RESEARCH PAPER

In silico screening of bioactive compounds derived from Polyherbal Oil against Seborrhea dermatitis.

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Abstract :
This study uses phytochemical analysis and molecular docking techniques to investigate the medicinal potential of Ayurvedic herbs in controlling dandruff and encouraging hair growth. Phyllanthus emblica (Amla), Eclipta alba (Bhringraj), Hibiscus rosa-sinensis, Azadirachta indica (Neem), Zingiber officinale (Ginger), Cyperus rotundus (Nagarmotha), Acacia concinna (Shikakai), Solanum indicum (Dorli), Glycyrrhiza glabra (Liquorice), Dioscorea bulbifera (Amarkand), Citrus sinensis (Orange peel), Lawsonia inermis (Henna), Bacopa monnieri (Brahmi), Cocos nucifera (Coconut oil), Trigonella foenum-graecum (Fenugreek), Simmondsia chinensis (Jojoba oil), Rosmarinus officinalis (Rosemary oil), and Lavandula angustifolia (Lavender oil) were chosen for their traditional significance. The following phytochemicals were shown to be important bioactive components: alpha-tocopherol, linolenic acid, luteolin, kaempferol, quercetin, ascorbic acid, 6-gingerol, beta-caryophyllene, camphor, linalool, ursolic acid, and linolenic acid. They obtained their 3D conformer structures in SDF format from the PubChem database. The Protein Data Bank provided the protein targets, Dihydrofolate Reductase (PDB ID: 6IJ0) and Carbonic Anhydrase XII (PDB ID: 1JD0), which are linked to the regulation of hair growth and antifungal action. MOL software was used to prepare ligands and proteins, identify receptor sites, configure grid boxes, and run docking simulations. Significant binding affinities were found by the docking studies, suggesting that the phytochemicals and protein targets have persistent interactions. The findings imply that these natural substances may serve as efficient plant-based substitutes for dandruff and hair loss treatments. This research supports the development of herbal therapies for dermatological applications by fusing contemporary computational biology with traditional Ayurvedic expertise.

Keywords : Seborrhea dermatitis, Phytoconstituents, Polyherbal Extract, Molecular docking, Ligand-receptor interaction, Essential oils

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Introduction :
Human hair typically consists of follicles of anagen, catagen, and telogen phases. [1] Hair is a complex structure made by many components that act as a unit, with the biological purpose of protecting the scalp, enhancing physical attractiveness, preventing pre-greying, rusting of hair, and preventing dandruff [2]. Hair is thought to be the most important organ in humans that defines appearance, gender differences, offers protection from extreme temperatures, and plays a role in self-defense. Although hair loss is normal and prevalent as people age, it worries people more. The younger generation has begun to experience several hair loss issues as a result of various lifestyle changes, including stress, anxiety, junk food consumption, hair styling, hair coloring, etc. The issues of split ends, hair loss, and lice are getting worse these days. Alopecia Areata is an immune-mediated skin condition that causes non-scarring hair loss in the general population. Its incidence ranges between 1.7 and 2.1 percent, with young patients between the ages of 21 and 40 experiencing a higher incidence. There is no discernible difference in the incidence of the condition between males and females. Numerous products have been developed by the hair care business to support, strengthen, and enhance hair issues [3].

The skin condition known as seborrhea dermatitis typically affects areas of the body including the face, chest, and scalp that have a high density of sebaceous glands [4]. Those with weakened immune systems have a prevalence of 34–83%, while the general population has a frequency of 1-3 percent [5]. Age, gender, immunological deficiencies, neurological and behavioral disorders, low humidity or ambient temperature, and increased sebaceous gland activity are risk factors for this condition.

Changes in skin cell function are the cause of the clinical signs of seborrhea dermatitis, which include

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scaly skin, erythema, and itching. In patients with seborrhea dermatitis, Malassezia is most likely to induce a nonspecific immune response that might lead to alterations in skin function [6]. A normal part of the skin's flora, Malassezia affects the stratum corneum in patients with seborrhea dermatitis, producing lipase, which can lead to the production of free fatty acid compounds and an inflammatory process. Additionally, fatty acids can promote this fungus's growth [7].

Stratum corneumhyperproliferation and inadequate corneocyte differentiation can result from inflammation, which can change and damage the stratum corneum barrier's function, making it easier for Malassezia to enter and making it easier for water to exit the cells.[7]Keratolytic medicines are used to treat seborrhea dermatitis by removing the stratum hyperproliferativecorneum's outer layer. Furthermore, it is believed that coal tar slows down the stratum corneum's pace of formation.[8]Malassezia can be defeated by antifungals, and the inflammatory reaction can be lessened by anti-inflammatory drugs such corticosteroid [11].

Poor adherence, resistance, and some adverse effects of the currently utilized medications are issues. Long-term corticosteroid treatment may result in adverse consequences and low patient compliance [5,12]. When antifungals are used, a number of adverse effects may occur, such as burning, skin redness, and baldness [13] Malassezia has been found to be less sensitive to voriconazole and fluconazole.[14] Furthermore, a number of Malassezia strains exhibit ketoconazole resistance.[15,16] These issues make the creation of novel therapeutic agents for the treatment of seborrhea dermatitis even more urgent.

Many studies have been published over the years regarding the potential of plants as new therapeutic agents in the treatment of seborrhea dermatitis, and several compounds have been identified and tested for their activities related to the treatment of seborrhea dermatitis. Accordingly, it is necessary to review the clinical and in vitro test data regarding the activity of several medicinal plants that have the potential to treat seborrhea dermatitis, as well as what compounds play a role in these activities. Research on medicinal plants has a great deal of potential to produce compounds with new structures and bioactivity.

Many people believe that because they are "natural" and utilized extensively in many fields, plants and herbs don't have any negative effects, interactions, or contraindications. Sadly, this is untrue; simply consider that there are poisonous and deadly plants in nature that can even be fatal. For instance, a list of 21 adverse effects of therapeutic herbs was described by Gupta and Raina [17]. The plants that have been reported are primarily utilized orally. These include matricariarecutita (travel wickness), vicarosea (chemotherapeutics and diabetes), tylophoraasthmatica (asthma), prunusvirginiana (inflammation), allium sativum (cough), colchicum autumnale (gout, rheumatism), and cassia alata (constipation). Lists of adverse consequences of plants used locally, such seborrheic dermatitis, are rare.

Seborrhea dermatitis is a frequent inflammatory disease that affects areas of the skin (such as the face, scalp, and sternum) that have a high density of sebaceous glands. Although the exact origin is uncertain, species of the common skin yeast Malassezia are implicated. Patients with HIV and those with specific neurological conditions are more likely to develop seborrhea dermatitis. The symptoms of seborrhea dermatitis include dandruff, yellow, oily scaling on the face, along the hairline, and sporadic itching. Examination is used to make the diagnosis. Antifungals, topical corticosteroids, tar, and keratolytics are used as treatments. Seborrhea dermatitis is a frequent inflammatory disease that affects areas of the skin (such as the face, scalp, and sternum) that have a high density of sebaceous glands.

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Tabel 1: Plant Parts (Oil) & the medicinal uses of Phytoconstituents.

Sr. no	Plant Part(Oil)	Phytoconstituents	Medicinal Uses	Reference
1	Oil	Gallic acid	antiinflammatory, antiangiogenic, antimutagenic, antioxidative, and anticarcinogenic effects.	10.1016/j.fct.2010.02.034 10.4155/ppa.15.14
2	Oil	1,8 Cineole	anti-inflammatory, antioxidant, mucolytic/secretolytic, bronchodilatory, and antimicrobial effects	10.1002/jsfa.8600 10.1080/10286020.2020.1839432
3	Oil	Ferulic acid	antioxidant, antiallergic, hepatoprotective, anticarcinogenic, antibacterial, and anti-	https://doi.org/10.1017/S0043933918000740 https://doi.org/10.1016/j.btre.2014.09.002

			inflammatory activities	
4	Oil	Quercetin	anti-inflammatory, antihypertensive, vasodilator effects, antiobesity, antihypercholesterolemic and antiatherosclerotic activities	doi: 10.1155/2014/480258. doi: 10.1016/j.foodchem.2007.11.053.
5	Oil	Ascorbic acid	antioxidant	doi:10.17226/9810
6	Oil	Limonene	Antioxidant, Anti-inflammatory,Antinociceptive, Anticancer activities	https://journals.sagepub.com/doi/pdf/10.1177/1934578X0800300728
7	Oil	Thymol	anaesthetic, antiseptic, disinfectant	doi:10.1111/j.1399-302X.2005.00216.x
8	Oil	Camphor	decongestant. to treat sprains, swellings, and inflammation.	https://en.wikipedia.org/wiki/Camphor#Uses
9	Oil	Linalool	antimicrobial agent, Insectisides	https://en.wikipedia.org/wiki/Linalool
10	Oil	Alpha tocopherol	Antioxidant Supplementation in Atherosclerosis Prevention	https://pmc.ncbi.nlm.nih.gov/articles/PMC6361124/
11	Oil	Ursolic acid	anti-inflammatory, antioxidant, anticancer, and anti-apoptotic effects	https://www.sciencedirect.com/topics/medicine-and-dentistry/ursolic-acid
12	Oil	6 Gingerol	anti-inflammatory, antitumor	https://www.sciencedirect.com/topics/neuroscience/6-gingerol
13	Oil	Luteolin	anti-hypertensive, anti-diabetic, anti-asthmatic, anti-carcinogenic	https://www.sciencedirect.com/topics/biochemistry-genetics-and-molecular-biology/luteolin#:~:text=Luteolin%20is%20a%20bioactive%20polyphenolic,well%20as%20anti%2Dviral%20properties.
14	Oil	Kaempferol	antioxidant angiogenesis, inflammation,	https://pmc.ncbi.nlm.nih.gov/articles/PMC3601579/
15	Oil	Linolenic acid	lower the risk of cardiovascular disease, diabetes and premature death.	https://en.wikipedia.org/wiki/Linoleic_acid
16	Oil	Beta Carophyllene	Analgesic, anticancer, antinociception activities	https://pmc.ncbi.nlm.nih.gov/articles/PMC5083753/
17	STD	Minoxidil	hypertension, treatment of high blood pressure and pattern hair loss.	https://en.wikipedia.org/wiki/Minoxidil#:~:text=Minoxidil%20is%20a%20medication%20used,a%20topical%20liquid%20or%20foam.

Material and Methods :

1. Derivatives:

1.1 Amla :

Amla, commonly referred to as Indian gooseberry, is a rich source of vitamin C and offers numerous health benefits. The powdered form of Amla is a key ingredient in hair tonics, which are necessary for promoting hair growth and enhancing hair pigmentation. It strengthens the hair roots, enhances color, and boosts shine. The application of amla oil to

the hair roots promotes growth and improves pigmentation [19]. It is widely recognized for its effectiveness in reducing baldness and hair loss [20].
This benefit is attributed to its tannin content, including tannic acid, ellagic acid, gallic acid, iron, and antioxidants, which protect hair follicles from damage caused by free radicals and dandruff [21]. This research identified Linolenic acid as one of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. Phytochemicals found in Amla, such as linolenic acid, were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database [23].

1.2 Bhringraj :

Bhringraj, commonly known as false daisy, is a therapeutic herb that enhances hair growth. This widely used Ayurvedic component aids in improving blood circulation to the scalp, thereby stimulating hair growth [25] that may have been hindered by various factors, such as dandruff. Additionally, it addresses scalp issues related to dandruff and irritation, ensuring that hair growth is not compromise [26].
This research identified Luteolin as one of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. This research identified Luteolin as one of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. Phytochemicals found in Bhringraj, such as Luteolin, were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

1.3 Hibiscus :

Hibiscus, also known as 'gudhal', is an exceptionally advantageous component for hair [27]. It promotes hair growth, facilitates regrowth, and addresses hair loss. This plant is rich in amino acids, Vitamins A and C, as well as alpha hydroxy acids, along with various other nutrients that significantly benefit both hair and scalp health [28]. These properties help maintain a healthy scalp and reduce the likelihood of dandruff.
This research identified Kaempferol and Quercetin as two of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. This research identified Kaempferol, Ascorbic acid and Quercetin as three of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. Phytochemicals found in Hibiscus, such as Kaempferol and Quercetin were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

1.4 Neem :

Neem is beneficial for cleansing the scalp by unclogging pores and promoting hair growth. Its regenerative properties are vital for treating dandruff [29]. Additionally, neem possesses antiseptic and healing qualities, making it suitable for various hair issues [30]. Dandruff can be alleviated by rinsing with neem leaves. In hair care practices, neem is commonly utilized alongside other Ayurvedic herbs such as amla, and shikakai, which are essential for maintaining healthy hair, enhancing growth, reducing hair loss, and increasing volume. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. This research identified Quercetin and Kaempferol as two of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. Phytochemicals found in Neem, such as Quercetin and Kaempferol were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

1.5 Ginger :

Ginger serves as an excellent hair conditioner, rich in minerals and essential oils, which enhances hair manageability, softness, and shine [31]. It provides relief for itchy scalps, dryness, and dandruff. Additionally, it possesses natural anti-inflammatory and antiseptic properties that promote a healthy and clean scalp [32]. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. This research identified 6 Gingerol and Kaempferol as two of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. Phytochemicals found in Ginger, such as 6 Gingerol and Kaempferol were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

1.6 Nagarmotha :

Nagarmotha, also referred to as Nut grass, is primarily utilized for treating scalp disorders. It is particularly effective in managing dandruff, which is a fungal condition, as nagarmotha combats the fungus responsible for it. Consistent application of nagarmotha enhances hair texture, imparts shine, and promotes hair growth. Additionally, it effectively reduces hair loss and delays premature graying. This research identified 1,8 cineole and Ascorbic acid as two of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. Phytochemicals found in Nagarmotha, such as 1,8 cineole and Ascorbic acid were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

1.7 Shikakai :

Shikakai serves as an effective anti-dandruff solution due to its distinctive capability to cleanse the scalp gently. It is particularly beneficial in addressing chronic dandruff resulting from excessive oil production on the scalp. Regular use of Shikakai aids in eliminating surplus oil and alleviating dandruff. As one of the most valuable Ayurvedic herbs for hair-related issues, particularly hair loss, Shikakai not only cleanses the scalp of dirt and excess oil but also encourages hair growth, attributed to its astringent properties. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules.

1.8 Dorli :

In Ayurveda, the term 'Brihati' typically denotes the desiccated root of the Solanum indicum plant, a highly spiny, extensively branched perennial undershrub predominantly found in the warmer regions of the country, thriving at elevations up to 1500 meters. Traditionally, Brihati is employed in the treatment of various respiratory conditions such as asthma, catarrh, and both dry and spasmodic coughs, as well as dropsy, cardiovascular diseases, chronic fevers, colic, scorpion stings, difficulties in urination, and parasitic worm infestations. Additionally, the fruits of the plant are utilized for medicinal purposes due to their notable analgesic, antipyretic, anti-inflammatory, and central nervous system depressant effects [24]. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules.

1.9 Liquorice :

Common English liquorice or American English licorice is a common name for Glycyrrhizaglabra, [33,34] a flowering plant that belongs to the Fabaceae family of beans and whose root is used to extract a sweet, aromatic flavouring [35].The herbaceous perennial legume known as liquorice is indigenous to Southern Europe, North Africa, and West Asia [36]. Liquorice is sold as a dietary supplement and utilized as a flavoring in beverages, tobacco, confections, and medications [35,37]. Herbalism and traditional medicine have both made use of liquorice extracts [35].The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules

2.0 Amarkand :

The term "Amarkand" is made up of two distinct words. "Kand" represents tubers, and "Amar" denotes immortal. The term "Amarkand" is frequently used to refer to one species from the genus Dioscorea (Dioscoreabulbifera, family: Dioscoreaceae) and thirty closely related plant species from the genus Eulophia (Orchidaceae). Amarkand has long been regarded as a superior health-promoting substance. The tribal regions of India regularly use rizhomes, or tubers of Amarkand, as food and as a medicinal substance to promote lifespan and improved health [38,39]. In the field of Ayurveda, As a stimulant, anabolic, tonic, diuretic, astringent, digestive, and gentle purgative, Amarkand is typically recommended [40]. Furthermore, several ancient literature have also emphasized the benefits of using these species to cure debility, joint edema, blood clotting, and ear discharge [40]. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. This research identified 6 Gingerol and Beta Caryophyllene as two of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. Phytochemicals found in Amarkand, such as 6 Gingerol and Beta Caryophyllene were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

2.1 Orange peel :

In 2008, 122.09 million tons of citrus were produced globally. Oranges make up over 60% of all citrus produced globally. Oranges accounted for 2.14 million of the 3.23 million tons of citrus fruit produced in

Egypt in 2008 [41]. With 1,300 species and over 140 genera, the genus [42] Citrus is a member of the Rutaceous, or Rue, family. Citrus Sinensis (orange), Citrus parades (grapefruit), Citrus lemon (lemon), Citrus reticulate (tangerine), Citrus grandis (shaddock), Citrus aurantium (sour orange), Citrus medicinal (citrus), and Citrus aurantifolia (lime) are some of the important fruits in the Citrus genus. Studies that investigate the existence of polyethoxylated flavones in byproducts made from processing citrus fruit are currently of great interest to the citrus industry since their beneficial effects suggest potential value-added applications for these compounds as specialty ingredients and nutraceuticals.

The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. This research identified Linolenic acid and Limonene as two of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. Phytochemicals found in Orange peel , such as Linolenic acid and Limonene were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

2.2 Heena :

The henna plant, Lawsoniainermis, is a tiny tree or shrub that is grown as a commercial and decorative dye crop in many areas [43]. It is primarily found in south Asia, northern Australia, and the tropic, sub-tropic, and semiarid regions of Africa (tropical Savannah and tropical arid zones) [44]. The only species of the Lawsonia genus, Lawsoniainermis, is used to make henna, a dye. It is also referred to as hina, the henna tree, the mignonette tree, and the Egyptian privet [45]. Since ancient times, henna has been used to color leather, silk, and wool as well as skin, hair, and fingernails. The Arabian Peninsula, Indian Subcontinent, portions of Southeast Asia, Carthage, and other regions of North Africa and the Horn of Africa have all historically used henna. Other skin and hair dyes with the same name, like black and neutral henna, are not made from the henna plant [46,47]. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. This research identified Linolenic acid and Luteolin as two of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. Phytochemicals found in Henna , such as Linolenic acid and Luteolin were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

2.3 Brahmi :

Often used in ayurvedic medicine, Bacopamonnieri is a medicinal creeping perennial of the Scrophulariaceae family. It has small rectangular leaves and white to purple flowers (see Image. Bacopa). This herb is also known as thyme-leaved gratiola, water hyssop, brahmi, and the herb of grace [48]. The Hindu mythological term Brahmi signifies "Brahma," or the "supreme creator [49]." Bacopamonnieri, Centellaasiatica (Gotu kola), or a mix of the two plants have all been referred to as Brahmi [49]. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. This research identified Ascorbic acid one of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. Phytochemicals found in Brahmi , such as Ascorbic acid were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

2.4 Coconut Oil :

To keep the scalp healthy and hygienic, people all around the world utilize items like oils, shampoo, and other cosmetics [52,53]. The most popular product among them for improving hair growth and scalp health in Asian and African nations, including India, is coconut oil [53,54]. The way that coconut oil works is not well understood. First, it is believed that the oil's main fatty acid, lauric acid, has antifungal properties that stop bacteria from growing [53,54,55]. Second, because it reduces trans-epidermal water loss (TEWL) with prolonged use, coconut oil is known to have a biophysical effect on the skin barrier function [56,57]. Nevertheless, the impact of topical coconut oil treatment on the scalp microbiota has not yet been thoroughly investigated in any research.

The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. This research identified Alpha tocopherol as one of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. Phytochemicals found in Coconut oil, such as Alpha tocopherol were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features

distinct chemical structures sourced from the Substance database [23].

2.5 Fenugreek Seed/Oil :

The mild type of seborrhic dermatitis, known as "dandruff," is an inflammatory skin disorder marked by an unusually high amount of dead scalp shedding and flaking.

Dandruff can be effectively treated using natural herbs. One such herb is "fenugreek," which aids in the destruction of a particular kind of fungus that causes dandruff. Fenugreek seeds are incredibly potent and excellent at combating baldness, hair loss, and thinning hair. In addition to being a strong source of protein and nicotinic acid, fenugreek seeds promote hair development. Numerous experts have verified that fenugreek has a significant amount of lecithin, a natural emollient that gives hair strength and health. It hydrates hair as well [58].

The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. This research identified Linolenic acid as one of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. Phytochemicals found in Fenugreek oil, such as Linolenic acid were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

2.6 Jojoba Oil :

In order to restore the normal health of skin and hair, jojoba oil is utilized extensively in the pharmaceutical business, particularly in cosmetics. The leaf extract treats sensitive skin tension by acting as an anti-inflammatory agent when coupled with extracts from other plants [60]. Bath oil, body oil, cleansing creams, cleansing pads, cleansing scrubs, nourishing face cream, facial oil, hair conditioner, hair oil, makeup remover, and shaving cream are among the jojoba cosmetic items that are currently available on the market [61,62,63,64].

2.7 Rosemerry Oil :

By promoting circulation, rosemary essential oil may help keep hair follicles from starving to death and experiencing hair loss.

In addition to promoting hair growth, people use essential oil of rosemary to avoid dandruff and premature graying. Although more research is required, it may also assist with dry or itchy scalps. By raising nerve growth factor, rosemary may help nerve tissue, per researchTrusted Source. This could promote healthy skin and hair growth. This capacity to repair nerve endings may help revitalize scalp nerves, perhaps reviving hair development [65].

The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. This research identified Camphor, Linalool as two of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. Phytochemicals found in Rosemerry oil, such as Camphor, Linalool were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

2.8 Lavender Oil :

A novel, safe, and organic substitute for somewhat dangerous pharmaceutical compounds is provided by essential oils. The Lamiaceae family includes lavender, or Lavandula, as one of the often studied therapeutic herbs [67]. Since ancient times, the purple-blue flowers of this shrub have been used to treat a variety of illnesses. Lavandula angustifolia, Lavandula latifolia, Lavandula stoechas, and Lavandula intermedia are the most widely utilized varieties of lavender [68].It is grown for commercial purposes all over the world. It is grown in the Indian states of Uttar Pradesh, Himachal Pradesh, and the Kashmir valley. Anxiolytic, anti-inflammatory, antinociceptive, antioxidant, and antibacterial properties have all been documented [68,69]. Lavender essential oils are one example of a herbal product that may help with issues including drug addiction, side effects, invasive treatments, and antibiotic resistance. Due to the emergence of drug resistance, these characteristics make lavender a particularly valuable therapeutic herb in the present era [70].

The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules [22]. This research identified Ursolic acid as one of the derivatives. The 3D conformer structures of these derivatives were obtained in SDF format from the PubChem Database, which is also referred to as the Library of Drug Molecules. Phytochemicals found in Lavender oil, such as Ursolic acid were extracted and examined through PubChem. PubChem provides open access to information regarding chemical compounds and their biological functions. The Substance database offers chemical data contributed by various individuals to PubChem, while the compound database features distinct chemical structures sourced from the Substance database [23].

Figure 1: Gallic acid

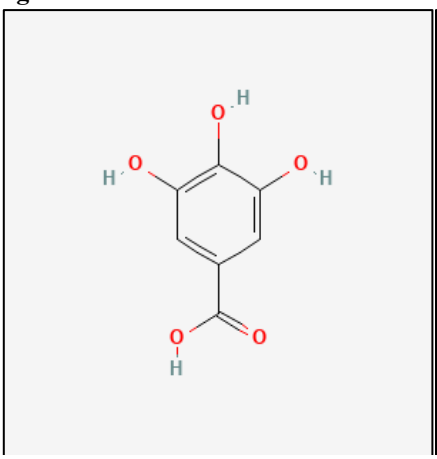


Figure 2: 1,8 Cineole

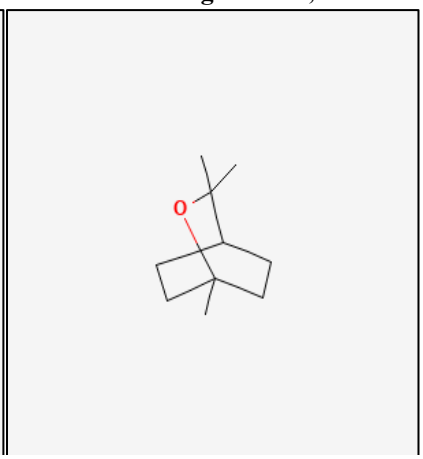


Figure 3: Ferulic acid

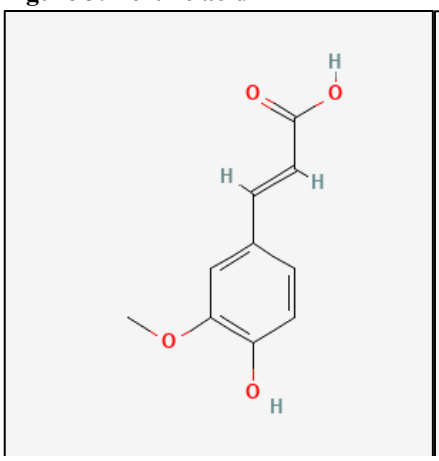


Figure 4: Quercetin

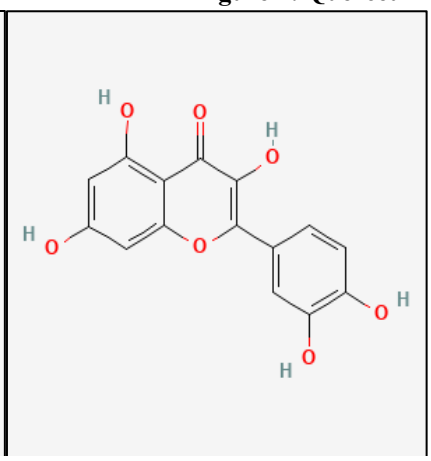


Figure 5: Ascorbic acid

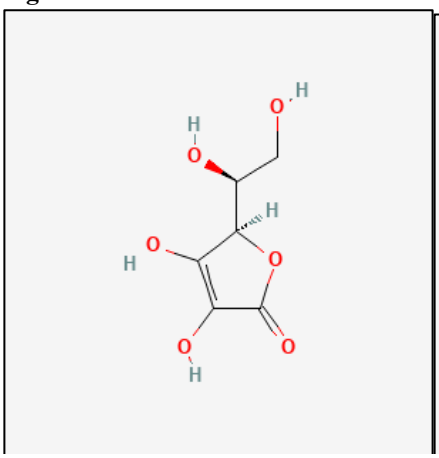


Figure 6: Limonene

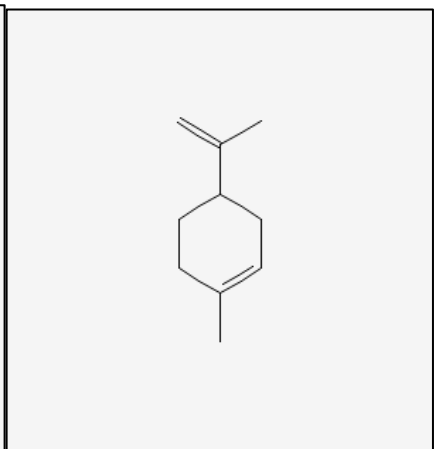


Figure 7: Thymol

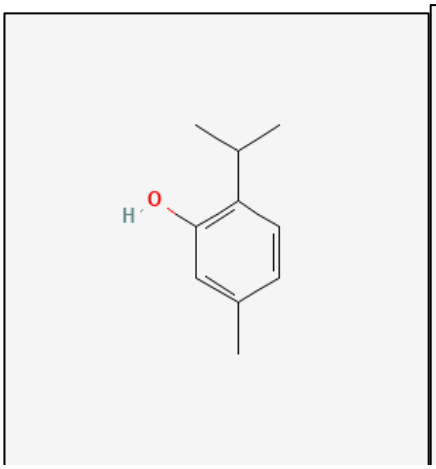


Figure 8: Camphor

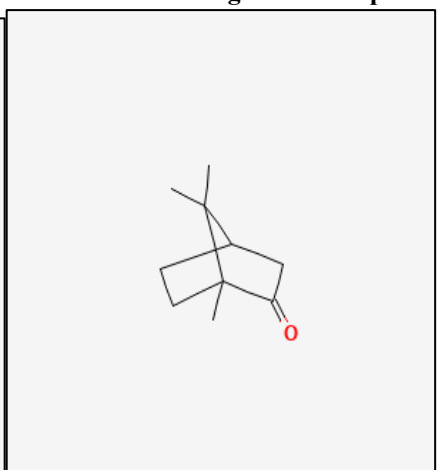


Figure 9: Linalool

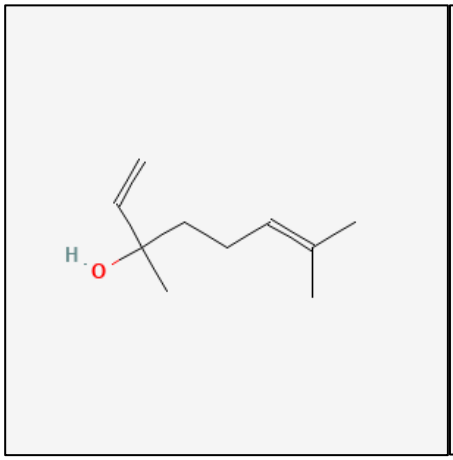


Figure 10: Alpha tocopherol

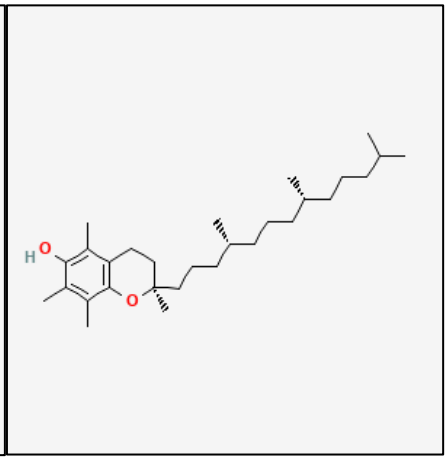


Figure 11: Ursolic acid

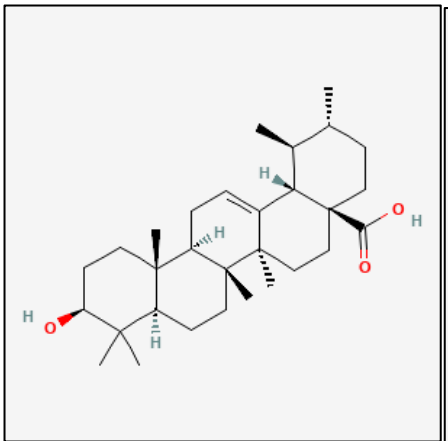


Figure 12: 6 Gingerol

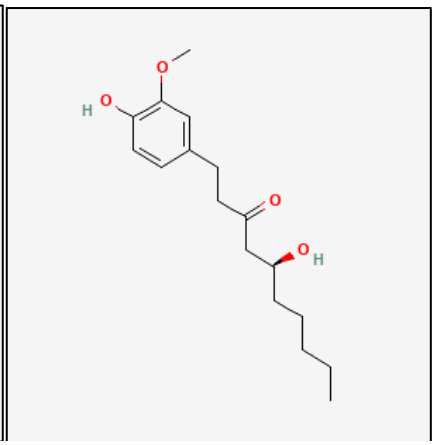


Figure 13: Luteolin

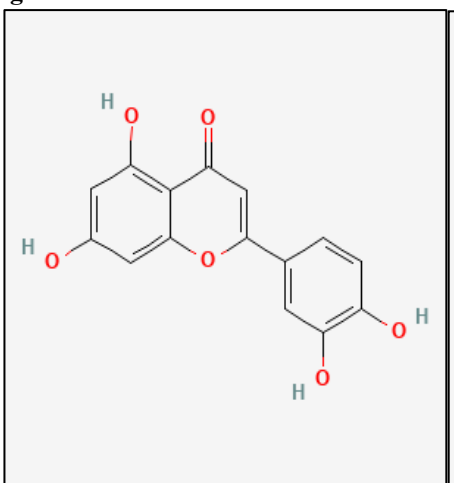


Figure 14: Kaempferol

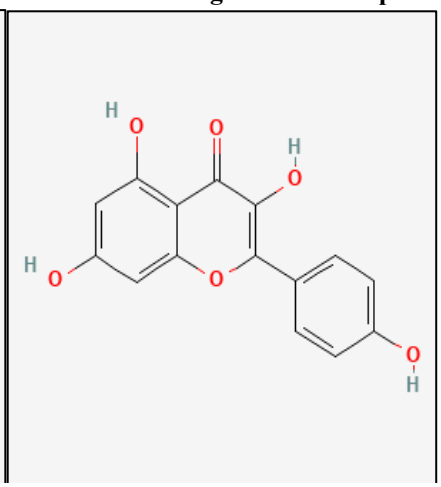


Figure 15: Linolenic acid

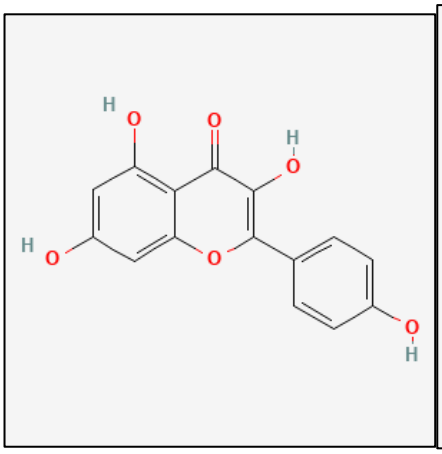


Figure 16: Beta Carophyllene

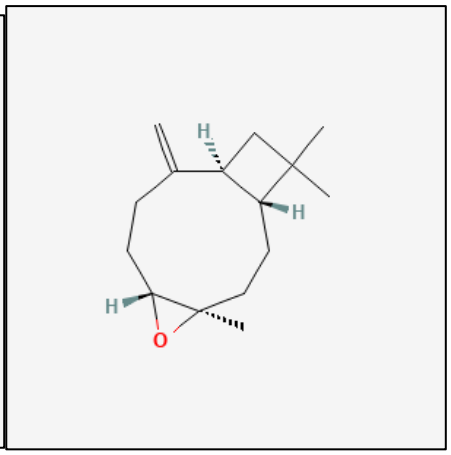
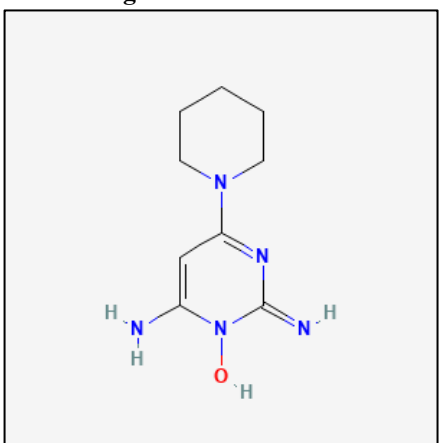


Figure 17: Minoxidil



2. Ligand Preparation:

I. **Access Data Sources: -** Visit the following websites:
   1. Dr. Duke's
   2. IMPACT

II. **Search for the Plant: -** Use the search function to find the plant of interest. Locate the desired phytoconstituent (compound) listed under the plant.

III. **Retrieve Phytoconstituent Structure: -** Copy the name of the phytoconstituent. Paste it into the PubChem search bar and run the search.

IV. **Download Structure Data: -** Once the compound page opens, click on the structure image. Select the option to Download Coordinates. Choose the SDF format for downloading. Save the file.

V. **File Management: -** Open the downloaded .SDF file using Notepad or a text editor. Rename the file using the phytoconstituent's name for easier identification.

VI. **Final Step: -** Ensure all files are clearly named and arranged grammatically for future reference.

Table No.2: Proteins & PDB ID

Sr. No.	Protein	PDB ID
1.	Carbonic anhydrase xii complexed with acetazolamide	1JD0
2.	DihydrofolateReductasecarbonic anhydrase I in complex with the 4-({[4-chloro-3-(trifluoromethyl)phenyl]carbamoyl}amino)phenyl sulfamate inhibitor	6IJ0

Figure 18: 1JD0

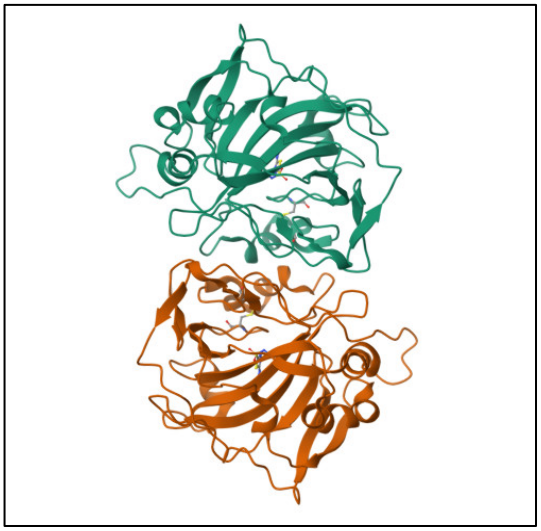
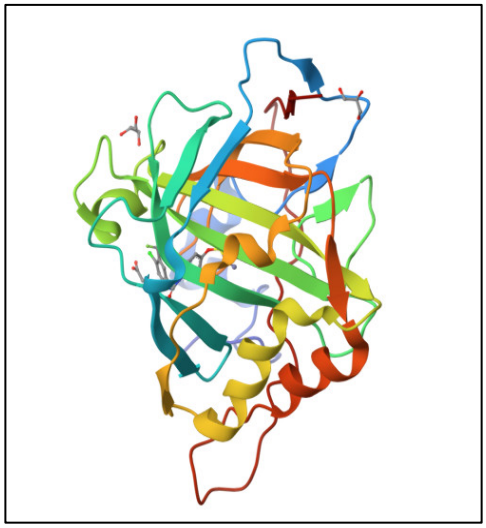


Figure 19: 6IJ0



3. Protein Preparation:

Therapeutic Target Database Workflow

I. **Search and Select a Disease: -** Begin by searching for and selecting the disease of interest.

II. **Click on the Target: -** Click on the corresponding target to open its detailed information.

III. **Find the Receptor Information: -** Scroll down to locate the receptor information (e.g., 1XKK).

IV. **Open in Protein Data Bank (PDB): -** Use the receptor ID (e.g., 1XKK) to search in the Protein Data Bank.

V. **Download the Structure: -** Download the receptor structure in PDB format.

4. Docking Procedure: (MOL Software)

I. **Open Software and Load File: -** Open the software. Load the file named IXKK-PDB.

II. **Prepare Receptor: -** Click on Receptor. Convert to PDB format. Delete water molecules.

III. **Fix Missing Chains: -** Unhide high missing side chains. remaining chains are hidden—unhide them.

IV. **Color and Inspect Ligand: -** Select the drug. Right-click and choose Colour (e.g., orange) for clarity.

V. **Pocket and Interaction: -** Select Pocket Ligand Interaction.

VI. **Separate Drug Molecule: -** Select the drug again. Right-click and choose Move from Object.

VII. **Set Up Docking Project: -** Select Drug Docking → New Project Setup Receptor. Enter Project Name: IXKK. Select Define Site Around Selected Molecule → click OK.

VIII. **Grid Box Configuration: -** Click on the green option (grid box). Double-click on it to remove the grid box if needed.

IX. **Extract Ligand: -** Select the drug. Change colour for better visibility (e.g., orange). Go to Extract Ligands.

X. **Run Docking: -** Go to Docking → Dock Chemical Table. Click Check Name → Click OK [50].

Result and Discussion: -

1. Ramchandran Plot: -

Figure 20: 1JD0

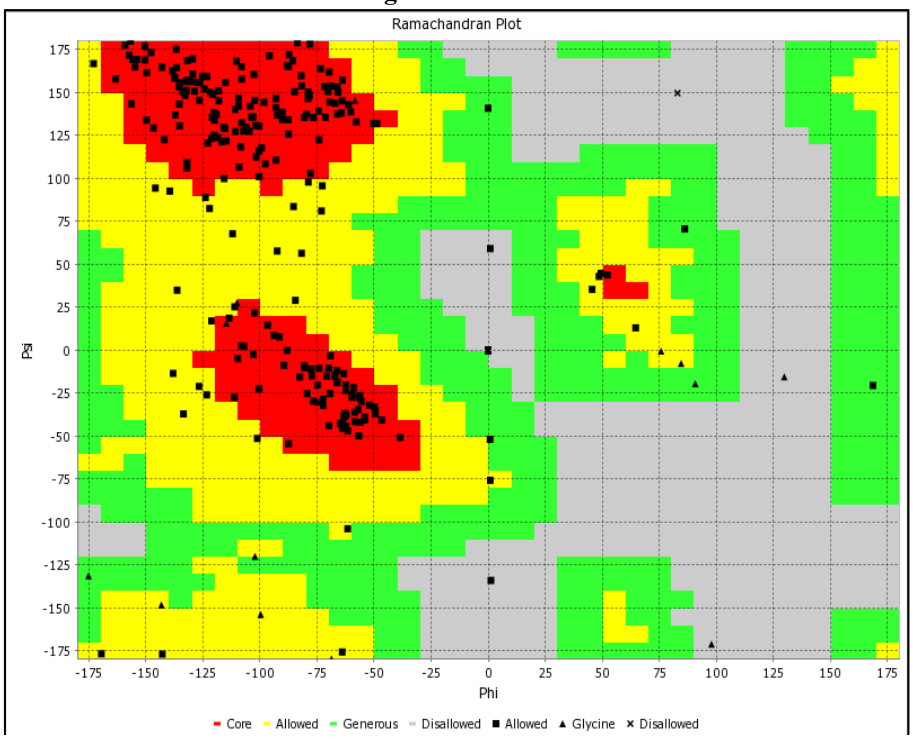
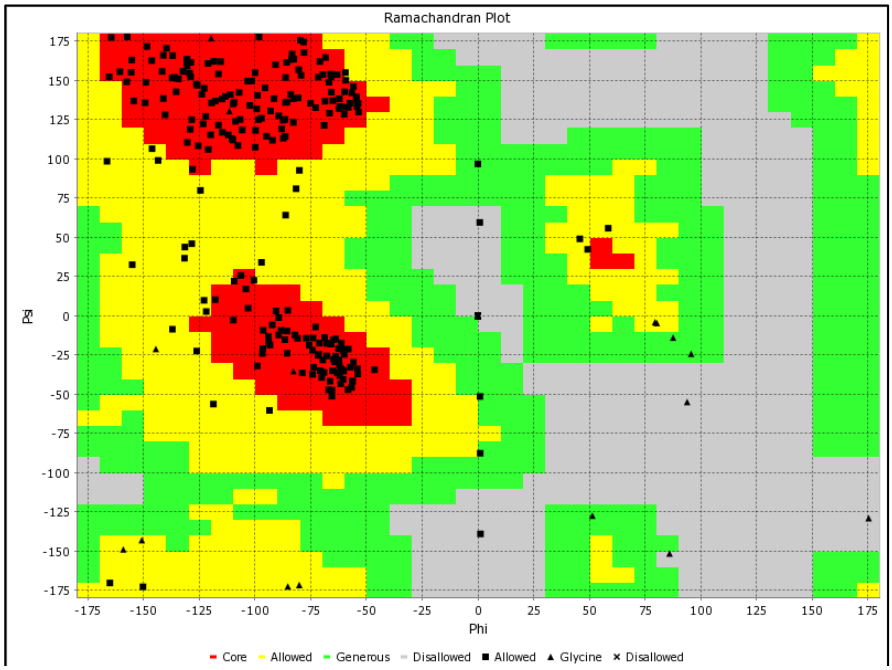
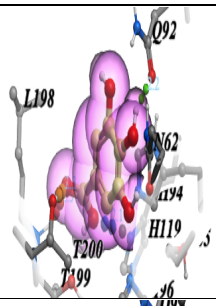
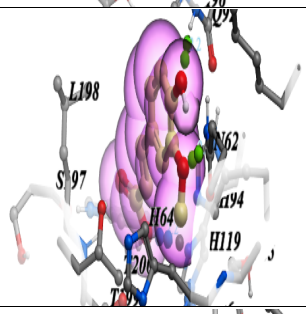
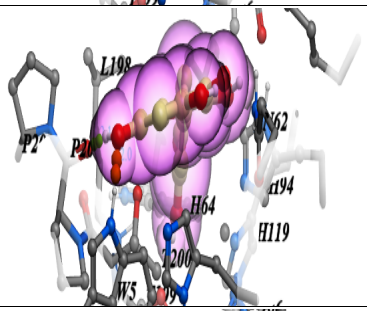
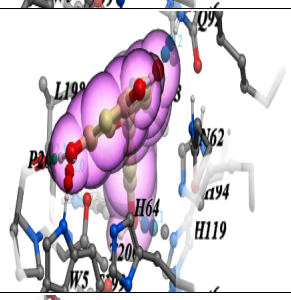
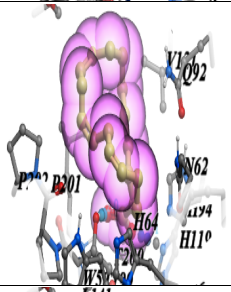
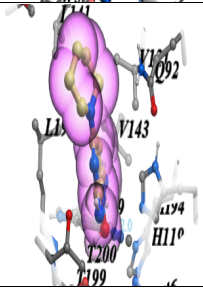


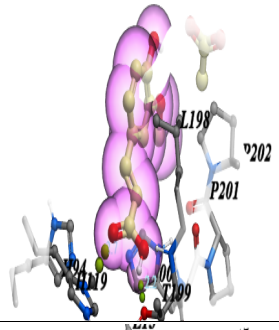
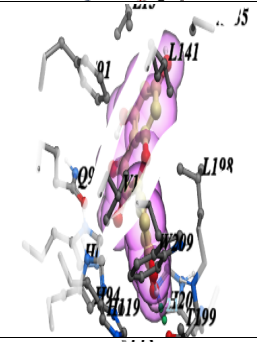
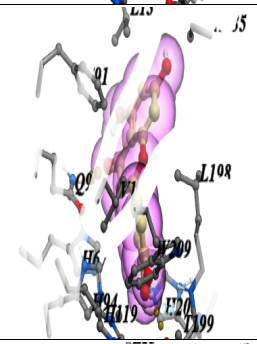
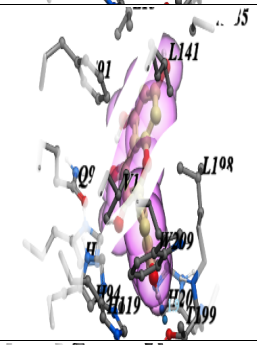
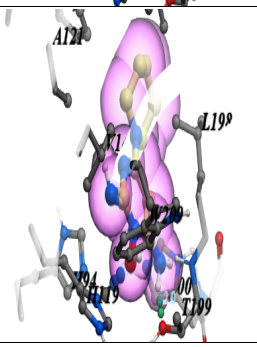
Figure 21: 6IJ0



5. Ligand Drug Docking : (Table no 3)

Sr No	Ligand	Phytoconstituents	Structures

1	1JD0	Gallic acid	
2	1JD0	Ferulic acid	
3	1JD0	Quercetin	
4	1JD0	Luteolin	
5	1JD0	Linolenic acid	
6	1JD0	Std Minoxidil	

7	6IJ0	Ferulic acid	
8	6IJ0	Quercetin	
9	6IJ0	Luteolin	
10	6IJ0	Kaempferol	
11	6IJ0	Std Minoxidil	

6. Amino acid (2D structure):

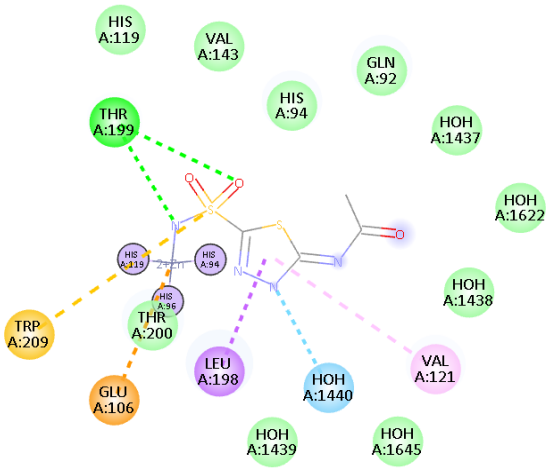


Figure 22: 1JD0 & Gallic acid

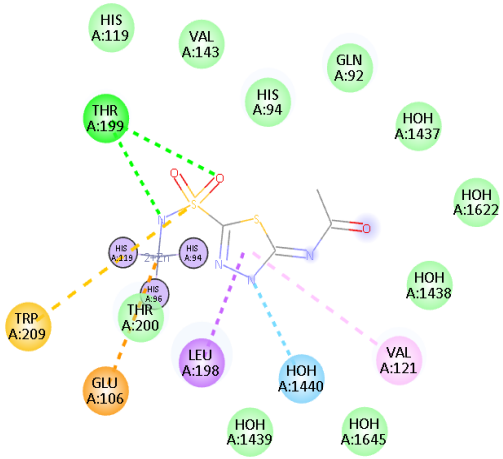


Figure 23: 1JD0 & Ferulic acid

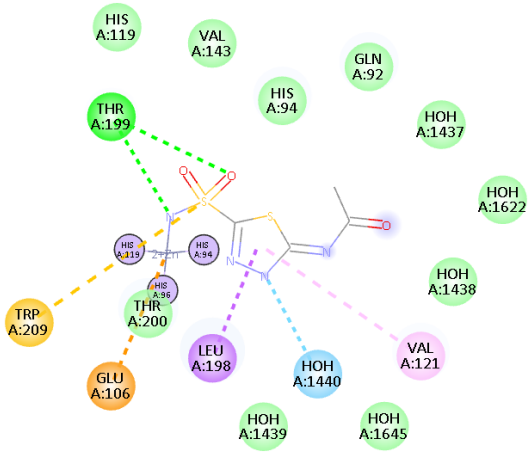


Figure 24: 1JD0 & Quercetin

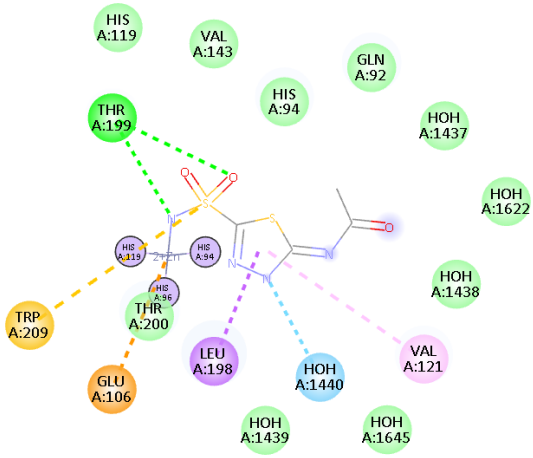


Figure 25: 1JD0 & Luteolin

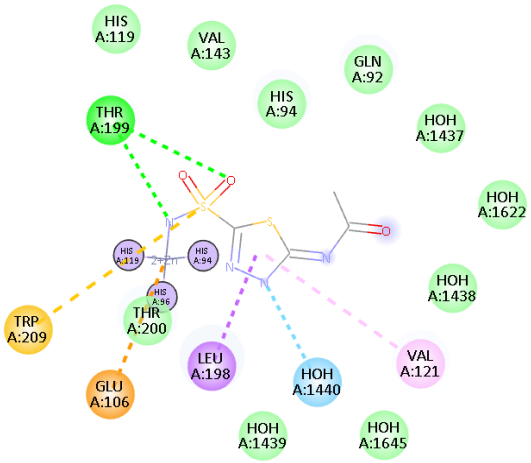


Figure 26: 1JD0 & Linolenic acid

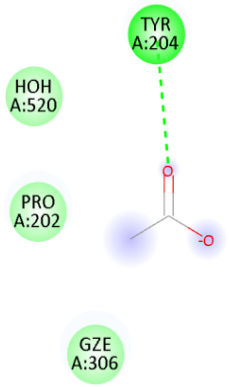


Figure 27: 6IJ0 & Ferulic acid

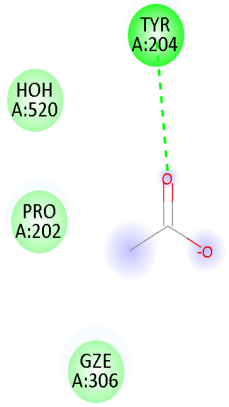


Figure 28: 6IJ0 & Quercetin

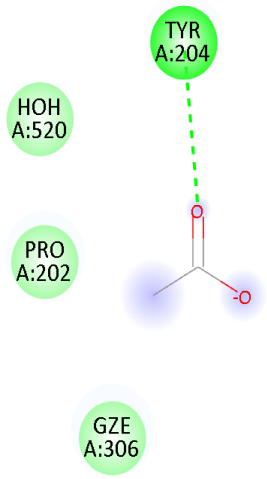


Figure 29: 6IJ0 & Luteolin

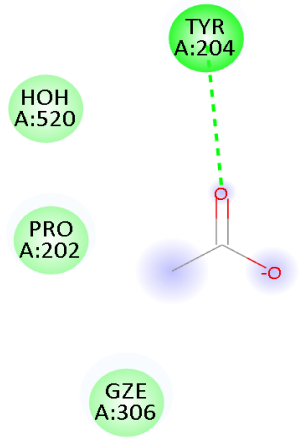


Figure 30: 6IJ0 & Kaempferol

7. Binding Energy : (Table no 4)

Sr No	Phytoconstituents	1JD0	6IJ0
1	Gallic acid	-22.9	-10.95
2	Ferulic acid	-12.35	-17.66
3	Quercetin	-17.18	-19.35
4	Luteolin	-18.46	-17.91
5	Linolenic acid	-18.18	-9.77
6	Kaempferol	-10.02	-18.06
7	Std Minoxidil	-12.79	-13.42

Our model is based on the ligand based pharmacophoric features of already known active compounds of the plant species. Structures of health beneficial phytochemicals i.e Gallic acid, Ferulic acid, Quercetin, Luteolin, Linolenic acid, present in Polyherbal oil were extracted and analyzed using DR DUKE'S& the proteins are downloaded using Therapeutic Target Database and open (TTD) the protein dada bank (PDB) & that is PDBID (1JD0, 6IJ0) They have good binding energy.

Conclusion: -

The study highlights the antidrandruff potential of phytoconstituents derived from polyherbal oil through in silico molecular docking. Among the compounds analysed, Gallic acid and Quercetin demonstrated the strongest binding affinity with both 1JD0 and 6IJ0 proteins, indicating its potential as a lead molecule for Antidrandruff drug development. Other compounds, such as Linolenic acid ,Ferulic acid ,Luteolin and Kaempferol also exhibited promising interactions. These findings suggest that polyherbal oil contains bioactive compounds with significant therapeutic potential, which could be further explored in in vitro and in vivo studies for drug formulation.

Reference:

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