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Research Article
doi: 10.61705/6pjgdk14
Ace J. Addict., 7 (1): 70-81 | 2026

"Pharmacognostic and Phytochemical Evaluation of Aegle marmelos and Bergenia ligulata: Molecular Docking Insights into Their Potential Antipsoriatic Activity"

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OPEN ACCESS

Key Words
Psoriesis, Aegle marmelos, Bergenia ligulate, Quercetin, Rutin, Phytochemical screening, Molecular docking, IL-17RC

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Received: 19 Oct 2026
Accepted: 30 Oct 2026
Published: 16 Nov 2026

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ABSTRACT

Red, scaly lesions are the hallmark of psoriasis, a persistent immunoinflammatory skin condition. The possible anti-inflammatory and antioxidant qualities of natural phytoconstituents have drawn attention. With an emphasis on quercetin and rutin, this study sought to assess the phytochemical makeup and possible antipsoriatic action of *Aegle marmelos* and *Bergenia ligulata*. Plant materials were gathered, dried, ground into a powder, and extracted. Foreign matter analysis, drying loss, and extractive value calculation were all part of the pharmacognostic assessment. Alkaloids, flavonoids, steroids, and carbohydrates were found after preliminary phytochemical screening The aluminum chloride colorimetric method was used to determine the total flavonoid concentration, and thin-layer chromatography (TLC) was used to identify substances that resembled flavonoids. Using AutoDock 4.2 and Discovery Studio, molecular docking was used to assess how quercetin and rutin interacted with the IL-17RC receptor (PDB ID: 6HGA). For *Aegle marmelos* and *Bergenia ligulata*, the drying value losses were 9% and 5.8%, respectively. Alkaloids, flavonoids, and sugars were found in both plants, but only *Aegle marmelos* had steroids. *Aegle marmelos* has a higher total flavonoid concentration (143.91 mg QE/g extract) than *Bergenia ligulata* (35.7 mg QE/g extract). TLC revealed molecules that resembled quercetin and rutin. Binding energies of −8.2 kcal/mol for rutin and −7.3 kcal/mol for quercetin were found through docking. These results point to possible antipsoriatic action.

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INTRODUCTION

Psoriasis is a complex chronic immunoinflammatory skin disease affecting an estimated 125 million people worldwide. This condition is often associated with a large number of comorbidities, including cardiovascular diseases, chronic kidney disease, uveitis, mental health issues, metabolic syndrome, inflammatory bowel disease, and psoriatic arthritis. Such comorbidities substantially increase the disease burden and therapeutic complexity. We have topical medicines, systemic medicines, phototherapy and biologic therapies to treat psoriasis and these are often used in combination to try and get the best control of the disease. Meanwhile, a significant number of people with psoriasis are turning to complementary and alternative therapy (CAM), with documented Herbal therapies are the most popular form of with a prevalence that varies from 2% to 70% worldwide. CAM includes mind and body therapies and natural products such as herbs, vitamins and dietary supplements.[1] People choose complementary and alternative medicine (CAM) for a variety of reasons, including curiosity, dissatisfaction with conventional medicines, perceived decreased toxicity, and a preference for natural treatments. Herbal products, while generally perceived as safe, can cause clinically important interactions and adverse events (AEs), especially in patients with co-morbid conditions and in the pediatric population. [2]

It is mainly inherited and is characterized by red, scaly, itchy patches. Most commonly the whole scalp is involved but it may extend to forehead, back of neck or behind the ears, chest, arms, elbows, in the armpits, under breasts, around the genitalia, knees, legs, toenails and fingernails [3].It can occur at any age and affects men and women equally, as well as children, adults and the elderly. It is more common in people aged 15-35. “According to the National Psoriasis Foundation.Psoriasis has both genetic and environmental components. There are three forms of psoriasis, mild, moderate and severe. Rashes appear when psoriasis is mild, and the skin becomes scaly when it is intermediate. In extreme circumstances, the skin's surface may have red areas that itch.Type of psoriasis : Plaque Psoriasis: The Most common form of psoriasis.[4] About 80–85% of those who have psoriasis have this type. Guttate Psoriasis: It is usually triggered by a bacterial infection such as streptococcal throat infection and often starts in childhood or young adulthood and affects about 18% of all psoriasis patients. Inverse Psoriasis: Also known as Flexural Psoriasis. About 18% of those who have psoriasis have this type. Postural Psoriasis: Less than 5% of patients who have psoriasis have this type. Nail Psoriasis: About 50–80% of those who have psoriasis have this type. Although the exact cause of psoriasis is unknown, the immune system, genetics, and environmental factors are some of the contributing causes. Genetics: It plays a major role in the development of this disease.[5] Ten percent of people in general have genes that make them. Quercetin is a member of the flavonol class, which is not made by the human body. quercetin has demonstrated a wide range of pharmacological activity, including antiviral, anticancer, and the treatment of inflammatory, metabolic, and allergy illnesses as well as ocular and cardiovascular conditions and arthritis [6]. Inhibits NF-κB signaling pro-inflammatory cytokines (TNF-α, IL-6, IL-17)Antioxidant scavenges ROS Inhibits MAPK pathway Rutin, a common dietary flavonoid usually nontoxic naturally derived compound exhibits a diverse range of useful biological properties such as anticancer, antioxidant, antidiabetic, anti-inflammatory, antibacterial, antifungal, neuroprotective, card ioprote ctive, hepatoprotective, n ephroprotective, haematoprotective, antiarthritis, anthelmintic, testicular protection, etc. Below is a brief description of rutin's primary biological characteristics.[7] Flavonol glycoside (quercetin + rutinose sugar) Inhibits NF-κB signaling pro-inflammatory cytokines (TNF-α, IL-6, IL-17, IL-23) Stabilizes capillaries Reduces oxidative stress.[8]

Placing molecules in the right configurations to engage with a receptor is known as molecular docking. When molecules bind to one another to form a stable complex, a natural process called molecular docking takes place in a cell in a matter of seconds . Docking types Docking comes in two varieties. 1. Rigid docking 2. Flexible docking .Rigid Docking Assuming that the molecules are stiff, we seek to change one of the molecules in three dimensions so that it best fits the other molecules in terms of a scoring function. Both the presence and absence of receptor binding activity can result in the development of the ligand's conformation . Flexible Docking Our goal is to uncover confirmations of the receptor and ligand molecules as they occur in complex, taking into account molecular flexibility in addition to transformation [9]. Virtual screening of thousands of compounds is possible in a short time using molecular docking, thereby reducing the number of unnecessary experiments. This speeds up the drug discovery process and makes it more cost-effective. Molecular docking plays an important role

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in the study of structure based drug design, enzyme inhibition, and protein-ligand interactions. It gives important information about molecule stability, hydrophobic interactions and hydrogen bonding in the active site of the target protein. Researchers use this information to improve the biological activity of lead compounds. In recent years, molecular docking has been playing an important role in the development of anti-viral, anti-cancer, anti-inflammatory and anti-bacterial drugs. Molecular docking has also been found very useful in medicinal chemistry, bioinformatics and herbal drug studies. Several researchers are used docking experiments to assess phytochemicals from therapeutic plants against targets causing disease[10].



Fig. No 1 : Parts of *Aegle Marmelos*



Figure No 2 : Plant of *Bergenia Ligulata*

MATERIAL METHODS :

Collection and preparation of crude drug :

Collection of plant material Leaves of the Aegle marmelos were found and collected from the native place. Bergenia ligulate rhizomes were procured from local market. Aegle marmelos leaves and Bergenia ligulate rhizome were washed and dried at room temperature and then extracted. The dry leaves and rhizome are separately ground and the extraction of the ground leaves and rhizome is filtered through an 80-mesh sieve during the maceration process.[11]

Analysis of crude drug

1.Foreign matter

The sample of Aegle marmelos and Bergenia ligulata shall be free from any visible signs of mould growth, slime, stones, rodent droppings, insects or any other potentially hazardous impurities. They must also be checked for foreign matter. Spread a suitable amount of the sample in a thin layer on a sanitized plate or tray. Then it is examined carefully in the daylight by the naked eye, for any possible foreign particles. Any material suspected to be foreign material is isolated and sent to a Petri plate for further analysis. The separated particles are viewed in daylight through a 10x magnifying glass to confirm their identity. The percentage of foreign matter is then calculated with respect to the weight of the sample taken for analysis. Finally, the observed value is recorded in the laboratory data register.[12]

2.Loss on Drying

Loss on drying test is one of the important analytical techniques to determine the amount of water and volatile materials present in a sample. This technique determines the weight loss, which is related to the moisture and volatile content, by drying the sample under the specified conditions. For effective drying, 2 g of the powder sample is carefully transferred to a petri dish do that the sample is evenly dispersed. The dish is the dries in hot air oven for 105^{o} for five hours to remove excess moisture and volatile ingredients. After the first period of drying, the dish is removed from the oven and cooled in desiccator to prevent absorption of moisture. Weigh the dish and record the weight loss initially. The dish is placed back in the oven for another half hour to make sure it is

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thoroughly dried out. It is then removed and cooled in the desiccator and reweighed to obtain the final weight.The loss on drying (LOD) value calculated as the weight loss of the sample as a percentage provides important information about the moisture and volatile contents of the sample. LOD = Initial Weight – Final Weight – 100%.This process is often employed in the food and drug industries to evaluate the stability and quality of their products.

Average = Differences of sample / Total no. of sample

Percentage of LOD = Average × 100 / Weight of Sample Taken.[13]

3. Extraction value

a.Determination of alcohol soluble extractive value

Five grams of the air dried coarse powder were macerated with 100 ml of 90% ethanol in a closed flask for twenty four hours, shaking at regular intervals for the first six hours and standing for the next eighteen hours. It was then filtered quickly taking care not to lose any of the solvent. Twenty five millilitres of the filtrate were evaporated to dryness, dried at 105° C. and weighed in a shallow tarred dish. The air dried medication was used to determine the percentage of ethanol soluble extractive value.[14]

b.Determination of water soluble extractive value

Accurately weigh out 5 grams of the coarsely ground medication. Macerate with 100 milliliters of chloroform water in a closed flask for 24 hours, stirring vigorously for the first six hours and allowing to stand for eighteen. It was then rapidly filtered with care, to avoid loss of solvent. Then 25 ml. of the filtrate were evaporated to dryness in a shallow dish having a tarred bottom, dried at 105 degrees C. and weighed. The percentage of water-soluble extractive was determined using air-dried drug.[15]

c.Extraction process

Maceration is one of the oldest and simplest methods of extraction and consists of soaking the plant material in solvents at room temperature. Depending on the target chemicals and the desired result, extraction is an important first step in the isolation of bioactive molecules. The reason it is available is because it is simple and requires little equipment. The plant material is crushed or finely milled to increase its surface area for better solvent penetration.Then the material is immersed in a solvent, e.g. water.Depending on the type of material, solvent and target chemicals, the solvent is in contact with the material for a long time – usually a few hours up to several days. Stirring and sometimes shaking can be used to enhance the extraction process. After maceration , the solvent with the extracted chemicals are separated from the solid plant material by filtration . Usually the solvent is evaporated to get a concentrated extract which can be used for further research or applications.[16]

Table no 1 : Phytochemical test:

Phytochemicals	**Tests**	**Procedure**	**Observation of *Aegle marmelos***	**Observation *Bergenia ligulata***
Alkoloid	Mayer's test	2 ml of extract + drop of mayer's reagent	Precipitates formed.	Precipitates
	Dragandroff's test	2-3 ml of extract + few drops of dragendroff reagent	Orange brown precipitate	Orange brown precipitated
Flavonoids	With concentrated sulfuric acid	2 ml of extract +few drop of sulfuric acid	Yellow-orange color observed	Yellow orange colour was observes
Steroides :	Salkowski reaction	2ml of extract + 2 ml of chloroform + 2 ml of concentrated H_2so_4	Reddish chloroform layer with greenish fluorescence	Chloroform layer appeared red + acid layer was observed with greenish yellow florescence
Carbohydrates	Felhing's test	1ml of Fehlings A+ Felhling B solution + boil for 1 min +	Brick red precipitate formed	First yellow, then brick red precipitated was

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		Equal volume of extract in boiling water for 5-10 min		observed.
	Benedict's test	Equal volume of benedict's reagent + extract solution +test tube in boiling water bath for 5 min	Green colored solution observed.	Solution was observed green.

4.TOTAL FLAVANOID CONTENT (TFC)
Total Flavonoid Content:
Determination of Total Flavonoid Content (TFC)
The total flavonoid content (TFC) of the samples was determined using the colorimetric method of Bertolino et al. with slight modification. Briefly, 1 mL of the extracted sample was added to 4 mL distilled water into a test tube. The mixture was then well mixed and 0.3 mL of 5% sodium nitrite ($NaNO_2$) solution was added and left for five minutes. Then 0.3 mL of 10% aluminium chloride ($AlCl_3$) was added and the reaction mixture was maintained at room temperature for 1 min. Then 2 mL of 1M sodium hydroxide (NaOH) was added and mixture was allowed to react for 1 min at room temperature. The mixture was then brought to final reaction volume of 2.4 mL with addition of distilled water and allowed to develop the color for 15 min at room temperature in the dark. For the standard calibration curve, rutin and quercetin standard solutions with different concentrations were prepared by taking 1, 2, 3 and 4mL aliquots of the standard solution and adding ethanol to a final volume of 10mL. The absorbance of the resultant solutions was determined at 510 nm using a UV-visible spectrophotometer. Total flavonoid content was determined using the respective standard calibration curves and expressed as milligrams of rutin equivalent (RE) or quercetin equivalent (QE) per 100 g of sample (mg RE/100 g or mg QE/100 g sample).[17]

THIN LAYER CHROMATOGRAPH (TLC):
Thin-Layer Chromatography (TLC)
Analysis of Aqueous Extracts
Preliminary phytochemical screening of aqueous extracts of Aegle marmelos and Bergenia ligulata was carried out with thin layer chromatography (TLC). For TLC plates preparation, 5 g of gel-G was mixed with 10 mL of distilled water to prepare smooth and uniform slurry. Clean glass plates were uniformly coated with the slurry and dried at room temperature. The plates were dried and activated for 1 hour at 100^{o} C in hot air oven ti remove moisture and to improve the adsorption efficiency.
After activation, a baseline was drawn approximately 1 cm from the bottom edge of each TLC plate. The aqueous extracts were placed on the designated line as tiny spots at equal spacing between each spot using capillary tubes. The mobile phase was a solvent solution of toluene, formic acid and ethyl acetate in the ratio of 5:4:0.5 (v/v/v). The prepared TLC plates were placed vertically in the developing chamber presaturated with the solvent solution to keep the sample spots above the solvent level.The solvent was then allowed to run up the plate by capillary action until the desired distance was reached. The solvent front was marked as soon as the plates were taken out of the chamber. The bands and spots were separated, dried and examined. The spots appeared on the TLC plates were separated and the pattern of the spots helped to detect the presence and pattern of distribution of phytochemical ingredients which made it easier to identify the substances found in the aqueous extracts.[18]

MOLECULAR DOCKING
PREPARATION OF PROTEIN STRUCTURES
The experimental coordinates of IL-17RC (PDB ID: 6HGA) arrangements were taken from PDB (rcsb.org/pdb/). Ligands were eliminated from the binding sites of both IL-17RC for docking research studies. Heteroatoms were removed and also polar hydrogen atoms were added to protein structures, and also partial atomic charges were assigned. The proteins were saved in PDB format; atomic solvation parameters were assigned and converted finally into PDBQ format.

PREPARATION OF LIGANDS
Potential chemicals found in the chosen plants were utilized as ligands in this investigation, and medicinal plants with anti-inflammatory qualities were chosen from earlier research. quercetine and Rutin from Aegle marmelos , Bergenia ligulate . The 6HGA protein structure was optimized, purified, and

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prepared for docking with the help of Discovery Studio Visualizer 2019 by removing unwanted water molecules, bound ligands from the proteins Structure and saved again in a pdb file format to the same folder.

PROTEIN -LIGANDS DOCKING

AutoDock 4.2 was used to dock ligands against IL-17RC. A popular molecular docking program in the public domain is called AutoDock. It employs the Lamarckian genetic algorithm to generate a set of potential conformations and incorporates components such as AutoGrid and AutoTors. This software deals with the flexible docking of ligands directly into a known protein structure. The ligands were allowed torsional flexibility while the proteins for each docking were kept stiff. AutoTors was used to specify the rotatable bonds in the ligands, and AutoGrid was used to calculate grid maps. Grid points of 40x40x40 with 0.675 were used for the search. A˚ spacing for Quercetin and 40x40x40 with 0.503A˚ spacing for Rutin in three dimensions constructed in x, y, and z directions on the macromolecule binding site. There are 50 docking runs with 150 participants in each docking experiment. All other parameters were set to their default values. The binding energy and bound conformations of docked structures are provided by the AutoDock results.

MOLECULAR DOCKING PROTOCOL WITH DISCOVERY STUDIO

The Discovery Studio application was used to carry out molecular docking. It gave the ligands complete flexibility, which aids in the creation of ligand conformation. Using a default option, the crystal structure was created using Discovery Studio's "prepare protein" procedure. The "prepare ligand" process in Discovery Studio was utilized to prepare the chosen phytoconstituents that were employed as ligands. Additionally, docking was carried out a grid-based molecular docking technique that makes use of CHARMm force fields. The docking study's default settings were top hits (10), random conformations (10), orientations to refine (10), force field (CHARMm), and employ full potential (false). The total docking energy, is used to evaluate the results.

RESULT AND DISCUSSION

Physicochemical Evaluation of Crude Drug

The physicochemical evaluation of the crude drugs Aegle marmelos and Bergenia ligulata was performed to determine their purity and quality. During the foreign matter analysis, no visible impurities such as stones, insects, fungal growth, or other extraneous materials sample, indicating that the drug was clean and free from contamination. Likewise, the Bergenia ligulata sample showed no signs of mold, slime, rodent droppings, insects, or any undesirable matter, which reflects proper handling and good quality of the crude drug.

The moisture content of the samples was determined by the loss on drying (LOD) test. The LOD value of Aegle Marmelos was found to be 9% w/w, whereas Bergenia ligulata exhibited a lower value of 5.8%w/w. The comparatively lower moisture content of both drugs was within acceptable limits, suggesting that they are suitable for further analysis and medicinal applications.

Overall, the results of the physicochemical studies relealed that both Aegle marmelos and Bergenia ligulata possess good quality and purity. The absence of foreign matter and the acceptable moisture content indicate that the crude drugs were proper processed and stored. These findings support their suitability for subsequent pharmacognostic and phytochemical and phytochemical investigations and provide a basis for their safe and effective use in herbal formulations and research studies.

Table No 2 : Physicochemical Evaluation of Crude Drug

Sr.no	Parameter	Result obtained *Aegle marmelos*	Result obtained *Bergenia ligulate*
1	Foreign Matter	No visible foreign particles, insects, stones, or fungal growth were observed.	The sample must not have any obvious signs of mold growth, slime, stones, rodent droppings, insects, or anything else that could be harmful when checked.
2	Loss on Drying	9%w/w	5.8%w/w

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Extractive value

The extractive values of Aegle marmelos and Bergenia ligulata were evaluated using alcohol and water as extraction solvents, and the findings are presented in Table No. 3. The alcohol-soluble extractive value of Aegle marmelos was found to be 0.29% w/w, while Bergenia ligulata showed a markedly higher value of 14.6% w/w. Likewise, the water-soluble extractive value of Aegle marmelos was 0.66% w/w, whereas Bergenia ligulata exhibited a higher value of 18.2% w/w.

These results suggest that Bergenia ligulata possesses a greater quantity of extractable constituents than Aegle marmelos. In both plant samples, the water-soluble extractive values were higher than the alcohol-soluble extractive values, indicating that a larger proportion of their phytochemical constituents are polar in nature and readily soluble in water. The comparatively higher extractive values observed in Bergenia ligulata may be attributed to the presence of a higher concentration of bioactive compounds. Therefore, the extractive values obtained in the present study can be considered important parameters for assessing the quality, purity, and standardization of these crude drugs.

Overall, the findings indicate that Bergenia ligulata contains a richer amount of extractable phytoconstituents than Aegle marmelos. Furthermore, the higher water-soluble extractive values in both samples suggest that water is a more effective solvent for extracting their active constituents. These observations support the medicinal significance of both plants and provide valuable information for their pharmacognostic evaluation and quality control.

Table No 3 : Extractive value

Sr no.	parameters	Results obtained *Aegle marmelos*	Results obtained *Bergenia ligulate*
1.	Alcohol Soluble Extractive Value	0.29%w/w	14.6%w/w
2.	Water Soluble Extractive Value	0.66%w/w	18.2%w/w

Phytochemical screening

Preliminary phytochemical screening of Aegle marmelos and Bergenia ligulata was carried out to identify the presence of important secondary metabolites, and the results are summarized in Table No. 4. The analysis revealed the presence of alkaloids in both plant samples, as confirmed by positive results in Mayer's and Dragendorff's tests. Flavonoids were also detected in both plants through the concentrated sulphuric acid test, indicating the occurrence of compounds with potential antioxidant activity.

Steroidal constituents showed a variation between the two plants. Aegle marmelos gave a positive result in the Salkowski reaction, indicating the presence of steroids, whereas Bergenia ligulata did not show a positive response, suggesting the absence of steroidal compounds. Furthermore, carbohydrate analysis by Fehling's and Benedict's tests confirmed the presence of carbohydrates in both plant samples.

The findings indicate that both Aegle marmelos and Bergenia ligulata are rich sources of bioactive phytoconstituents, particularly alkaloids, flavonoids, and carbohydrates. The presence of these compounds may contribute to the therapeutic properties of the plants, including antioxidant, antimicrobial, anti-inflammatory, and other pharmacological activities. The presence of steroids exclusively in Aegle marmelos suggests a difference in the chemical composition of the two species, which may influence their medicinal applications.

Overall, the preliminary phytochemical screening demonstrated that both plants possess several important classes of secondary metabolites. However, Aegle marmelos exhibited the presence of steroids in addition to alkaloids, flavonoids, and carbohydrates, whereas Bergenia ligulata lacked steroidal constituents. These results provide valuable information regarding the chemical composition of the plants and support their use in traditional medicine. Furthermore, the phytochemical profile obtained in the present study can serve as a basis for further pharmacological investigations, quality control, and standardization of these medicinal plants.

Table No 4 : Preliminary Phytochemical Screening

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Phytochemicals	Tests	*Aegle Marmelos*	*Bergenia Ligulate*
Alkoloid	Mayer's test :	Present (+)	Present (+)
	Dragendroff's test :	Present (+)	Present (+)
Flavonoids	With con. Sulphuric acid :	Present (+)	Present (+)
Steroids	Salkowski reaction:	Present (+)	Absent(-)
Carbohydrates	Fehling's test :	Present (+)	Present (+)
	Benedict's test :	Present (+)	Present (+)

Total flavonoid content (TFC)

The total flavonoid content (TFC) of Aegle marmelos and Bergenia ligulata extracts was estimated using the aluminium chloride colorimetric method, with quercetin employed as the standard reference compound. The results presented in Table No. 6 revealed that Aegle marmelos contained a considerably higher amount of flavonoids, with a value of 143.91 mg QE/g extract, whereas Bergenia ligulata showed a total flavonoid content of 35.7 mg QE/g extract.

The standard calibration curve of quercetin exhibited good linearity, with the regression equation y = 0.0023x + 0.0079 and a correlation coefficient (R^2 = 0.9675), indicating that the method used for flavonoid estimation was reliable and reproducible. The significantly higher flavonoid content observed in Aegle marmelos suggests that this plant possesses a richer source of phenolic compounds and flavonoids than Bergenia ligulata. As flavonoids are well known for their antioxidant, anti-inflammatory, and free radical scavenging properties, the higher TFC of Aegle marmelos may contribute to its greater therapeutic potential.

Table No 5 : Total Flavonoids content (TFC)

Sr.no	parameters	Results obtained *Aegle marmelos*	Results obtained *Bergenia Ligulate*
1.	Total Flavonoids Content	143.91 mg QE/g extract	35.7 mg QE/g extract

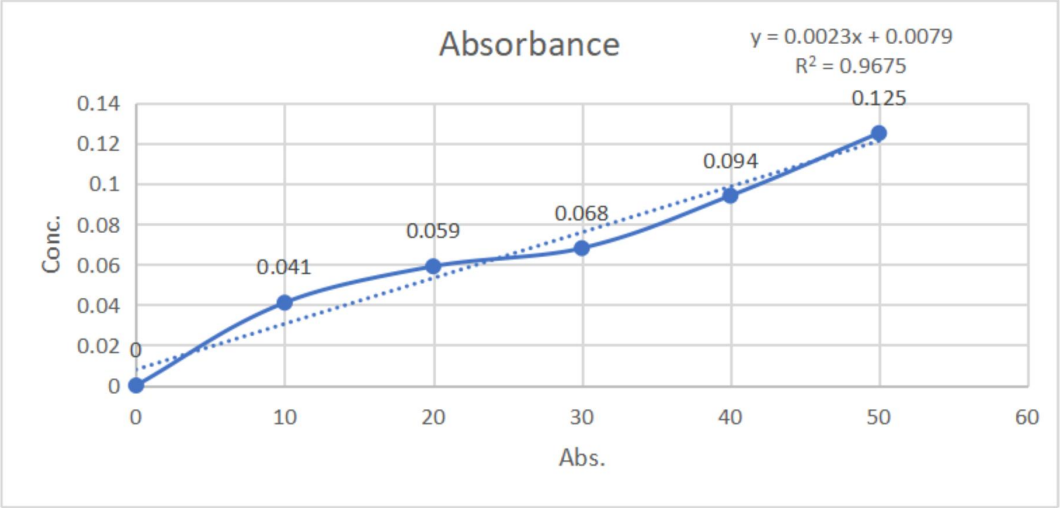
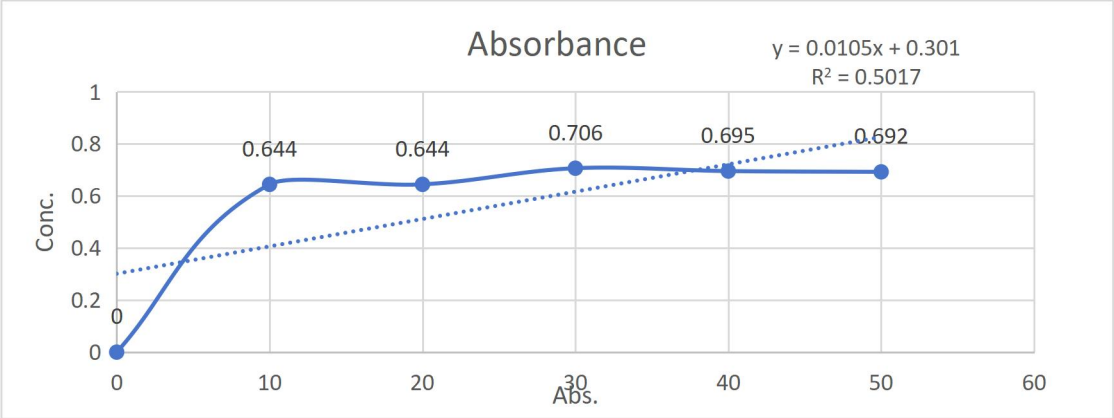


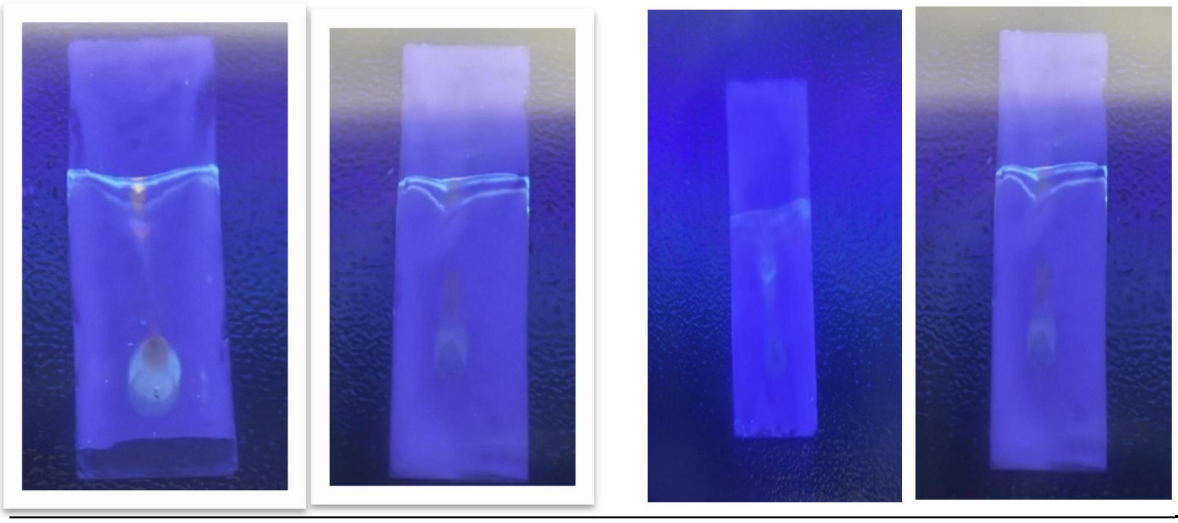
Fig No 3 : Total Flavonoid Content Graph *Aegle marmelos*

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Thin Layer Chromatography (TLC) Analysis

Thin Layer Chromatography (TLC) was performed to further characterize the phytochemical constituents present in the aqueous extract of Aegle marmelos leaves and to confirm the presence of flavonoid compounds. The extract was prepared in ethanol at a concentration of 10 mg/mL and applied to silica gel TLC plates using capillary microtubes. Approximately 10 µL of the sample was spotted on the plate, maintaining a distance of 1 cm from the bottom edge and side margins. The chromatographic separation was carried out using a mobile phase consisting of toluene, ethyl acetate, and formic acid in the ratio of 5:4:0.5 (v/v/v). The TLC plates were developed in a pre-saturated migration chamber over a distance of about 3.5 cm, dried in a hot air oven, and subsequently examined under white light as well as ultraviolet light at 254 nm and 365 nm The chromatographic analysis revealed the presence of several distinct spots, particularly in the aqueous extract, indicating the occurrence of multiple phytoconstituents. The aqueous extract exhibited a greater number of fluorescent spots under long-wave UV light (365 nm), suggesting a rich chemical composition and a high diversity of flavonoid compounds. Comparison of the Rf values of the separated spots with those of standard compounds provided evidence for the presence of important flavonoids. Certain spots showed Rf values comparable to those of standard rutin (Rf = 0.72) and quercetin (Rf = 0.63), thereby confirming the presence of rutin- and quercetin-like flavonoids in the extract. The TLC findings were consistent with the results obtained from preliminary phytochemical screening, which demonstrated the presence of flavonoids in the plant extract. The combined evidence from phytochemical tests and chromatographic profiling supports the occurrence of bioactive flavonoids in Aegle marmelos. Although some extracts showed fewer spots despite positive preliminary screening results, this variation may be attributed to the low concentration of flavonoids present or to the limitations associated with the solvent system employed. Overall, TLC analysis provided valuable qualitative evidence for the presence of quercetin and rutin and further highlighted the rich flavonoid profile and chemical complexity of the aqueous extract of Aegle marmelos.



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Fig. No 5 : Thin layer chromatography *Aegle marmelos* and *Bergenia Ligulate*

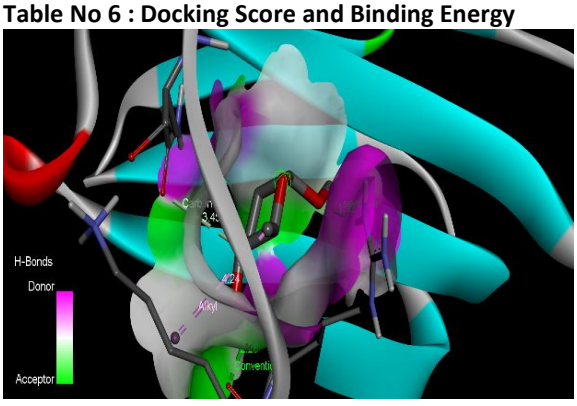
Molecular docking

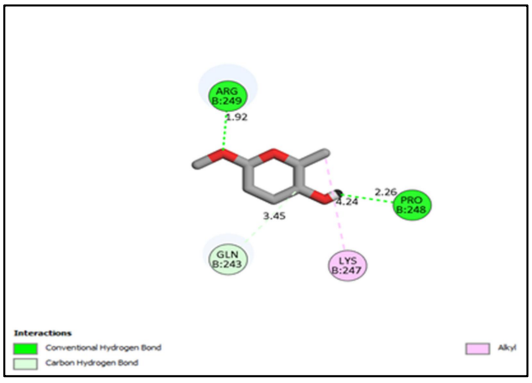
In the present study, molecular docking studies were performed to evaluate the antipsoriatic potential of phytoconstituents quercetin and rutin obtained from Aegle marmelos and Bergenia ligulata against IL-17RC receptor (PDB ID: 6HGA). The plant materials were successfully collected, dried, powdered and extracted . Preliminary phytochemical and analytical studies by UV spectroscopy, TLC.identified the presence of important flavonoids, such as quercetin and rutin, in the extracts. The protein structure of IL-17RC was prepared by removing water molecules, ligands and heteroatoms, and adding hydrogen atoms and partial charges. The ligands quercetin and rutin were downloaded from the PubChem database and converted into suitable docking formats for analysis. Molecular docking was performed successfully using AutoDock 4.2 and Discovery Studio software. The study was designed to Studio Software The present study aimed to evaluate the antipsoriatic potential of two flavonoids (quercetin and rutin) extracted from Aegle marmelos and Bergenia ligulata through molecular docking against IL-17RC receptor (PDB ID: 6HGA), an important protein involved in psoriasis inflammation. Docking Results (Table 6) revealed that both compounds showed good interaction with the IL-17RC receptor. Rutin had a binding energy of -8.2 kcal/mol with four hydrogen bonds, while quercetin had a slightly lower binding energy of -7.3 kcal/mol with three hydrogen bonds.

Docking Score and Binding Energy

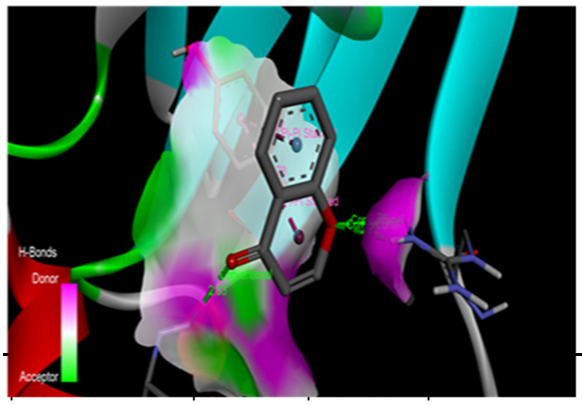
This means that both compounds have good affinity to the receptor with the rutin complex being slightly more stable. Protein–Ligand Interactions (Table 7) were as follows: Rutin formed hydrogen bonds with ARG249, PRO248, and GLN243 and hydrophobic interaction with LYS247. Quercetin stabilized the ligand in the active site of the receptor by hydrogen bonds with ARG249, GLN241, and TYR238.

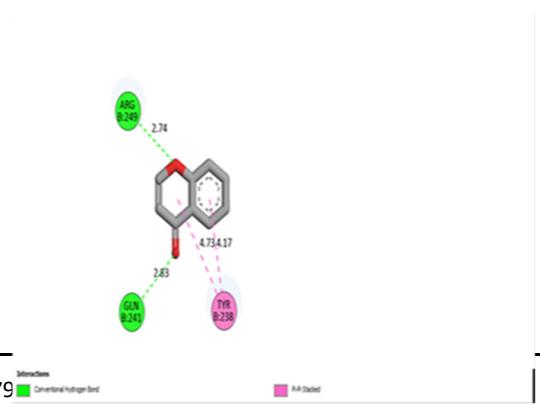
Table No 6 : Docking Score and Binding Energy





Interaction between Rutin and 6HGA 3D Structure 2D Structure





Interaction between Quercetin and 6HGA 3D Structure 2D Structure

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doi: 10.61705/6pjgdk14
Ace J. Addict., 7 (1): 70-81 | 2026

Sr. no	Ligand name	Target protein	PBD ID	Binding Engery	No .of H - Bonds	Amino Acid Interaction
1.	Rutin	IL-17RC receptor	6HGA	-8.2	4	ARG249,PRO248, GLN243, LYS247
2.	Quercetin	IL-17RC receptor	6HGA	-7.3	3	ARG249, GLN241, TYR238

Protein–Ligand Interaction Analysis

Table No 7: Protein -Ligand Interaction Analysis

Ligand	Interaction	Amino Acid Residue	Bond Distance
Rutin	Hydrogen Bond	ARG249	1.92 Å
	Hydrogen Bond	PRO248	2.26 Å
	Hydrogen Bond	GLN243	3.45 Å
	Hydrophobic Bond	LYS247	4.24 Å
Quercetin	Hydrogen Bond	ARG249	2.74 Å
	Hydrogen Bond	GLN241	2.83 Å
	Hydrogen Bond	TYR238	4.17 Å
	Hydrophobic Bond	TYR238	4.73 Å

Stabilized the ligand in the active site of the receptor by hydrogen bonds with ARG249, GLN241, and TYR238. Both flavonoids fitted well into the binding pocket with stable interactions via hydrogen bonding and hydrophobic contacts as confirmed from 3D and 2D interaction visualizations. These interactions imply that both compounds could inhibit IL-17RC-mediated inflammatory signaling in psoriasis. Between the two, quercetin showed higher interaction in terms of receptor binding efficiency possibly due to its smaller molecular size which facilitates better entry into the active site. Rutin also displayed high binding, but with a somewhat lower receptor complementarity, likely due to its larger glycoside structure. Overall, the docking study suggests that both quercetin and rutin are promising natural compounds that may exhibit antipsoriatic activity. Their ability to bind stably to IL-17RC points to their potential to reduce inflammation associated with psoriasis. Molecular docking also proved to be a reliable and cost-effective method for screening herbal compounds before further laboratory and clinical evaluation.

CONCLUSION

The present study evaluated the phytochemical constituents and potential antipsoriatic activity of Aegle marmelos and Bergenia ligulata through physicochemical analysis, preliminary phytochemical screening, total flavonoid content estimation, thin-layer chromatography (TLC), and molecular docking studies. The physicochemical evaluation revealed the absence of visible foreign matter and loss on drying values of 9% w/w for Aegle marmelos and 5.8% w/w for Bergenia ligulata. Phytochemical screening confirmed the presence of alkaloids, flavonoids, and carbohydrates in both plants, while steroids were detected only in Aegle marmelos. The total flavonoid content was higher in Aegle marmelos (143.91 mg QE/g extract) than in Bergenia ligulata (35.7 mg QE/g extract). TLC analysis indicated the presence of rutin- and quercetin-like flavonoids in the Aegle marmelos extract. Molecular docking against the IL-17RC receptor (PDB ID: 6HGA) demonstrated favourable binding interactions for both flavonoids. Rutin exhibited a binding energy of −8.2 kcal/mol with four hydrogen bonds, whereas quercetin showed −7.3 kcal/mol with three hydrogen bonds. These findings suggest that both compounds may have potential in the development of plant-based antipsoriatic agents, with rutin demonstrating stronger predicted binding affinity. However, these results are preliminary and based on phytochemical analysis and computational predictions. Further in-vitro, in-vivo, toxicity, and clinical studies are required to confirm their biological activity, safety, and therapeutic effectiveness in psoriasis.

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