

IN SILICO INVESTIGATION, FORMULATION AND EVALUATION OF NON-AEROSOL BASED ANTI PERSPIRANT FOAM FOR SCALP

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Article Received: 04 August 2026 | Article Revised: 25 August 2026 | Article Accepted: 14 September 2026

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DOI: <https://doi.org/10.5281/zenodo.22797725>

How to cite this Article: Dr. R. Sundhararajan, J. Seraphine Joyce, A. Abdul Hadee, K. Abdul Kalam, J. Abdullah, B. Abul Hazan Abrar (2026) IN SILICO INVESTIGATION, FORMULATION AND EVALUATION OF NON-AEROSOL BASED ANTI PERSPIRANT FOAM FOR SCALP. World Journal of Pharmaceutical Science and Research, 5(9), 853-862.



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ABSTRACT

Scalp hyperhidrosis is a challenging condition for topical pharmaceutical delivery because the hair-bearing scalp may limit direct contact of conventional liquid formulations with the skin surface and eccrine sweat-duct openings. The present study was designed to investigate, formulate and evaluate a non-aerosol antiperspirant foam containing aluminium chloride hexahydrate for scalp-oriented topical application. Traditional aerosol formulations demands the usage of propellents and specialized container. The scientific rationale of the formulation was supported by an exploratory in silico investigation and preliminary drug-excipient compatibility considerations. Aluminium chloride hexahydrate was selected as the antiperspirant active because aluminium-containing species are associated with temporary obstruction of the distal eccrine sweat pathway. The proposed formulation system included Poloxamer 407 as a formulation and rheology variable, Cocamidopropyl Betaine as part of the foam-generating surfactant system, propylene glycol and glycerin as formulation modifiers, phenoxyethanol as a preservative component and purified water as the vehicle. Trial batches were formulated with intentions to compare for physical appearance, pH, viscosity or rheological behaviour, foamability, foam stability, drainage, density, spreadability, application characteristics, content consistency and stability. The study provides a formulation-development framework for a localized foam dosage form intended for a difficult hair-bearing site.

KEYWORDS: Aluminium chloride hexahydrate; Antiperspirant foam; Scalp hyperhidrosis; Topical foam; Poloxamer 407; In silico investigation.

INTRODUCTION

Hyperhidrosis¹ is excessive sweating beyond that required for normal thermoregulation. It may affect localized regions or occur more generally, and common sites include the axillae, palms, soles, face and scalp. Primary focal hyperhidrosis generally occurs without an identifiable systemic cause, whereas secondary hyperhidrosis may be associated with systemic disease, medication or other medical conditions.

Scalp or Cranio facial hyperhidrosis presents a specific pharmaceutical challenge because the scalp is a hair-bearing anatomical site containing the epidermis, dermis, hair follicles, sebaceous glands, blood vessels, nerves and eccrine sweat glands. Excessive sweating of this region may cause persistent wetness, discomfort, difficulty maintaining hairstyles, visible perspiration and social or occupational inconvenience apart from aesthetic appeal.

The hair shaft is not the primary therapeutic target of a scalp antiperspirant. Instead, the formulation should preferentially reach the scalp surface and the openings of eccrine sweat ducts while minimizing unnecessary wetting and coating of the hair. Conventional liquid formulations may preferentially wet the hair, spread beyond the intended site or leave undesirable wetness and facilitates dripping.

Eccrine sweat glands are the principal glands responsible for thermoregulatory sweating. They consist of a secretory portion and a ductal system that transports sweat to the skin surface. Topical treatment for hyperhidrosis can be administered using antiperspirant substances that block the eccrine sweat gland duct or cause secretory cell atrophy, such as 20% aluminum hydroxide. Diversified studies it is safe to use for axillary and palmar regions, but there is scant data regarding its use on the face, probably due to the risk of irritability². Aluminium salts are established topical antiperspirant agents and act locally through a physicochemical process associated with the formation of aluminium-containing material that temporarily obstructs the distal eccrine sweat pathway.

Aluminium chloride hexahydrate was selected as the proposed active pharmaceutical ingredient because of its established topical antiperspirant role. However, its use in the present study is directed toward formulation development, and the formulated product could be considered as an initiative for utilizing the available in-silico methods to innovate ease the non-aerosol formulation avoiding time consumption.

Foam is a topical dosage form in which gas is dispersed within a liquid or semi-solid phase. For a non-aerosol system, the formulation and the mechanical foamer should be considered together because foam properties are influenced by surfactant concentration, liquid composition, viscosity, gas incorporation and dispensing conditions. A foam may offer localized application, reduced apparent liquid burden, controlled distribution and improved cosmetic acceptability for hair-bearing areas.

Literature survey supports the topical use of aluminium chloride hexahydrate and provides a dosage-form precedent for aluminium-salt foam systems. However, direct evidence for an aluminium chloride hexahydrate foam specifically developed and clinically validated for scalp hyperhidrosis remains limited. The present study therefore investigates a scalp-oriented non-aerosol antiperspirant foam through exploratory computational assessment, preliminary compatibility considerations, formulation development and physicochemical evaluation making use of standard laboratory resources.

MATERIALS AND METHODS

The Proposed Formulations Include

- Aluminium Chloride Hexahydrate,
- Poloxamer 407,
- Cocamidopropyl Betaine,
- Propylene Glycol,
- Glycerin,
- Phenoxyethanol and
- Purified Water.

Equipment

The usage of an analytical balance, beakers, measuring cylinders, magnetic stirrer, calibrated pH meter, viscometer, mechanical foaming dispenser, graduated cylinders were employed accordingly.

In silico investigation

Software used –Pharmdex.

The computational method utilized in this study was **Pharmdex**, a clinical-grade system exploring machine-learning algorithms to forecast API-excipient compatibility, expediting pharmaceutical formulation investigations. The Pharmdex software was employed as a supportive exploratory investigation rather than proof of the antiperspirant mechanism. Aluminium chloride hexahydrate is an inorganic hydrated ionic compound, and its accepted antiperspirant action is primarily a localized physicochemical process involving aluminium-containing species, sweat constituents and temporary obstruction of the distal sweat pathway.

Preliminary drug–excipient compatibility assessment

Preliminary compatibility assessment focused on aluminium chloride hexahydrate in combination with propylene glycol, glycerin and phenoxyethanol. Computational observations and physicochemical reasoning were considered preliminary screening information and final assessment was supported by experimental datas, including visual examination, pH monitoring, and stability evaluation.

Drug–Excipient Combination	Primary Role of Excipient	Assessment Status
Aluminium chloride hexahydrate + Propylene glycol	Solvent/Humectant	Provisional; requires experimental confirmation
Aluminium chloride hexahydrate + Glycerin	Humectant	Provisional; requires experimental confirmation
Aluminium chloride hexahydrate + Phenoxyethanol	Preservative component	Provisional; requires experimental confirmation

Formulation design

A series of trial formulations were prepared by keeping the active ingredient and major formulation components at predetermined levels while varying the concentration of Poloxamer 407. The purpose is to investigate the influence of this formulation variable on viscosity, flow, foam behaviour and overall physical characteristics.

Ingredient	Pharmaceutical role	F1 5%	F2 10%
Aluminium chloride hexahydrate	Antiperspirant active	5g	10g
Poloxamer 407	Formulation/rheology variable	5g	5g
Cocamidopropyl Betaine	Surfactant/foam-supporting component	4ml	4ml
Propylene glycol	Solvent/Humectant	5ml	5ml
Glycerin	Humectant	3ml	3ml
Phenoxyethanol	Preservative component	0.8ml	0.8ml
Purified water	Vehicle	77.2ml	72.2ml

Method of preparation

Purified water was measured and the required amount of Poloxamer 407 was dispersed using an appropriate method. The humectant and solvent components were incorporated under controlled stirring. Aluminium chloride hexahydrate was dissolved or dispersed according to the established laboratory procedure. Cocamidopropyl Betaine was incorporated carefully to minimize premature foaming, followed by phenoxyethanol. Purified water was added to the final volume, and the formulation was allowed to deaerate before filling into a suitable mechanical foaming container. The exact mixing time, speed, temperature, order of addition and final pH was reported from the actual laboratory procedure.

Evaluation of the prepared formulations Physical appearance

The final formulation was examined for colour, clarity, homogeneity, phase separation, precipitation and other visible changes.

pH

The pH was measured using a calibrated pH meter and compared with routine pH paper recorded in replicate where appropriate.

Viscosity or rheological behaviour

Viscosity was measured using a Ostwald viscometer at a defined temperature. The spindle or geometry, speed and measurement conditions were documented.

Foamability

A defined quantity of formulation was dispensed through the intended mechanical foamer and foam formation assessed using a consistent procedure.

Foam stability and drainage

An established comparison approach was used to evaluate liquid drainage and foam volume or height at predetermined intervals.

Foam density may be determined by measuring the mass of a known foam volume using a standardized method.

Spreadability and application characteristics

The formulations was assessed for ease of dispensing, localized application, spreading and residue.

Stability studies

Stability evaluation was assessed based on changes in appearance, pH, foam performance and other relevant quality attributes under the actual selected storage conditions and study duration.

Selection of optimized formulation

The refined formulation was chosen based on established quality criteria instead than relying on a singular metric. Physical stability, pH, viscosity, foamability, drainage and application characteristics were all considered together.

RESULTS AND DISCUSSION

The In Silico (Pharmdex) API-Excipient compatibility study provided the necessary suggestions for arrived formulation.

In silico results

The compatibility analysis conducted using InSilico demonstrated findings indicating appropriate excipients that are compatible with the active pharmaceutical ingredient (Aluminium chloride Hexahydrate), as illustrated in Fig (1), Fig (2), and Fig (3).

Drug–excipient compatibility results

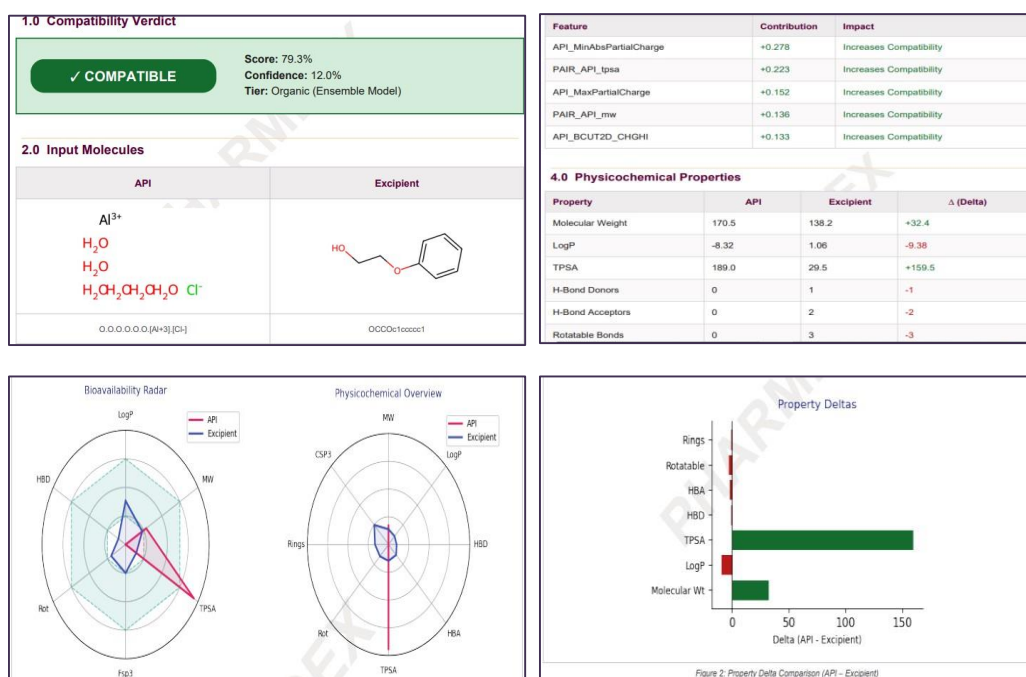
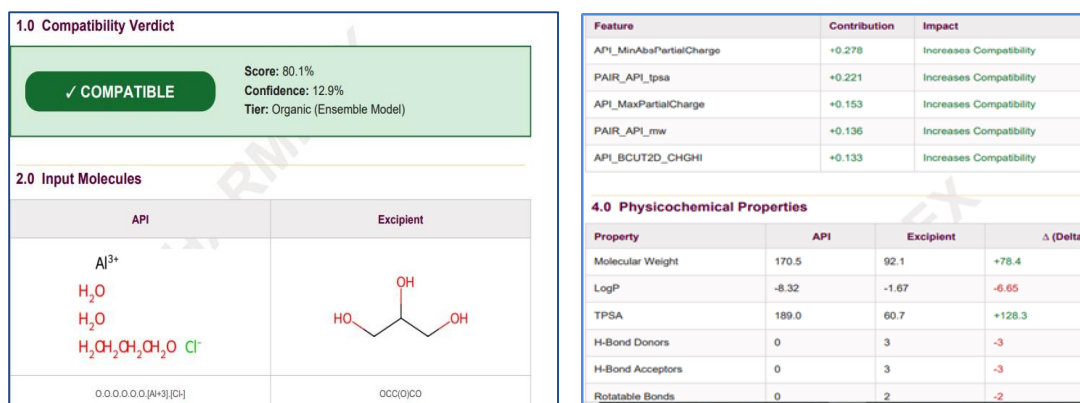
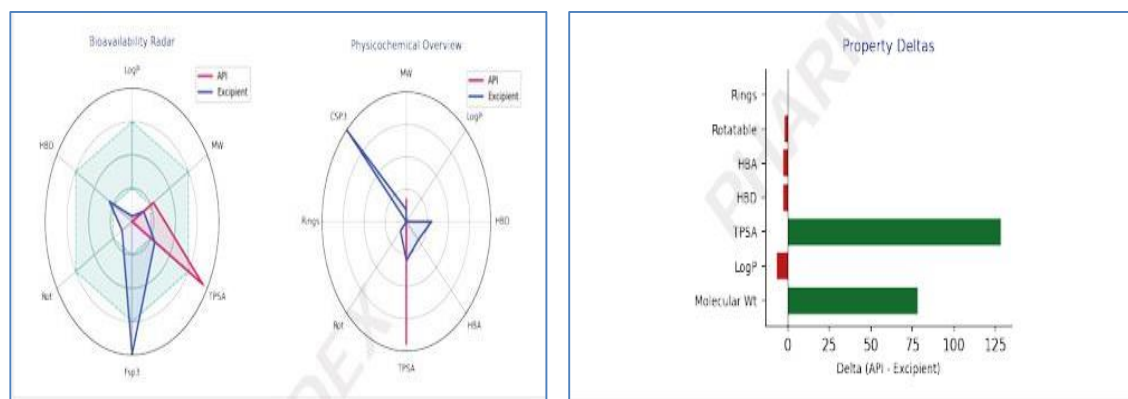


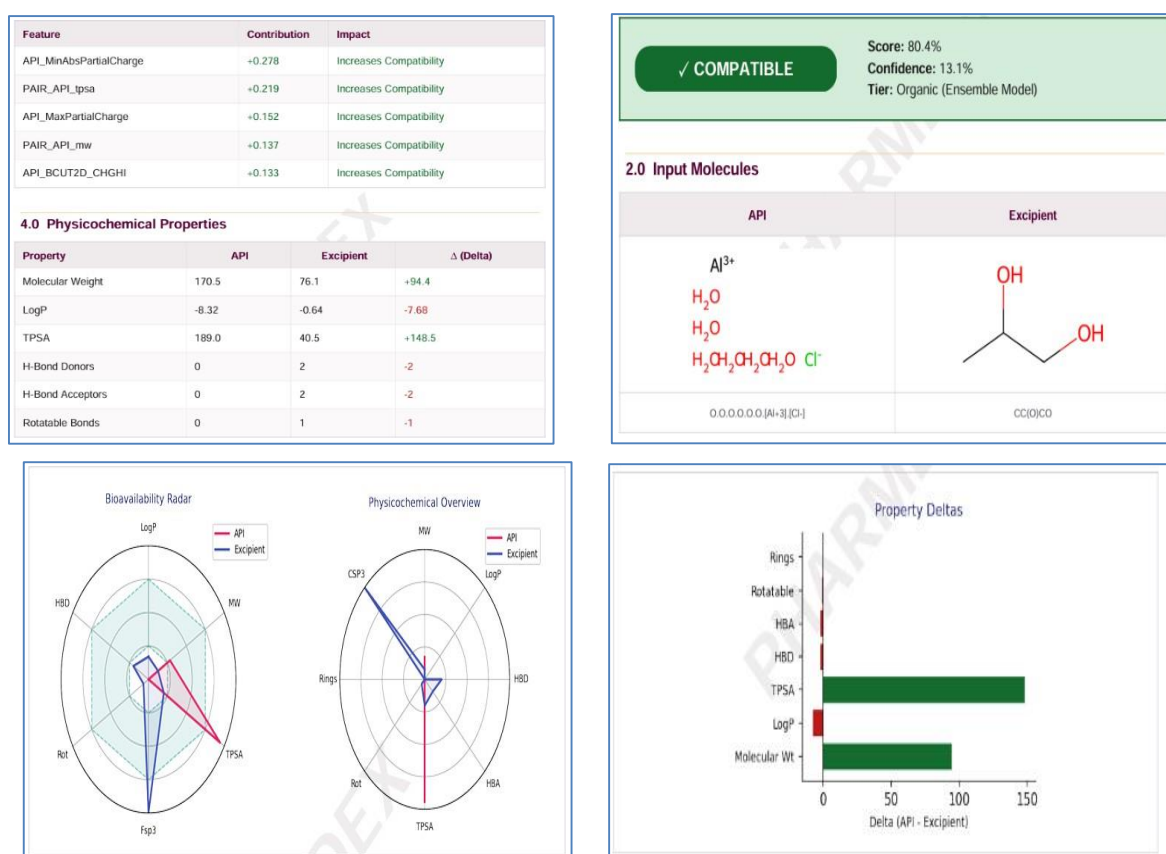
Fig. 1: Compatibility of Aluminium chloride Hexahydrate with phenoxy ethanol.





Bioavailability Radar (left) & Physicochemical Overview (right) Property Delta Comparison (API - Excipient)

Fig. 2: Compatibility of Aluminium chloride Hexahydrate with glycerin.



Bioavailability Radar (left) & Physicochemical Overview (right) Property Delta Comparison (API - Excipient)

Fig. 3: Compatibility of Aluminium chloride Hexahydrate with propylene glycol.

Formulation

The corresponding measured data was used to analyze the final composition, pertinent observations made during formulation development, and any impact of variation in Poloxamer 407.



Evaluation results

pH

The pH was measured using a routine pH paper [Universal Indicator strips]. The pH range is about 5 to 5.5 [Fig (4)]



Fig. 4.

The normal pH of the scalp is slightly acidic, generally ranging from approximately 4.5 to 5.5. Therefore, the pH of the developed antiperspirant foam was evaluated with consideration of Scalp pH compatibility and formulation stability.

Viscosity or rheological behavior

Viscosity was measured using a Ostwald viscometer at a defined temperature. The spindle or geometry, speed and measurement conditions were documented. The viscosity of the formulation was 35.2cST[3.52 cp/sec]

Foamability

The foamability results showed that the formulation exhibited good foam-forming ability.

The formulation produced a foam volume about 6ml/per pump.[fig(5)]

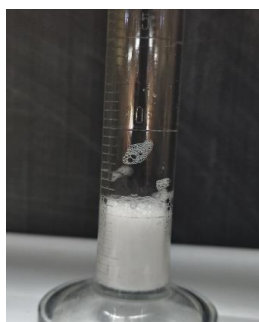


Fig. 5.

Foam stability and drainage

The foam stability of the formulated antiperspirant foam was evaluated by measuring the volume of foam remaining at predetermined time intervals after foam generation. The foam volume was recorded at 0,10,20 and 30 minutes. The percentage of foam stability was calculated by comparing the foam volume at each time interval with the initial foam volume. A formulation showing minimum reduction in foam volume over time was considered to possess better foam stability.

Initial amount = 25ml [Fig(6)] At 10 mins = 22ml [Fig(7)] At 20 mins = 20ml [Fig(8)] At 30 mins = 18ml [Fig(9)]



Fig(6)



Fig(7)



Fig(8)



Fig(9)

Percentage of foam stability

$$\text{Foam Stability (\%)} = \frac{\text{Foam volume at specified time}}{\text{Initial foam volume}} \times 100$$

At 10 mins = 88%

At 20 mins = 80%

At 30 mins = 72%

Spreadability

The spreadability of the formulated antiperspirant foam was evaluated to determine its ability to spread uniformly over the scalp surface with minimum effort. A suitable quantity of the foam was applied onto the selected surface, and its spreading characteristics were observed. The formulation was assessed for ease of application, uniform distribution and smooth spreading. Good spreadability indicates that the foam can be applied evenly over the scalp surface.

Approximately foam spread about 10cm of diameter at minimum effort [Fig(11)]



Fig(10)

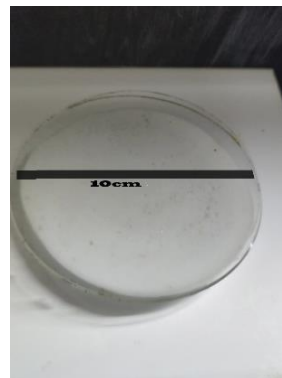


Fig (11)

Foam density

The density of the prepared antiperspirant foam formulations was determined and found to be within an appropriate range. The formulations produced a light and uniform foam with consistent density, indicating satisfactory foam formation and physical stability.

Formula

Density of foam = **Weight of foam / Volume of foam**

Weight of foam = 1g Volume of foam = 10ml Density of foam = 0.1g/ml

DISCUSSION

The In Silico (Pharmdex) API-Excipient compatibility study provided crucial suggestions for formulation creation that reduced the down time needed for unintentional numerous trials.

The first line of treatment for hyperhidrosis is known to be topical treatments containing aluminum chloride.

In tropical nation such as India, hyperhidrosis is a prevalent illness that necessitates prompt intervention. Aluminum salts can clog the distal sweat gland ducts, according to multiple studies. One theory explaining this blockage is because the metal ions precipitate with mucopolysaccharides, causing damage to the duct's lumen's epithelial cells and creating a clog that prevents the production of sweat.

Although it is a common ingredient in antiperspirants, people with hyperhidrosis require a special approach.

Aluminum salts have established their efficacy in treating palm hyperhidrosis using gel formulations, whereas cranial hyperhidrosis necessitates a distinct approach via foam application, which has been effectively explored in this work.

CONCLUSION

The present study provides a scientific and pharmaceutical framework for the development of a non-aerosol based aluminium chloride hexahydrate antiperspirant foam intended for scalp-oriented topical application. The rationale is based on the localized physicochemical action of aluminium salts, the anatomical challenges of the hair-bearing scalp and the potential practical advantages of a foam dosage form.

The project integrates exploratory In silico investigation, preliminary drug–excipient compatibility assessment, formulation development and physicochemical evaluation. The developed foam designed for scalp application aligns with the characteristics of foam and may be regarded as a viable approach for scalp formulation. The In silico tool (Pharmdex) additionally offers essential data on API-excipient compatibility. Although Aluminum hexa hydrate salts are deemed safer than other Aluminum salts for topical application, future research may encompass validated active-content analysis, prolonged stability testing, sophisticated rheological characterization, microbiological preservation evaluation, skin compatibility assessments, and duly sanctioned clinical validation.

ACKNOWLEDGEMENTS

The authors would like to express their sincere gratitude to MOHAMED SATHAK A J COLLEGE OF PHARMACY for providing guidance, facilities and support for the completion of this research work.

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