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PREVENTION OF *Staphylococcus aureus* CAUSING ECZEMA BY *Glycyrrhiza glabra*

SUSHREE SUSMITA PALEI[1], KABYASHREE DIPTIMAYEE SWAIN[1], DEBASMITA DAS[1], MUKUNDJEE PANDEY[1,2*] AND DIPANKAR BHATTACHARYAY[1]

[1]Centurion University of Technology and Management, Odisha, India.
[2]Go to Market Laboratory, Gram Tarang, Odisha, India.

AUTHORS' CONTRIBUTIONS

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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Short Research Article

ABSTRACT

Glycyrrhiza glabra is one of the therapeutic plants that show the adequacy for the disorder. Thus, the present study is an attempt to check the efficacy of *G. glabra* in the prevention and cure of eczema. "Phytochemicals" are non-nutritive compounds found or obtained from plants. It has been reported that *Glycyrrhiza glabra* plant extract is used to manage eczema, which has different phytochemical compounds. Eczema is caused by the causal organism, such as *Staphylococcus aureus.* Aspatate-semialdehyde-dehydrogenase is one of the key enzymes involved in its biochemical pathway. By using "Biovia Discovery Studio", the "molecular docking of the phytochemicals" with the enzymes was studied. The strength of the interaction was evaluated based on "-CDOCKER energy and-CDOCKER interaction energy". "High positive values for both the parameters indicated that out of different phytochemicals" 3-bromo-2-pentanol and liquiritigenin can effectively deactivate the aspatate-semialdehyde-dehydrogenase enzyme thereby interrupting the life cycle of *S. aureus*. The phytochemicals screening of the *G. glabra* root revealed the presence of alkaloids, glycocides, carbohydrates, starches, phenolic compounds, flavonoids, proteinsetc. The showed the memory enhancement, antimicrobial, anticancer activity. Many plants with their optional metabolites have a long history of use in current western medication and specific frameworks of customary medication and are the wellsprings of significant medications, such as "atropine, codeine, dioxin, morphine, quinine and vincristine and so on". The utilization of home-grown medication in have created nations has extended forcefully in the last of the twentieth century. The pharmacological treatment of sickness started a while in the past with the utilization of herbs.

Keywords: Phytochemical; *Glycirrhiza glabra*; *Staphylococcus aureus*.

1. INTRODUCTION

Since ancient occasions, for treatment and fix of illnesses has been one essential worries of humankind. Nearby specialists had used local plants and herbs for a considerable length of time everywhere throughout the world to treat an assortment of infirmities and these have displayed clear pharmacological exercises [1]. The variety name Glycyrrhiza was derived from the Greek glykys, for (sweet) and rhiza, for (root). The species name glabra was gotten from the Latin glaber, which implies (smooth) or (uncovered) and

**Corresponding author: Email: mukundjee.pandey@cutm.ac.in;*

alludes to the smooth husks. The plant regular name were: Arabic: Sus, Irik Sus; English: licorice, licorice-root; Hindi: Mulhatti, Jethima [2]. The plant showed a wide range of pharmacological activities including antimicrobial, antioxidant, anticancer, hypolipidemic, cardiovascular, central nervous, respiratory, immunological, anti-inflammatory, analgesic antipyretic and many other pharmacological effects [3].

The information of plant properties was acquired by an ancient society that passed down from generation to generation until today. Plants show the various "pharmacological activities such as antimicrobial, antioxidant, anticancer, hypolipidemic, cardiovascular, central nervous, respiratory, immunological, anti-inflammatory, analgesic antipyretic also [3].

Nature has been a wellspring of therapeutic specialist a large number of years. The restorative estimation of plants lies in some compound substances that produce a distinct phytochemical activity in the human body is called phytochemicals, which can be utilized for a helpful reason. The phytochemicals might be gotten from various pieces of plant-like bark, leaves, root, stem, natural product, bloom, etc. A significant number of therapeutic plants are utilized as species and food thing. They additionally assumed a significant job in numerous prescriptions like allopathic medication, natural medication, aromatherapy [4].

The stem, roots and leaves were screened to got rough methanol (MeOH), chloroform, ethyl acetic acid derivation (ELOAC), n-butanol (Bt-OH) and fluid portions [5].

Medicinal plants are the foundation of many drugs prescribed today in the modern medicinal system. For example, the herb foxglove is the source for digital and the herb salicin is the source for aspirin, vincristrine, and vinblastine from Vinca minor atropine from *Atropa belladonna*, newly ensuring scientific techniques and approaches have been used in the growing area of medicinal plant research, for investigation of constituents and determination of the biological activity of medicinal plants. Plants that demonstrated anticancer, antioxidant, anti-inflammatory, immunostimulatory and antimicrobial properties have believed research attention [5]. Most usually utilized a piece of *G. glabra* is root. It is sweet in taste and alleviating in nature and has antibacterial and mitigating properties [6].

Mulethi belongs to Family: Fabaceae. Its extract is used to cure diseases like eczema. Mulethi is known to contain phytochemicals like phloretin-3-5-Di-C-glucoside, cornstarch, 3-Bromo-2-pentanol, rosmarinicacid, (+)catechins, 1-hexanol, liquiritigenin, linalool-oxide, tannic acid, cortisone, sucrose, cholesterol, pyraine, glycyrrhizin and liquiritin. Licorice root extracts are beneficial in the treatment of eye disease, throat infection, peptic ulcer, liver disease, joint disease, arthritis condition, immunodeficiency, cancer, diabetes, eczema, kidney disease, etc. It has also been shown that extracts help regulate the estrogen–progesterone ratio and gastrointestinal system [7].

Mulethi is a sweet root and used to get ready for different medications. Its underlying foundations are used to fix skin issues, ulcer, jaundice and so forth there is a high likelihood that these phytochemicals assume a significant job in relieving dermatitis. Anyway, there is no report distinguishing the particular phytochemical capable to fix skin inflammation. A gathering of microscopic organisms has a place with genous *Staphylococcus aureus* that causes eczema [8].

Mulethi has been proven as an extraordinarily fruitful plant, which is as yet significant in present-day age-medication because of its flexibility and tirelessness [8]. Proof for the helpful impacts of chosen plants is commonly founded on tests exhibiting a natural action in an important in vitro bioassay or trials utilizing creature models [9].

An enormous individual from an organic dynamic mix has been confined from *Glycyrrhiza* species where triterpene, saponins and flavonoids are the fundamental constituents which show wide natural movement [9,10]. The microbes which is answerable for skin inflammation is a coccus-molded Gram-positive microscopic organisms disease *S. aureus* is a typical microorganisms illness that impacts the skin. Dermatitis is where patches of skin become aggravated, irritated, red, split and unpleasant of human skin. Humans become tainted most habitually through debased water or food, stress, organisms, hot and cold temperature [11].

A large number of the restorative plants are utilized as flavors and food things. They additionally assumed a significant job in numerous medications like allopathic medication, natural medication, elective medication, homeopathy and fragrance based treatment [12].

This investigation tries to find the recognizable proof of the phytochemical of *G. glabra* useful to cure skin inflammation caused by *Staphylococcus aureus sp.*

Table of phytochemicals:

1	Liquiritigenin
2	3-bromo-2-pentanol
3	Geraniol
4	Terpinen-4-ol
5	Linalool
6	Isocoumarine
7	(+)-catechin
8	Cornstarch
9	Liquirtin
10	Rosemarenicacid
11	Sucrose

2. MATERIALS AND METHODS

2.1 Software Used

"Discovery Studio Module of Biovia software (Dassault Systemes of France)" was utilized for investigation. The product uses "machine learning techniques" to predict the level of "molecular interaction" [13].

2.2 Methodology

2.2.1 List of phytochemicals

Phytochemicals" are created by plants as optional metabolites to shield them from predators. The potential dangers to plants incorporate microscopic organisms, infections, and growths. At the point, these plants or their parts are devoured by people these "phytochemicals" ward off dangers to wellbeing. A few phytochemicals have been utilized as toxic substances and others as customary medication. Distributed works demonstrated that *G. glabra* contains phloretin-3-5-d-C-glucoside, cornstarch, 3-Bromo-2-pentanol, rosmarinic corrosive, (+)-catechins, 1-hexanol, liquiritigenin, linalool-oxide, tanic corrosive, cortisone, sucrose, cholesterol, pyrazine, glycyrrhizin, liquiritin, chrysin. It has just been set up that *G. glabra* plant having a place with Fabaceae family can possibly help controlling skin inflammation. This work is centered around recognizable proof of the specific phytochemical liable for repressing and controlling of skin inflammation.

2.2.2 Enzyme found in *Staphylococcus aureus*

It has been accounted for that dermatitis can cause because of *S. aureus* invasion. Different "metabolic cycles" have been found in the bacterial life cycle for its endurance. These metabolic cycles are controlled by various chemicals. Brenda protein database was utilized to distinguish and list various chemicals found in *S. aureus* microscopic organisms. It has been discovered that aspartate semialdehyde dehydrogenase catalyst (protein database code 3VOS) is associated with threonine digestion and exceptionally significant for the endurance of the specific organism.

2.2.3 Molecular docking

Molecular docking technique" has been utilized to recognize the phytochemical from the plant remove, that go about as a ligand and structure a solid covalent bond with the bacterial protein to effectively hinder the microorganism. The "Discovery studio module of Biovia programming" was utilized for recognizing sub-atomic communication and perform sub-atomic docking. In this procedure first the sdf documents for the phytochemicals found in the *G. glabra* plant were downloaded from the site. The protein database code of the aspatate Semialdehyde dehydrogenase compound was recognized from the site. The dynamic site of the catalyst was distinguished by the "receptor depression" convention found under the "receptor-ligand connection" menu. Atomic docking was finished utilizing the "CDOCKER convention of Biovia software" under "receptor-ligand cooperation". The compound particle was treated as the receptor atom and the phytochemical was treated as the ligand. The high positive estimation of those pointers introduced decent cooperation between the ligand and the receptor. Subsequently, the collaborations with high qualities may show the significant phytochemical liable for restoring the malady.

3. RESULTS AND DISCUSSION

Fig. 1 shows the dynamic site of the aspatate semialdehyde dehydrogenase catalyst. It shows up as light green shading. CDOCK is a sub-atomic elements (MD) mimicked strengthening based calculation. It is a framework based atomic docking strategy and improved for exactness. The ligand adaptations were acquired by "Molecular Dynamic Methods".

"-CDOCKER" vitality was determined dependent on inward ligand strain vitality and receptor-ligand association vitality. "-CDOCKER communication" connotes the vitality of the non-reinforced association between the protein and the ligand. The standards for best communication was picked dependent on a) high positive estimation of -CDOCKER vitality and b) small contrast between -CDOCKER vitality and -CDOCKER collaboration vitality [14].

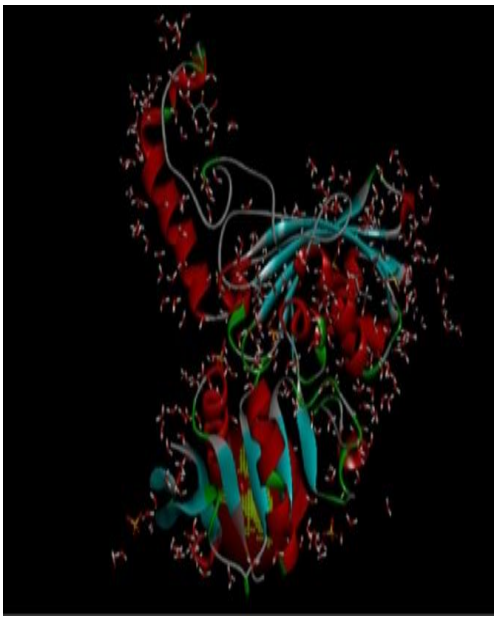

Fig. 1. Active site of aspatate semialdehyde dehydrogenase enzyme

Table 1 shows that aspatate semialdehyde dehydrogenase-liquiritigenin association has the most noteworthy positive estimation of -CDOCKER energy (9.73518) and least estimation of the distinction (7.79372) between - C DOCKER cooperation vitality and - C DOCKER vitality followed by 3-bromo-2-pentanol. Consequently the outcomes showed that liquiritigenin and 3-bromo-2-pentanol can adequately deactivate the aspatate semialdehyde dehydrogenase compound in this manner intruding on the natural pattern of *Staphylococcus aureus sp.* Higher positive qualities for liquiritigenin demonstrated that it was the most dynamic fixing against *Staphylococcus aureus sp.*. Then again, Geraniol, terpinen-4-ol, linalool, isocoumarine, (+) - catechins can deactivate the protein to a little degree (negative - CDOCKER vitality however positive - CDOCKER connection vitality). Cornstarch, Rosemarie corrosive, sucrose, liquirtin can't deal with Aspatate Semialdehyde dehydrogenase catalyst. Subsequently, the key phytochemicals forestalling Eczema brought about by *Staphylococcus aureus sp.* are liquiritigenin and 3-bromo-2-pentanol.

Table 1. "Results of C Docking of phytochemicals" with aspatate semialdehyde "dehydrogenase (receptor)"

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and -CDOCKER energy
1	Liquiritigenin	9.73518	17.5289	7.79372
2	3-bromo-2-pentanol	6.00051	12.9721	6.97159
3	Geraniol	-24. 9095	25.2743	50.1838
4	Terpinen-4-ol	-20. 992	10.2946	31.2866
5	Linalool	-152. 676	-49. 3661	-202. 0421
6	Isocoumarine	-70. 5088	-36. 8245	-33. 6843
7	(+) -catechin	-238. 31	-109. 961	-128. 349
8	Cornstarch	Failed	Failed	NA
9	Liquirtin	Failed	Failed	NA
10	Rosemarenic acid	Failed	Failed	NA
11	Sucrose	Failed	Failed	NA

4. CONCLUSION

It was recently realized "*Glycyrrhiza glabra"* has restorative activity against Eczema. *S. aureus sp.* causes the Eczema sickness. "Molecular docking activity" was performed utilizing "Discovery studio module of Biovia programming", to recognize and assess the photochemical (Phloretin-3-5-Di-C-glucoside, Cornstarch, 3-Bromo-2-pentanol, rosmarinic corrosive, (+)- catechins, 1-Hexanol, liquiritigenin, linalool-oxide, tanic corrosive, cortisone, sucrose, cholesterol, PYRAZINE, glycyrrhizin, liquiritin and so forth) and these phytochemicals have a critical deciphering collaboration with the fundamental chemical Aspatate Semialdehyde dehydrogenase of the pathogenic microorganism . It was discovered that liquiritigenin and 3-bromo-2-pentanol can shape solid bond with the protein effectively repressing the metabolic pattern of the microorganism. geraniol, terpinen-4-ol, linalool, isocoumarine were seen as very little successful in deactivating the compound of the organism. cornstarch, sucrose, rosemeric corrosive, liquirtin cannot deactivate the protein. Along these lines, this investigation could clarify that the nearness of (liquiritigenin and 3-bromo-2-pentanol gave the therapeutic qualities to *Glycyrrhiza glabra* against Eczema brought about by *Staphylococcus aureus sp.*

DISCLAIMER

The products used for this research are commonly and predominantly use products in our area of research and country. There is absolutely no conflict of interest between the authors and producers of the products because we do not intend to use these products as an avenue for any litigation but for the advancement of knowledge. Also, the research was not funded by the producing company rather it was funded by personal efforts of the authors.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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