.edu/chimera/. 2016

17. Segal BH, DeCarlo ES, Kwon-Chung KJ, Malech HL, Gallin JI, Holland SM. *Aspergillus nidulans* infection in chronic granulomatous disease. Medicine (Baltimore), 1998; 77(5):345-354.

18. Verweij PE, Brandt ME. *Aspergillus*, *Fusarium* and other opportunistic moniliaceous fungi. Edn 9, ASM Press, Washington D.C., 2007, pp. 1802-1838.

19. Joo H, Otto M. Molecular basis of in-vivo biofilm formation by bacterial pathogens. Cell Chemical Biology, 2012; 19(12):1503-1513.