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Research Article

BINDING AFFINITY ANALYSIS OF 16-O-ACETYL LEUCOTYLIC ACID WITH HYDROPHOBIN

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ABSTRACT

Microbial pathogens are omnipresent and forms a matrix around the cell surface known as biofilm. Biofilms acts as a barrier to the antibiotics, thus providing resistance to the cells. With the increasing reports of biofilm mediated drug resistant there is a need to search for the antibiofilm agents. In present study, the potential of 16-O-Acetyl-Leucotylic Acid, produced from *Myelochroa aurulenta* (Lichen) was investigated against class I hydrophobin protein. Hydrophobins are the the proteins present outside the cell in the biofilm matrix. The virtual docking of ligand in the binding sites of hydrophobin were performed for the analysis of interaction between two. The successful docking of ligand into the protein binding sites exhibited the potential of 16-O-Acetyl Leucotylic acid as an antibiofilm agent.

INTRODUCTION

Pathogenic fungi are responsible for many human diseases all around the globe and the antifungal agents have been used since long time for the cure of fungal infection. These infectious pathogens secretes polysaccharides outside the fungal cell which surrounds the cell and form a layer or matrix, known as biofilm (Donlan, 2002). It has been observed that biofilm encapsulated cells are more resistant to mortality when compared to detached cells (Uppuluri *et al*., 2010). In recent years, biofilm mediated cell resistance to antifungal agents has become a major concern (Fanning and Mitchell, 2012; Borghi *et al*., 2015). Hydrophobins, a type of protein secreted by the cell is one of the component of fungal biolfilm (Kwan *et al*., 2006; Morris *et al*,. 2012; Khalesi *et al*., 2014). In present study, the binding affinity of 16-O-Acetyl-Leucotylic Acid with class I hydrophobin was investigated. 16-O-acetyl-leucotylic acid, produced by the lichen *Myelochroa aurulenta,* is known for its antiproliferative property (Tokiwano *et al*., 2009).

MATERIALS AND METHODS

Targeted Protein

Protein structure was downloaded from RCSB: Hydrophobin protein EAS (PDB ID: 2FMC) (RCSB, 2017).

Ligand Accession

16-O-Acetyl-Leucotylic Acid three dimensional structure has been downloaded from PubChem compound database (NCBI, 2017).

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The pre dock adjustment was made via CADD Group Chemoinformatics Tools and User Services (CADD, 2017; Wang *et al*., 2006).

Molecular Docking

Before docking active binding sites were analyzed via Metapocket 2.0 (Zhang *et al*., 2011). The protein was prepared before docking via deleting solvents and unwanted residues (Dunbrack, 2004). Virtual docking was performed with the help of AutoDock Vina (Trott and Olson, 2010). The docked files were visualized with the help of Chimera 1.11.2 (Chimera, 2016).

RESULTS AND DISCUSSION

The binding affinity results of ligand and the targeted protein were listed in Table 1. The hydrogen bonds calculated between the ligand and the targeted protein has been presented in the Fig 1 and 2. The presence of hydrogen bonds, after the docked ligand-molecule, exhibited the good interaction between these two. The aforementioned interaction resulted into the successful docking of 16-O-Acetyl-Leucotylic Acid in the binding sites of hydrophobin protein EAS (PDB ID: 2FMC). The interaction of ligand with the hydrophobin protein gives the clue about the potential of ligand as antibiofilm agent which might be useful in future for the disintegration of hydrophobin chains present in the biofilm matrix.

Table1 Docking results of Hydrophobin (PDB ID: 2FMC) with 16-O-Acetylleucotylic Acid

S.No.	Binding site	Score	RMSD l.b.	RMSD u.b.	HBond (all)	HBond Ligand Atom	HBond Receptor Atom	Ligand	Amino acid residue	Bond Length A°
1	1	-4.2	0.0	0.0	1	1	1	O4	Met 22	2.107
2	1	-3.0	3.585	5.659	0	0	0	-	-	-
3	1	-2.9	2.381	4.651	0	0	0	-	-	-
4	1	-2.9	3.448	5.72	0	0	0	-	-	-
5	1	-2.7	3.511	7.399	0	0	0	-	-	-
6	1	-2.7	3.635	7.541	2	1	2	O5	Gly44 Cys45	2.050 3.657
7	2	-1.0	0.0	0.0	0	0	0	-	-	-
8	2	-0.9	2.043	8.47	0	0	0	-	-	-
9	2	-0.9	3.633	6.674	0	0	0	-	-	-
10	2	-0.9	3.543	7.243	0	0	0	-	-	-
11	2	-0.8	3.616	6.723	0	0	0	-	-	-
12	2	-0.8	3.829	6.364	0	0	0	-	-	-
13	2	-0.7	3.7	6.536	0	0	0	-	-	-
14	2	-0.6	2.527	4.653	0	0	0	-	-	-
15	2	-0.5	2.675	4.267	0	0	0	-	-	-
16	2	-0.5	3.655	6.724	0	0	0	-	-	-
17	3	13.3	0.0	0.0	1	1	1	O5	Gln 20	2.103
18	3	15.0	1.428	8.618	0	0	0	-	-	-

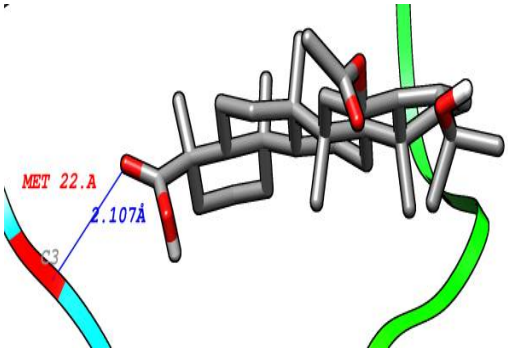

Fig 1 Hydrogen bonds at binding site 1.

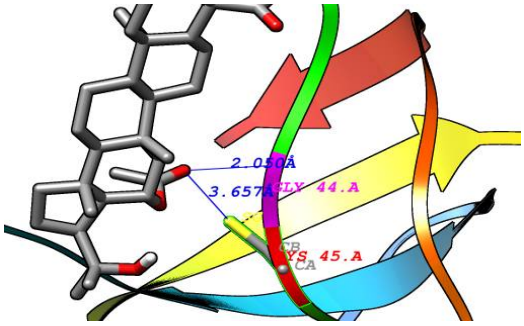

Table 1 S. No. 1 (Left); Table 1 S. No. 6 (Right).

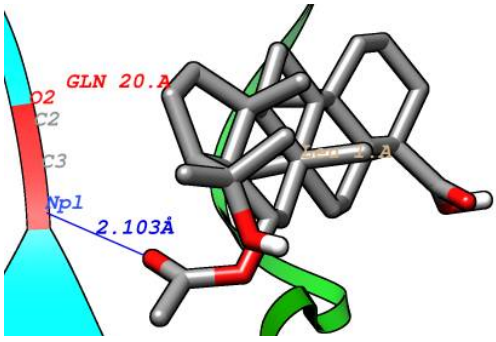

Fig 2 Hydrogen bonds at binding site 3. Table 1 S. No. 17.

CONCLUSION

The successful virtual docking of 16-O-Acetyl-Leucotylic Acid (ligand) in the binding sites of hydrophobin protein provides the hint about the potential of 16-O-Acetyl-Leucotylic Acid use as an antibiofilm agent in near future.

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