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Traditionally used lichen (*Thamnolia* sp.) compound binding affinity with aggregative adherence fimbria

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Abstract
Lichens are used traditionally all over the world. Two of such lichens viz. *Thamnolia vermicularis* and *T. subuliformis* used ethnically as tea by the folks of Yunnan, China. Thamnolic acid a compound produced by the thallus of aforementioned lichen species was investigated in present study for its binding affinity with the aggregative adherence fimbria protein of pathogenic bacteria of human intestine. Aggregative adherence fimbria protein is responsible for the recognition and adhesion of pathogen and causes the infection. The binding affinity was evaluated via Auto Dock Vina and further visualized by Chimera. The successful docking of thamnolic acid within the binding sites of targeted protein provides the insight into the potential of thamnolic acid against intestinal infection. Thus, the ethnically used tea of lichen might be helpful against the pathogenic intestine infection of humans.

Keywords: Ethnic, Lichen, *Thamnolia,* Thamnolic acid

1. Introduction
Lichens are consortium of photo and mycobiont and known for their biological activities and ecological significance (Hawksworth, 2000; Molnar and Farkas, 2010). Lichens have been used traditionally and ethnomedicinally, one of such lichen is *Thamnolia vermicularis* and *T. subuliformis* used traditionally as tea by the folks of Yunnan Province of China (Wang *et al*., 2001). Thamnolia sp. contains a specific compound thamnolic acid (Singh and Sinha, 2010). Aggregative adherence fimbria proteins are the proteins responsible for the host recognition and adhesion of the pathogenic bacteria *Escherichia coli* in the human intestine mucosa (Berry *et al*., 2014). The pathogenic strains of E. coli are responsible for diarrhoea and unirary tract infections (UTI) in the human intestine (Bennington-Castro, 2017). So, whether the ethnically used *Thamnolia* sp. tea have the potential against UTI was investigated.

2. Materials and Methods
2.1 Targeted Protein
Protein structure was downloaded from RCSB: Aggregative adherence fimbria proteins (PDB ID: 2MPV) (RCSB, 2017).

2.2 Ligand Accession
Thamnolic Acid three dimensional structure has been downloaded from PubChem compound database (NCBI, 2017). The pre dock adjustment was made via CADD Group Chemoinformatics Tools and User Services (CADD, 2017; Wang *et al*., 2006).

2.3 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).

3. Results and Discussion
The binding affinity of thamnolic acid into the binding sites of aggregative adherence fimbria protein were tabulated in Table 1. The virtual docking of ligand (thamnolic acid) into the binding sites of protein was successful with several hydrogen bonds at different conformations. The hydrogen bonds were represented in Fig 1. The binding of thamnolic acid might disturb the regular physiological function of aggregative adherence fimbria protein

Resulting into the inhibition of recognition and adherence of pathogen in human intestine. Thus, the traditional drink of *T. vermicularis* and *T. subuliformis* might be helpful against the UTI. The top of this paragraph illustrates a sub-subheading.

Table 1: Docking results of thamnolic acid in binding sites of aggregative adherence fimbria protein.

S. No.	Binding site	Score	RMSD l.b.	RMSD u.b.	Bond Length A°
1	1	-6.0	0.0	0.0	2.568 2.091
2	1	-5.4	1.874	6.387	2.550 1.985
3	1	-5.4	1.068	2.934	2.789 2.455
4	1	-5.3	1.763	5.461	2.467 2.426 2.379
5	1	-5.2	1.755	6.256	2.644 2.414
6	1	-5.0	1.541	2.608	-
7	1	-4.7	1.697	6.109	2.416
8	1	-4.4	2.07	7.302	2.402
9	1	-4.2	1.581	6.589	2.073
10	1	-4.1	2.098	6.941	-
11	2	-4.4	0.0	0.0	2.509 1.586 2.219
12	2	-3.8	1.839	3.954	-
13	2	-3.3	1.747	5.874	2.248 2.438
14	2	-3.2	1.473	5.874	1.903 2.407
15	2	-2.0	1.88	3.669	2.730 2.327
16	2	-1.9	1.789	2.575	2.802
17	3	-4.8	0.0	0.0	2.387 1.984
18	3	-4.0	2.008	3.951	1.912
19	3	-3.5	1.776	3.044	2.306
20	3	-3.2	2.023	4.661	-
21	3	-3.1	1.928	4.753	1.932 1.981
22	3	-2.2	1.938	4.872	-
23	3	-2.1	2.226	6.206	-
24	3	-1.9	2.092	5.062	1.758
25	3	-1.9	2.227	5.407	2.236

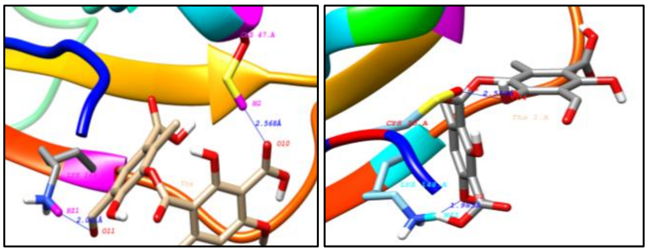

Fig 1: Hydrogen bonds representation for Table 1 S. No. 1 (Left) S. No. 2 (Right).

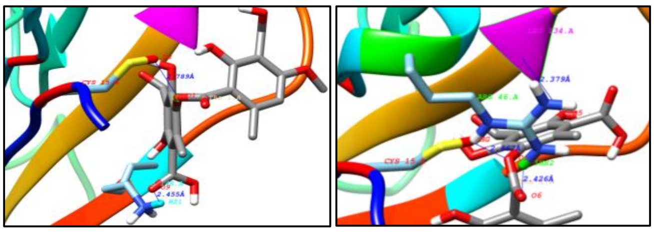

Fig 2: Hydrogen bonds representation for Table 1 S. No. 3 (Left) S. No. 4 (Right).

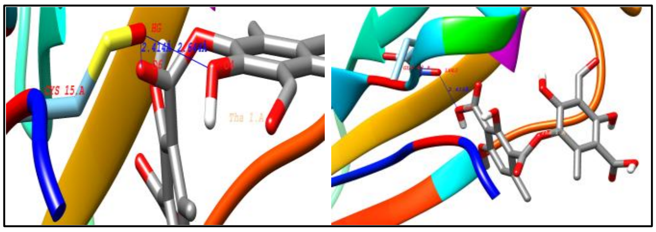

Fig 3: Hydrogen bonds representation for Table 1 S. No. 5 (Left) S. No. 7 (Right).

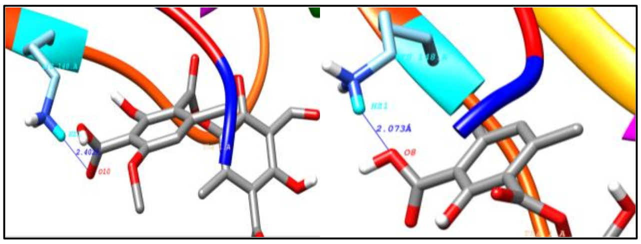

Fig 4: Hydrogen bonds representation for Table 1 S. No. 8 (Left) S. No. 9 (Right).

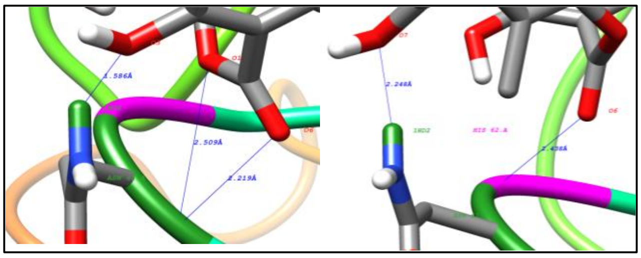

Fig 5: Hydrogen bonds representation for Table 1 S. No. 11 (Left) S. No. 13 (Right).

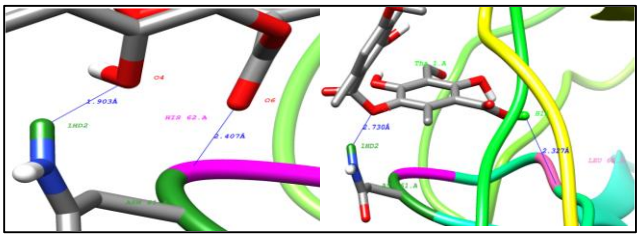

Fig 6: Hydrogen bonds representation for Table 1 S. No. 14 (Left) S. No. 15 (Right).

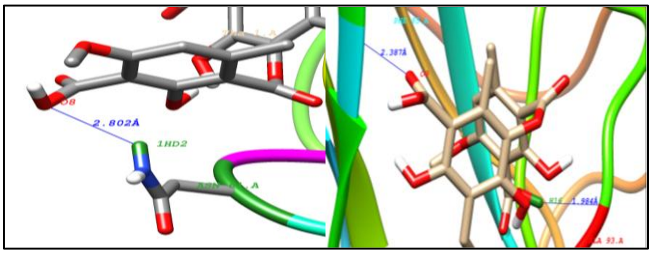

Fig 7: Hydrogen bonds representation for Table 1 S. No. 16 (Left) S. No. 17 (Right).

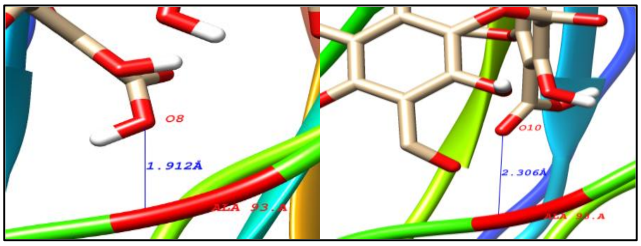

Fig 8: Hydrogen bonds representation for Table 1 S. No. 18 (Left) S. No. 19 (Right).

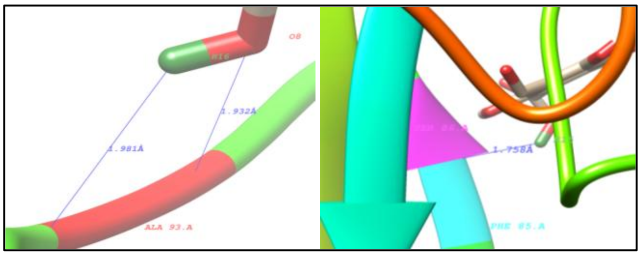

Fig 8: Hydrogen bonds representation for Table 1 S. No. 21 (Left) S. No. 24 (Right).

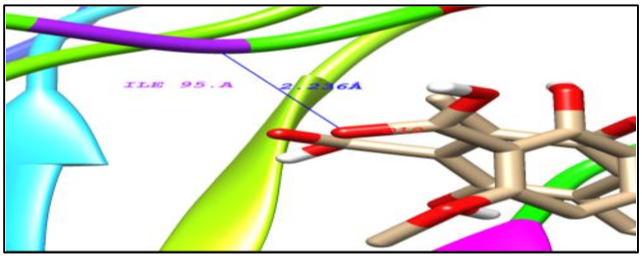

Fig 8: Hydrogen bonds representation for Table 1 S. No. 25.

4. Conclusion

The successful docking of ligand and protein in present study exhibited the potential of traditionally drinkable tea of *T. vermicularis* and *T. subuliformis* have the potential to fight against UTI.

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