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Phytochemical Screening and *In Silico* Analysis of Some Crude Stem Extracts against Skin Diseases

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Abstract— Curcumin is an important phytochemical present in curcuminoids (rhizome plants) essential; for control of skin diseases. The phytochemicals are more in *Zingiber officinale* followed by *Aloe barbadensis, Curcuma longa* and *Curcuma angustifolia.* Amino acids, Proteins, carbohydrates, tanins and terpenoids were almost present in all the selected plants. The plant *Curcuma angustifolia* aqueous extract has good composition of terpinoids and analysed for *in silico studies* of Curcumin with *Staphylococcus aureus, Streptococcus pyogenes* and *Trichophyton rubrum* proteins. Curcumin has shown good binding affinity with streptococcal superantigen (SSA) from *Streptococcus pyogenes (-90.62 KCal/Mol)* followed by exfoliative toxin B in *Staphylococcus aureus* (-85.01 KCal/Mol) and Aspartate Semialdehyde Dehydrogenase from *Trichophyton rubrum* (-82.96 KCal/Mol). Curcumin has shown good in silico activities against proteins/ antigens for skin diseases. Further isolation and identification through wetlab studies provide good scope in the field of phytochemistry.

Keywords— Phytochemical screening, *in silico* studies, curcumin

I. INTRODUCTION

Skin diseases are the major health problems in the present decades, produces rashes, skin lesions and disorders in several parts of human system like hair, nail, and mucosa. The solving of problems are key facts pertaining to epidemiology, physical examinations, clinical symptoms, diagnosis and treatment [1]. In the present healthcare system, Skin disease is noted as one of the top fifteen groups of medical conditions that was mostly prevalent with more cost spending on medicines and operations increased between 1987 and 2018 [2.3]. The impact on changes in quality of life made effects of 22 leading categories of skin diseases made the prevalence and economic burden in human life.

India is known for its rich biological diversity that contain medicinally important bioactive compounds that are using as traditional medicines in the treatment of diseases and disorders [4,5]. Phytochemicals are categorised as primary and secondary constituents that will exhibit medicinal and physiological activities. The main primary constituents like chlorophyll, proteins, sugars, amino acids and lipids are important in daily life whereas secondary constituents like Terpenoids, Tannins, Phlobatinins, Phenols, and Quinones are important of healthcare and metabolic activities.

II. RELATED WORK

Tannins, Phlobatinins, Phenols Quinones and Terpenoids play important pharmacological activities like anti-inflammatory and antifungal activities [6,7]. Curcumin, also known as diferuloylmethane is a phytochemical compound that shows good activity against skin diseases. turmeric contains curcumin as main component used for the treatment of wounds and skin diseases from ancient times in old Hindu medicine *[8]*. *Staphylococcus aureus,* β-hemolytic streptococci like *Streptococcus pyogenes, Herpes simplex* and *Trichophyton rubrum* are the most common microorganisms causing skin diseases [9]. The well known terpenoids like curcuminoids are found in turmeric, used for presence of aromatic qualities and play an important role in traditional herbal remedies. In the present study, Phytochemical screening of stem extracts of four different plants *(Curcuma angustifolia, Curcuma longa, Aloe barbadensis and Zingiber officinale)* from 4 solvents (A-Aqueous, E – Ethanol, M – Methanol, EA – Ethyl Acetate) were tested and analysed with curcumin for effects on microbial skin disease proteins streptococcal superantigen (ssa) from *Streptococcus pyogenes*, exfoliative toxin b in *staphylococcus aureus* and aspartate semialdehyde dehydrogenase from *Trichophyton rubrum*.

III. METHODOLOGY

A. Preparation of plant extracts

The stems of the four different plants (*curcuma angustifolia*, *curcuma longa*, *aloe barbadensis* and *zingiber officinale*) were removed from the plants and then washed under running tap water to remove soil and dust. the plant samples were air dried for few weeks and the stems were crushed into powder in a maxi and stored in polythene bags.
the plant powders were taken in different test tubes and solvents (a- aqueous, e – ethanol, m – methanol, ea – ethyl acetate) was added respectively such that plant powder soaked in it and shaken well. the solutions were then filtered with the help of filter paper. the filtered extracts of the selected plant samples were taken and used for further phytochemical analysis

B. Phytochemical analysis

there are different tests used for screening for phytochemicals such as carbohydrates (molisch test), aminoacids (ninhydrin test), protein (biuret test), terpenoids, tannins, phlobatinins, phenols and quinones.

1. **Test for aminoacids:**
   to 2ml of the extract, 2ml of ninhydrin reagent is to be added and keep the solution in hot water bath for 15 minutes. the formation of purple colour indicates the presence of aminoacids in the sample.

2. **Test for proteins:**
   to 2ml of extract, 2ml of biuret reagent is to be added. an appearance of violet colour ring indicates the presence of protein.

3. **Test for carbohydrates**:
   to 2ml of extract add 2 drops of molisch's reagent and mix the solution. nearly 2ml of conc.h_2so_4 is to be added drop by drop from the sides of the test tube. a reddish violet colour appearance at the junction of two layers immediately indicates the presence of carbohydrates.

4. **Test for terpenoids:**
   to 2ml of extract add 2ml of chloroform and 3ml of conc.h_2so_4. formation of a monolayer of reddish brown coloration of an interface shows a positive result for the terpenoids.

5. **Test For Tannins**:
   To 5ml of extract, few drops of 1% of lead acetate are to be added. An yellow coloured precipitate formed in the test tube shows the presence of tannins.

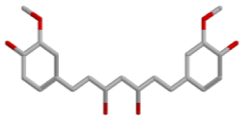
6. **Test For Phlobatinins :**
   To 2ml of extract add 1% aqueous HCL and boiled for few minutes. A red precipitate formed and deposited in the test tube is an evidence for the presence of phlobatinins.

7. **Test For Phenols:**
   To 2ml of extract, 3ml of ethanol and a pinch of $FeCl_3$ is to be added. The formation of greenish yellow color solution indicates the presence of phenols.

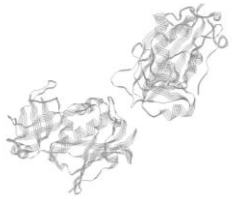
8. **Test For Quinones:**
   To 2ml of Extract, 3ml of Conc.HCl is to be added . Formation of green colour solution indicates the presence of quinones.

The structure of drug "curcumin" as pdb file was obtained from DrugBank. The structures of receptors 1BXT,1DT2 and 4ZHS as pdb files were obtained from Protein Data Bank. The activity of drug against skin disease causing proteins were analysed in the *in silico* studies. Docking studies were conducted using iGEMDOCK v2.1.

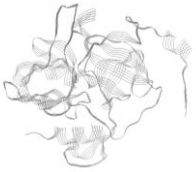
A.Structure of Curcumin



B.Structure of 1BXT



C.Structure of 1DT2



D. Structure of 4ZHS

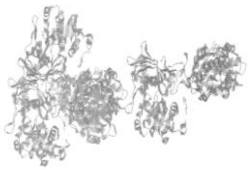


Figure 1: Drug and Receptors selected in present study

C. System Properties

Processor:	Intel(R) Pentium(R) Dual CPU E2160 @ 1.80GHz 1.80 GHz
Installed memory (RAM):	1.99 GB
System type:	32-bit Operating System

IV. RESULTS AND DISCUSSION

The phytochemical characteristics conducted in four different plants (*Curcuma angustifolia*, *Curcuma longa*, *Aloe barbadensis* and *Zingiber officinale*) were shown in Table 1. The phytochemicals are more in *Zingiber officinale* followed by *Aloe barbadensis*, *Curcuma longa* and *Curcuma angustifolia* (Table 1). Amino acids, Proteins, carbohydrates, tanins and terpenoids were almost present in all the selected plants. The plant *Curcuma angustifolia* aqueous extract has good composition of terpinoids and analysed for *in silico* studies of Curcumin with *Staphylococcus aureus*, Streptococcus *pyogenes* and *Trichophyton rubrum* proteins.

The docking of Curcumin with selected receptors were shown in Table 2. Curcumin has shown good binding affinity with streptococcal superantigen (SSA) from *Streptococcus pyogenes* (-90.62 KCal/Mol) followed by the exfoliative toxin B present in *Staphylococcus aureus* (-85.01 KCal/Mol) and Aspartate Semialdehyde Dehydrogenase from *Trichophyton rubrum* (-82.96 KCal/Mol). Curcumin has shown good *in silico* activities against proteins/ antigens for skin diseases. Further isolation and identification through wetlab studies provide good scope in the field of phytochemistry.

Curcumin is a yellow substance acts as a potent anti-inflammatory agent present in the roots of the plant Curcuma plants [10,11]. The compound has the ability to inhibit carcinogenesis of murine skin. Curcumin, a polyphenolic compound is derived from a dietary spice turmeric can both prevent and treat cancer [12,13]. The rhizomes also has rich in essential oils with biomedical significance for treatment of skin diseases. Phytochemical and *in silico* studies are very much important in the present decades to crack long history of traditional uses ranging from folk medicine to treatment of emerging diseases [14,15].

V. CONCLUSION and Future Scope

Curcumin is an important phytochemical present in rhizome plants. The compound has shown good activities and was important for metabolism of skin. To avoid skin diseases, curcuminoids are highly essential for humans.

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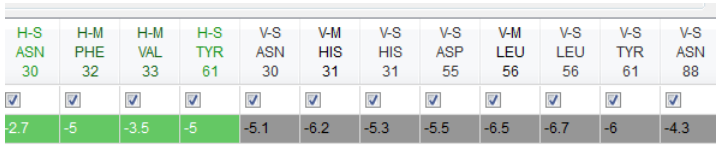
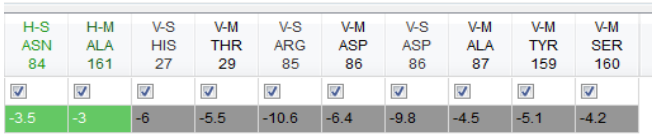
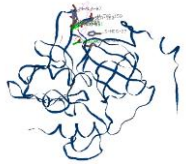
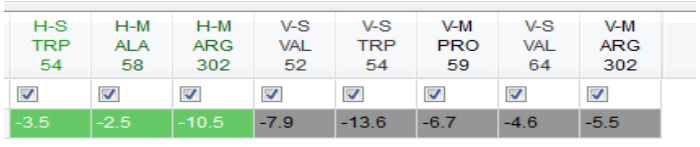
Table 1: Phytochemical characteristics of some medicinal plants

Name of the Compound	***Curcuma angustifolia***				***Curcuma longa***				***Aloe barbadensis***				***Zingiber officinale***			
	A	**E**	**M**	**EA**	**A**	**E**	**M**	**EA**	**A**	**E**	**M**	**EA**	**A**	**E**	**M**	**EA**
Amino acids	+	+	+	++	++	++	++	++	+++	++	+++	++	+++	+++	++	+++
Protein	++	++	+	+	++	+	+	+	_	+	+	++	+	+++	_	++
Carbohydrate	+++	++	_	_	++	++	+	+	+++	++	++	++	+++	+++	++	++
Terpenoid	+++	+++	+	--	++	+	++	++	_	++	++	+	++	+++	++	+++
Tannins	_	+	+	+	++	_	_	+	+	_	++	_	+	++	++	+
Phlobatinins	--	--	--	+	--	--	--	--	+	--	+	--	_	_	_	_
Phenols	_	_	+	_	_	_	_	_	+++	+	+	+	+	+	+	+
Quinones	_	_	_	_	_	_	_	_	++	+	+	++	_	_	_	_

Note: 1. A – Aqueous, E – Ethanol, M – Methanol, EA – Ethyl Acetate
2. +++Strongly positive (deep Intense colour); ++ Moderately positive ; + fairly positive; _Negative

Table 2: Binding energy (in Kcal/Mol), Binding site and Interaction profile of Curcumin with selected receptors

PDB	Energy	Binding site and Interaction profile
1BXT **STREPTOCOCCAL SUPERANTIGEN (SSA) FROM STREPTOCOCCUS PYOGENES** (bacterial superantigen affinities/ Pathogenic Strain)	**-90.62**	 
1DT2 *EXFOLIATIVE TOXIN B in Staphylococcus aureus* *(scalded skin syndrome)*	**-85.01**	 
4ZHS *Aspartate Semialdehyde Dehydrogenase from Trichophyton rubrum* *(Dermatophytoses/ Potential drug target)*	**-82.96**	 

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