

Formulation And Evaluation of Herbal Body Wash Containing *Mentha Gattefossei* for Anti-seborrheic Activity with in Silico Studies

Buddhbhushan Rambhau Gaikwad¹, Gopal Rajesh Bhakde², Shubham Bhagwan Korhale³,
Shruti Sanjay Dike⁴, Divya Valmik Pagare⁵, Tejasvi Tribhuwan⁶, Santosh Jain⁷
^{1,2,3,4,5,6,7} *Shri Sai College of Pharmacy Khandala, Tq. Vaijapur, Dist. Chh. Sambhajinagar*

Abstract—Seborrheic dermatitis is a common chronic inflammatory skin disorder associated with excessive sebum production, microbial growth, and scalp or skin irritation. Herbal formulations are gaining importance as safer and eco-friendly alternatives to synthetic skin-care products. The present study focuses on the development and evaluation of a herbal body wash containing *Mentha gattefossiei* for anti-seborrheic activity supported by molecular docking studies. The plant is known for the presence of bioactive phytochemicals such as pulegone, menthone, flavonoids, and phenolic compounds possessing antimicrobial, anti-inflammatory, and antioxidant properties.

The herbal body wash was formulated using extract of *Mentha gattefossiei* along with suitable natural excipients. The prepared formulation was evaluated for various physicochemical parameters including pH, viscosity, foamability, spreadability, appearance, and stability. Anti-seborrheic activity was assessed through antimicrobial studies against seborrhea-associated microorganisms such as *Malassezia* species and *Staphylococcus aureus*. Molecular docking analysis was performed to determine the binding affinity of selected phytoconstituents with target proteins involved in seborrheic dermatitis and microbial growth.

The docking results demonstrated significant interaction of active compounds with target receptors, indicating potential inhibitory activity.

Index Terms—Herbal body wash, *Mentha gattefossiei*, Anti-seborrheic activity, In-silico study.

I. INTRODUCTION

1.1. Antiseborrheic Activity

Antiseborrheic activity refers to the ability of a substance (drug, cosmetic ingredient, or therapeutic agent) to prevent, reduce, or control seborrhea — a

condition characterized by excessive sebum (oil) production and abnormal shedding of skin cells.

1.2. What is Seborrhea?

1.3. Seborrhea is a disorder of the sebaceous glands that leads to:

- Overproduction of sebum (oily secretion)
- Greasy, scaly skin or scalp
- Conditions like dandruff, seborrheic dermatitis, and acne^[1]

Seborrhea dermatitis is a skin disorder that usually appears on parts of the body that have high density of sebaceous glands, such as the face, chest, and scalp.

1 The prevalence is 1–3% in the general population and 34–83% in people with compromised immune systems.

2 Risk factors for this disease include age, gender, increased activity of the sebaceous glands, immune deficiency, neurological and psychiatric diseases, use of certain drugs, and low humidity or ambient temperature. ^[2,3]

II. MOLECULAR DOCKING

Molecular docking is such a structure-based drug design method that simulates the molecular interaction and predicts the binding mode and affinity between receptors and ligands. In recent years, this technology has been widely used in drug design research field. Using the compounds database to screen the docking potential pharmacophores is not only convenient for researchers to purchase, synthesize and complete follow-up pharmacological tests, but also greatly improves the efficiency and reduces the research cost. In addition, the emergence of the reverse molecular

docking technology could significantly improve the drug target predictive capacity and under-stand the related molecular mechanism for drug design. Finally, this review briefly introduces the latest progress ^[4-5]

III. HERBAL BODY WASH

The majority of body wash detergents and cosmetics are aqueous (10–20%) solutions of surfactants enhanced with different substances to improve the washing effect, attain the right consistency, color, fragrance, or product preservation. Body wash is a specific type of liquid that is used to clean the body while taking a shower. Gel body wash has a very liquid-like viscosity. Body wash, also known as shower gel, is an essential part of our everyday hygiene regimen since it makes bathing fun and helps remove pollutants, oils, and debris from the skin. In order to develop solutions that successfully cleanse, nourish, and protect the skin without irritating or drying it out, the science underlying body wash composition is crucial.^[6]

IV. MENTHA GATTEFOSSEI

- Common Name: Mentha Mentha gattefossei, Gattefosse's Mint Gattefosse's Horsemint
- Family: Lamiaceae
- Biological Source: Peppermint consists of dried leaves and flowering tops of Mentha piperita Linn
- Part Used: Leaf pulp(gel)
- Chemical Constituents: Peppermint contains volatile oil, resin, tannins and gum
- Properties: Cooling, moisturizing, soothing anti-inflammatory, Antiseborrheic
- Importance: Mentha gattefossei can be used as an ornamental plant in gardens, as a medicinal plant for treating digestive issues, and as a flavoring agent in food and drinks. ^[9]

V. MATERIALS AND METHODS

5.1 Materials

The leaves of spearmint (*M. spicata* L.) were obtained from Cameron Highland in Pahang, Malaysia. After harvesting, the leaves were separated and washed under tap water. Leaves were dried at 40°C in a

ventilated drying oven (1350FX, USA) for 24h and then stored at ambient temperature (22°C) in the dark. The samples were ground in grinding mill (MX-335, Panasonic, Malaysia) for 10s to produce a powder with an approximate size of 0.525 mm.

5.2 Formulation Table:

Table 5.2 Formulation table of herbal body wash

Sr No	Ingredient	Quantity for 20 ml	Function
1	Castile soap	8 ml	Cleansing agents
2	Guar gum	0.2 ml	Thickening agent
3	Mentha extract	0.5 ml	Anti seborrheic activity
4	Glycerin	1 ml	Moisturizer
5	Sodium benzoate	0.1 ml	Preservative
6	Rose oil	2.3 ml	Fragrance
7	Citric acid	Q .S	PH Adjacent
8	Distilled water	Q .S to 20 ml	Vehicle
9	Aloe vera	2 ml	Smoothing

5.3 Extraction

The commonly employed technique for separation of active substance from crude drug is called “Extraction” which involves the use of different solvents. The plant material used for extraction should be properly authenticated or identified. The choice of the plant material for extraction depends on its nature and the components required being isolated. The dried powdered plant material is commonly used for extraction. The fresh plant parts when used are homogenized or macerated with a solvent such as alcohol.

5.4 Procedure Of Formulation

1)Prepare Base

We have take 10 ml distilled water

We have add guar gum slowly with stirring to avoid lumps.

2)Add Soap Bas

We have mix soap base gently to avoid foam formation.

3) Add moisturizing agents

We added glycerin and aloe vera gel, mix well.

4) Add herbal extract

We added mentha extract and stir.

5) Add preservative

We dissolved sodium benzoate in a small amount of water and add.

6) Add fragrance

We added rose oil 2-3 drop.

7) Adjust PH

We added citric acid dropwise to maintain PH 5.5-6.

8) make up volume

We added distilled water to make final volume 20 ml.

9) Mix and pack

We Stir gently, filter if needed, and fill in a container.

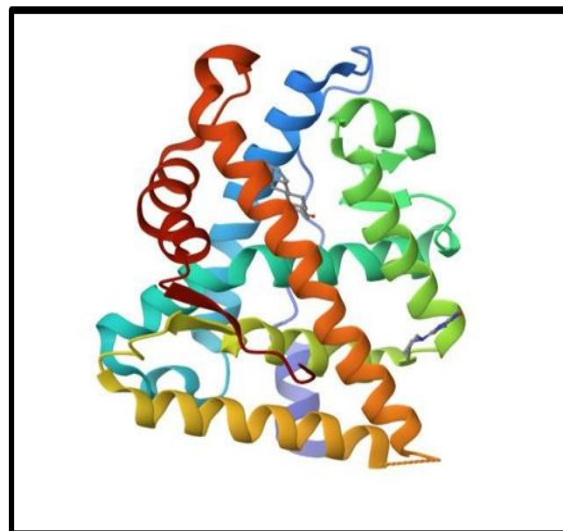
[14, 15]

6. Drug And Receptor Profile

The study analyzes the detailed profiles of receptors and phytoconstituents (ligands) using PASS and ADMET. We utilized cheminformatic websites like Drug Bank Online, PubChem and RCSB to gather data for this analysis.

6.1 Receptor Profile : (4K7A)

Receptor Name : Crystal structure of the androgen receptor ligand binding domain in complex with minoxidil



Classification and Structural Details Classification: TRANSCRIPTION

Organism(s): Homo_sapiens

Chains: A

Entity ID: Androgen receptor

Sequence Length: 249

DOI: <https://doi.org/10.2210/pdb4K7A/pdb>

6.2 Ligand profile (Standard Inhibitors):

Table. ligand profile of Metronidazole

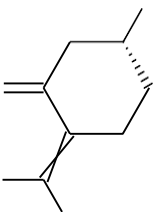
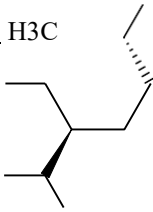
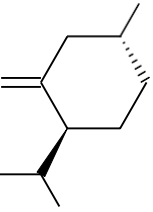
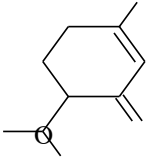
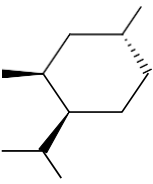
Parameters	Description
Structure	
Generic Name	Metronidazole
Synonyms	- metronidazole 443-48-1 - Metronidazole 2-Methyl-5-nitroimidazole-1-ethanol - Gineflavir
Brand Name	Flagyl, Metrogyl, Metro cream, Metrogel, Vandazole,
Molecular Formula	C ₆ H ₉ N ₃ O ₃
Molecular Weight	171.15 g/mol

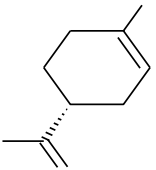
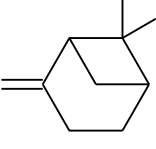
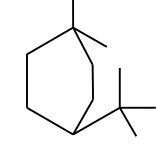
IUPAC Name	2-(2-methyl-5-nitroimidazol-1-yl) ethanol
Melting Point	159-163 °C
Solubility	Approximately 64.8 mg/mL
Side Effect	metallic taste, nausea, headache, dizziness, diarrhea, and dark urine.
Category	Metronidazole is a synthetic nitroimidazole antimicrobial agent

6.3 Ligand Profile (Phytoconstituents) :

The table below 7.1.3, shows the phytoconstituents selected for the Molecular Docking Study

Table Phytoconstituents Selected for the Molecular Docking Study

Chemical Name	Structure	IUPAC Name
Pulegone	$\begin{matrix} \text{CH}_3 \\ \text{O} \text{---} \text{H}_3\text{C} \\ \text{CH}_3 \end{matrix}$ 	(5R)-5-methyl-2-propan-2-ylidenecyclohexan-1-one
Menthone	$\begin{matrix} \text{CH}_3 \\ \text{O} \text{---} \text{H}_3\text{C} \\ \text{CH}_3 \end{matrix}$ 	trans-(2S,5R)-5-methyl-2-propan-2-ylcyclohexan-1-one
Neomenthone	$\begin{matrix} \text{CH}_3 \\ \text{O} \text{---} \text{H}_3\text{C} \\ \text{CH}_3 \end{matrix}$ 	trans-(2S,5R)-5-methyl-2-propan-2-ylcyclohexan-1-one
Piperitone	$\begin{matrix} \text{CH}_3 \\ \text{H}_3\text{C} \\ \text{CH}_3 \end{matrix}$ 	3-methyl-6-propan-2-ylcyclohex-2-en-1-one
Neomenthol	$\begin{matrix} \text{CH}_3 \\ \text{HO} \text{---} \text{H}_3\text{C} \\ \text{CH}_3 \end{matrix}$ 	(1S,2S,5R)-5-methyl-2-propan-2-ylcyclohexan-1-ol

D-Limonene	CH ₃ 	(4R)-1-methyl-4-prop-1-en-2-ylcyclohexene
α -pinene	CH ₃ CH ₃ CH ₃ 	2,6,6-trimethylbicyclo[3.1.1]hept-2-ene
β -pinene	CH ₃ CH ₃ H ₂ C 	6,6-dimethyl-2-methylidenebicyclo[3.1.1]heptane
Eucalyptol	CH ₃ O CH ₃ CH ₃ 	1,3,3-trimethyl-2-oxabicyclo[2.2.2]octane

VI. METHOD

Molecular Docking Using AutoDock Vina

6.1 Introduction

AutoDock Vina is a molecular docking software used to study the interaction between a ligand and a target protein. It predicts binding affinity, binding mode, and interactions between protein and ligand. It is widely used in drug discovery and pharmaceutical research.

6.2 Procedure

1. Protein Selection

- Download protein structure from RCSB-PDB in .pdb format.

2. Ligand Selection

- Download ligand structure from PubChem in .sdf format.

3. Create Docking Folder

- Create a folder and save protein and ligand files.

4. Protein Preparation in AutoDock

- Remove water molecules
- Add polar hydrogens
- Add Kollman charges
- Save as protein.pdbqt

5. Ligand Preparation

- Convert ligand .sdf to .pdb using PyMOL.
- Add hydrogens and Gasteiger charges.
- Detect torsions.
- Save as ligand.pdbqt

6. Grid Generation

- Open Grid Box in AutoDock.
- Set center coordinates (X, Y, Z) and grid size covering active site.

7. Create Config File

8. Run AutoDock Vina

Open Command Prompt and run:

```
vina.exe --config config.txt --log log.txt
```

9. Result Analysis

Observe:

- Binding affinity
- Hydrogen bonds
- Amino acid interactions

10. 2D Interaction Using BIOVIA

- Open docked complex in BIOVIA Discovery Studio Visualizer.
- Click:

- Analyze → Receptor–Ligand Interaction → 2D Diagram
- 3. Study:
 - Hydrogen bonding
 - Hydrophobic interactions
 - Amino acid residues involved

VII. RESULT

7.1 Drying and powdering of mentha gattefossei plant leaves:

Mature, healthy *Mentha Gattefossei* plants free of diseases or pests are selected for drying. Leaves are cleaned with water to remove dirt or soil, then shade-dried for 2-3 days to remove moisture. Dry leaves are brittle and easily crushed. The drying process continues until the desired dryness is achieved. Dried leaves are ground into a powder using an electric grinder and passed through a fine-mesh sieve to remove coarse particles. The powdered *Bougainvillea Spectabilis* leaves are stored in airtight containers.

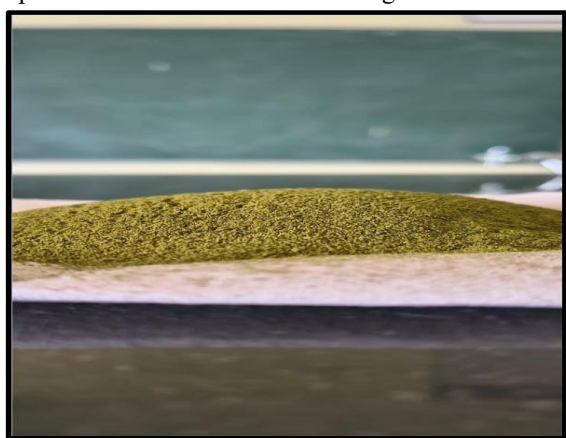


Fig Dried powder of Mentha Gattefossei.

7.2 Morphological study

It is a small aromatic perennial herb. The plant has a creeping or spreading growth habit with a pleasant mint odor. Root system is fibrous and develops from underground runners. Stem is soft, green, quadrangular (four-sided) and slightly hairy. It may be branched and creeping in nature. Leaves are simple, opposite, green, and aromatic. Shape is ovate to lanceolate with serrated (toothed) margins. Leaves contain essential oil glands responsible for mint fragrance. Flowers are small, bisexual, and pale purple to pinkish-white. Arranged in clusters or spikes. Fruit is a small nutlet containing tiny seeds.

7.3 Physicochemical Study:

Powdered drug parameters help in assessing the quality, safety, and purity of herbal materials

7.3.1 Physical appearance

Color: No significant change

Odor: Stable

pH: Stable

Consistency: No phase separation

VIII. PHYSICAL CHARACTERISTICS AND EXTRACTIVE VALUES OF EXTRACTS OF PLANT:

Hydroalcoholic extraction is a method used to extract active phytoconstituents from *Mentha* (mint) leaves using a mixture of water and alcohol (ethanol or methanol) as a solvent. This process helps to obtain both water-soluble and alcohol-soluble compounds such as flavonoids, terpenoids, phenolics, and essential oils from



FIG 9.4. PLANT EXTRACT

8.1 Preliminary Phytochemical Screening:

Phytochemical screening of *Mentha* herbal body wash is carried out to identify the presence of active phytoconstituents such as alkaloids, flavonoids, terpenoids, tannins, saponins, glycosides, and phenols.

Table 8.1 Phytochemical screening of leaves extract of *Mentha Gattefossei*

Sr. No.	Test	Result	Conclusion
1	Dragendorff's	Positive	Presence of Alkaloids
2	Shinoda Test	Positive	Presence of Flavonoids
3	Ferric Chloride Test	Positive	Presence of Phenolic compound
4	Salkowski Test	Positive	Presence of Terpenoid
5	Foam Test	Positive	Presence of Saponins
6	Keller-killiani	Positive	Presence of Glycoside

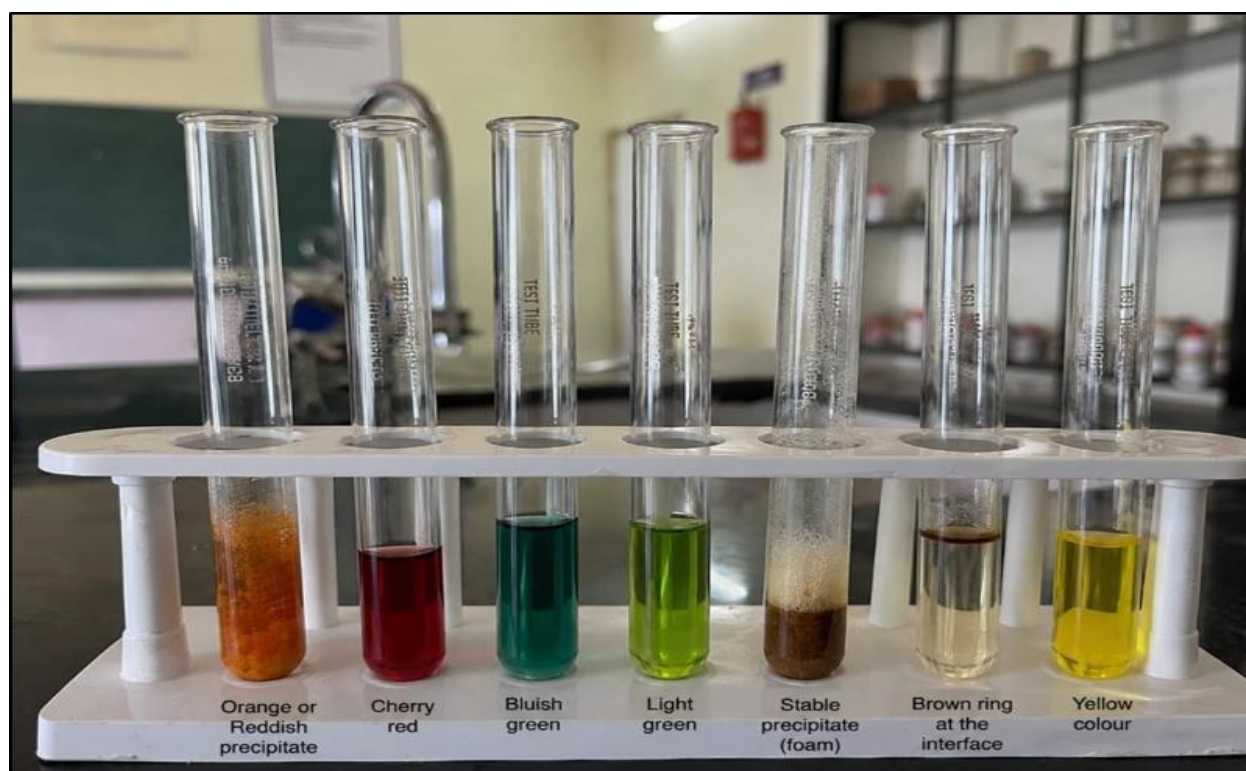


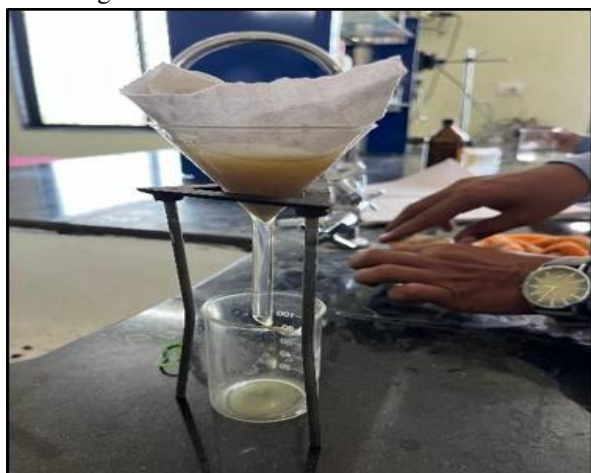
Fig 8.1 Phytochemical screening of leaves extract of *Mentha gattefossei* extract

IX. FORMULATION RESULT

The formulated *Mentha gattefossei* herbal body wash was successfully prepared and evaluated for its physicochemical and biological properties. The formulation showed acceptable physical appearance with a smooth texture, pleasant odor, and good consistency. The pH was found to be skin compatible, indicating suitability for topical application. The body wash exhibited satisfactory foaming ability and

viscosity, ensuring effective cleansing performance. Phytochemical screening confirmed the presence of bioactive compounds such as flavonoids, terpenoids, phenols, alkaloids, and saponins. Molecular docking and in silico studies suggested promising anti-seborrheic activity through favorable interaction of phytoconstituents with target proteins such as squalene epoxidase. Overall, the formulation demonstrated good stability, safety, and potential effectiveness for seborrheic skin management.

Fig 9. Formulation of Mentha Gattefossei



9.1 Evaluation Test:

9.1.1 Determination of pH:

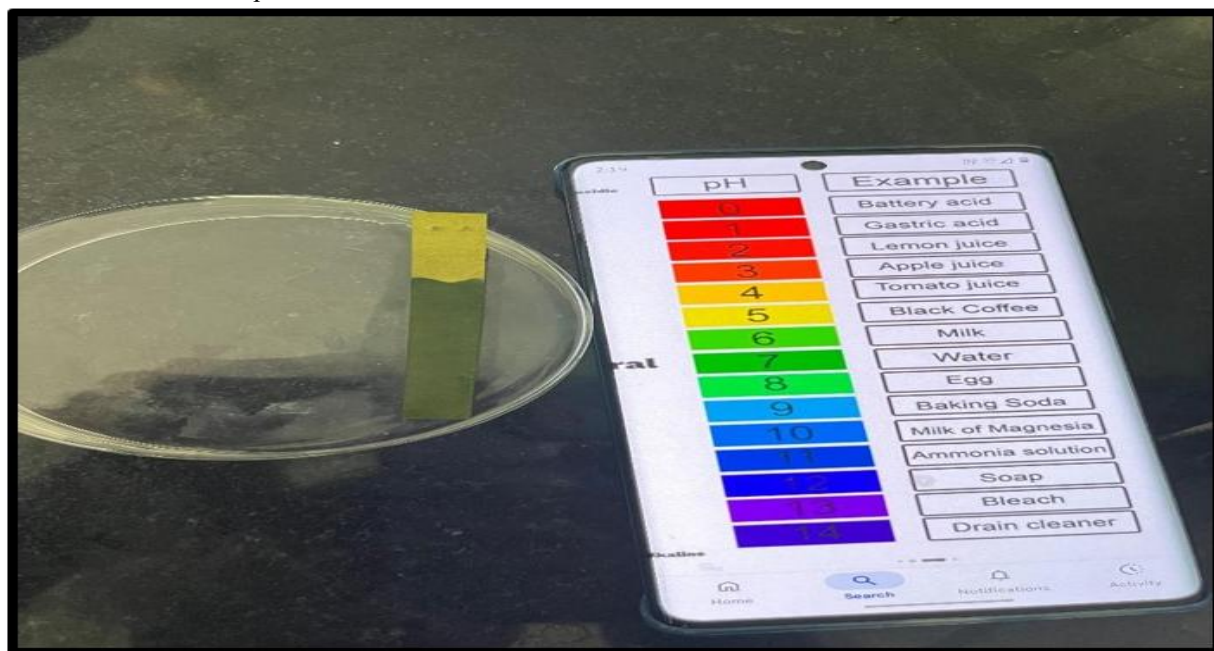


FIG 9.1.1. DETERMINATION OF PH

The Standard 10% Dilution Method (Recommended) While some liquid cleansers can be measured directly, standard cosmetic testing protocols (like Bureau of Indian Standards or general lab practices) recommend a 10% aqueous dilution. This lowers the viscosity of thick body washes, preventing the gel from coating and fouling the delicate glass electrode of a pH meter. Determination of ph test.

9.1.2 Determination of foaming index

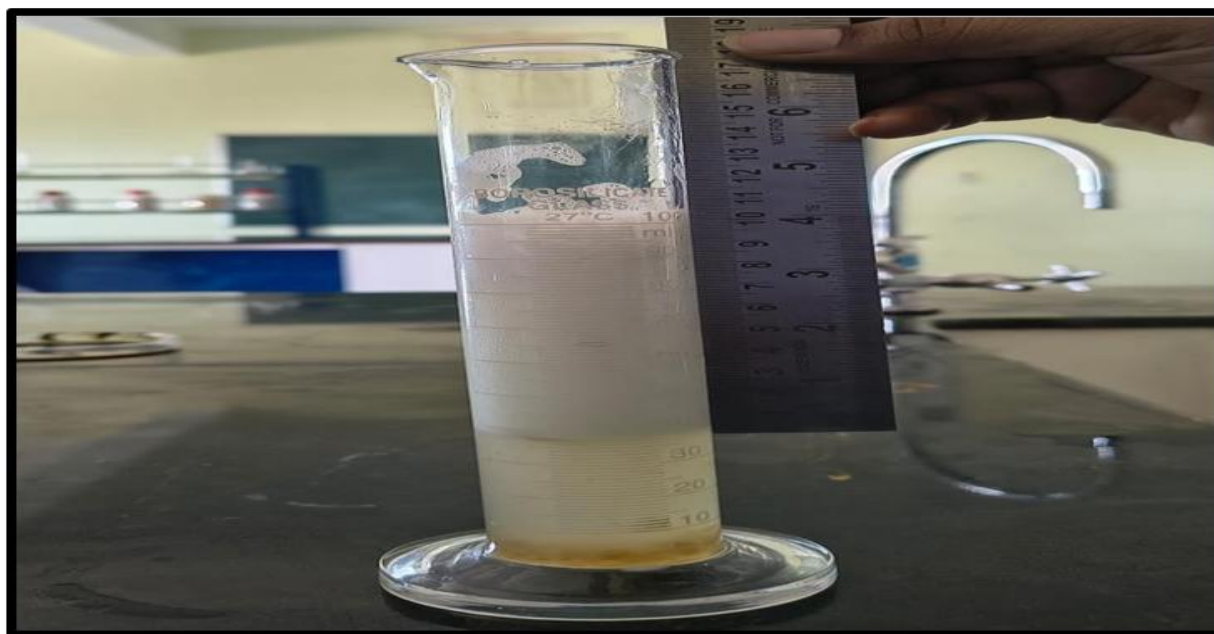


Fig 9.7.2. Determination of foaming index

The formulated herbal body wash showed good foaming ability, with a foam height of 10 cm, indicating satisfactory cleansing and surfactant properties. This suggests that the formulation has acceptable foam formation suitable for body wash application.

9.1.3 Viscosity:

Viscosity of Mentha Herbal Body Wash = 250 cP

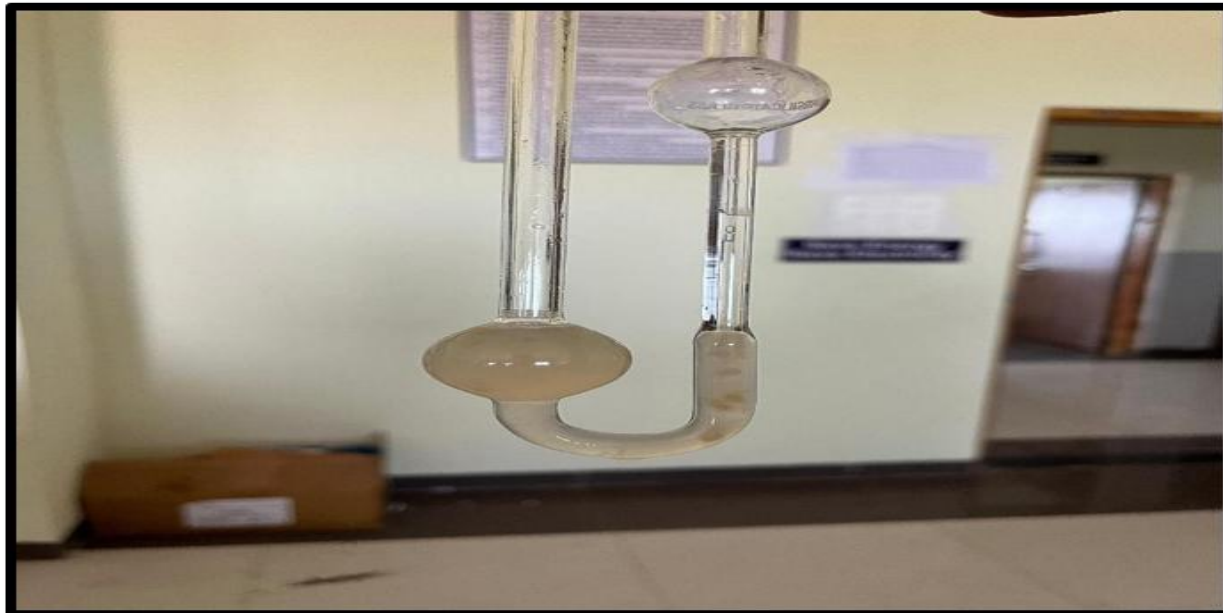


FIG 9.7.3.- VISCOCITY

Table No 9.1.3 - Evaluation Test

Sr. No.	Evaluation Test	Result
1.	Physical Appearance	+++
2.	pH Test	+++
3.	Spreadability Test	+++
4.	Foam Formation Test	++
5.	Viscosity Test	++

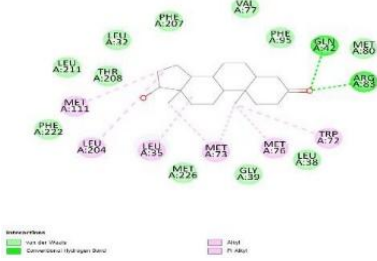
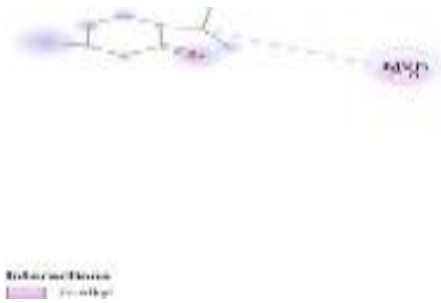
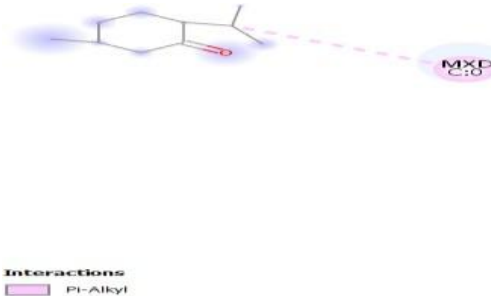
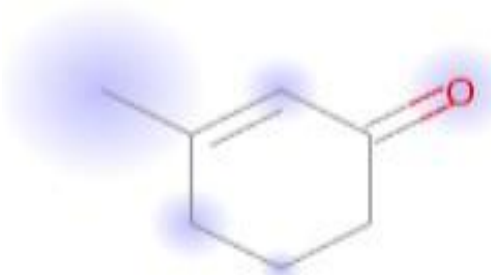
X. MOLECULAR DOCKING

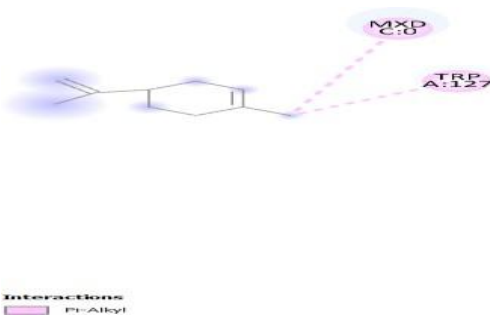
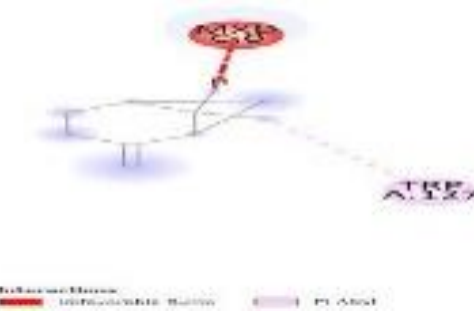
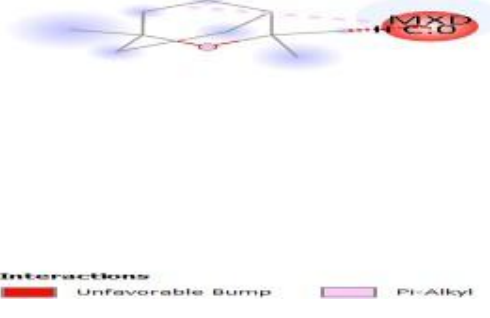
Molecular docking studies play a crucial role in modern drug discovery and can significantly expedite the identification of potential therapeutic agents for various diseases, including seborrheic disease. The results obtained from the Molecular docking of 4K7A receptor with Phytoconstituent using Biovia software are compiled in Table. 9.5.1. and Table. 9.5.2. as follows

Table 10. Molecular docking of 4K7A receptor with Standard..

Standard	2D Interaction	Affinity (kcal/mol)
Metronidazole		-4.0

Table 10. Molecular docking of 4K7A receptor with Phytoconstituents

Sr.No.	Standard	2D Interaction	Affinity (kcal/mol)
1.	Pulegone		-6.3
2.	Menthone		-4.4
3.	Neomenthone		-4.2
4.	Piperitone		-4.5

5.	D-Limonene		-6.3
6.	α -pinene		-4.6
7.	β -pinene		-4.6
8.	Eucalyptol		-4.6

XI. DISCUSSION

The present research work focused on the formulation and evaluation of *Mentha gattefossei* herbal body wash for seborrheic skin management. The plant leaves were successfully dried, powdered, and extracted using a hydroalcoholic extraction method. Phytochemical screening confirmed the presence of various bioactive constituents such as flavonoids, alkaloids, terpenoids, phenols, glycosides, and saponins, which are known for antimicrobial and skin protective activities. The formulated body wash showed good physical appearance, pleasant odor, smooth consistency, and acceptable stability. The pH of the formulation was found to be compatible with skin, indicating safety for topical use. The body wash also exhibited satisfactory foaming ability and viscosity, ensuring effective cleansing properties. Molecular docking studies revealed significant interaction between phytoconstituents and the 4K7A receptor. Pulegone and D-Limonene showed the highest binding affinity among the tested compounds, suggesting promising anti-seborrheic activity. The obtained results indicate that the formulated herbal body wash may serve as a safe and effective herbal alternative for skin cleansing and seborrheic condition management.