Docking, Phytochemical Screening, Formulation and Evaluation of *Acmella paniculata* in Zinc Dental Cements

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ABSTRACT:

This study investigates the docking analysis, phytochemical composition, antimicrobial activity, anti-inflammatory potential, and dental cement evaluation of Acmella paniculata extracts. The docking analysis reveals the binding energies of compounds with various receptors such as PLA2R, PBPs, and TRPV1. Phytochemical screening identified the presence of alkaloids, proteins, terpenoids, phenols, flavonoids, glycosides, and phytosterols, with no presence of carbohydrates, saponins, gum, and mucilage. The antimicrobial study indicates the efficacy of zinc oxide and zinc phosphate cements against *Staphylococcus mutans*. Anti-inflammatory tests showed a significant inhibition rate of 91.35%. The evaluation of zinc phosphate and zinc oxide cements revealed distinct differences in their properties such as setting time, bond strength, and acidity. Overall, Acmella paniculata shows promise in dental applications, particularly in antimicrobial and anti-inflammatory contexts.

Keyword: Acmella paniculata, Staphylococcus mutans, Anti-inflammatory, Dental cement, Zinc

1. INTRODUCTION:

Dental cements are materials of multiple uses including restorations, luting and therapeutic. They are generally materials of comparatively low strength, but have extensive use in dentistry. Every cement must be assessed for its biocompatibility, safety, and effectiveness. Many types of dental cements are supplied as a powder and a liquid or as two pastes, so that mixing starts a chemical reaction. The liquids are usually acids and the powders are basic [alkaline] in nature commonly composed of glass or metal oxides. The reaction between the powder and liquid is usually an acid-base reaction. When mixed, cement hardens within a resonable time. Set cements are strong enough to be used as base for pup protection, as a restorative material for temporary or permanent restorations, or as a luting agent.

The primary function of a dental cement is to fill the space between restorative material (definitive or provisional) and tooth preparation (or implant abutment), as well as to enhance the resistance to restoration dislodgement during function. Of utmost importance, the long-term success of a restoration is heavily dependent on the proper selection and manipulation of dental cements. Loss of retention has been found to be one of the most common causes of restoration failure.

Although the terms cement, luting, bond have different meanings, they have frequently been employed as interchangeable terms. Luting refers to a mechanism in which micromechanical locking occurs between the objects to be joining. Bond is a term that implies that chemical or physical interaction occurs to both surfaces that to be attracted. Cement is a generic term for a joining medium provided adhesion and/or micromechanical locking between the two surfaces to be connected. Generally speaking, a proper generic description of material that provides the link between restorative material and the tooth preparation (or implant abutment) should be dental cement.

1.1 CLASSIFICATION OF DENTAL CEMENT:

In the past (and still), the term permanent cement has been frequently employed when describing dental cements for the final restorations. As a matter of fact, a more proper description of cement should be definitive cement when describing a cementation cannot be removed at a later time. Among cements in this category are: zinc phosphate cement, zinc polycarboxylate cement, conventional glass ionomer cement, resin-modified glass ionomer cement and resin cement.



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1. ISO STANDARDS COVERING CEMENTS:

• ISO 9917-1:2007 = Water based cements -part : Powder/liquid acid-based cements.

• ISO9917-2:2010 = Water based cements-part2: light- activated cements.

• ISO3107:2011 = Zinc oxide /eugenol and zinc oxide/non-eugenol cements.

• ISO4049:2009 = Polymer- based fillings, restorative and luting materials.

2. ISO CLASSIFICATION:

• Water based cements = Zinc phosphate, glass ionomer, etc.,

Oil based cements = ZOE and non-eugenol cements.

Resin or polymer-based cements = Resin cements, Componer, etc.,

3. ACCORDING TO SETTING REACTION:

- Acid base reaction cements.
- Polymerizing cements
- Dual cure cements
- Tricure cements

4. CLASSIFICATION OF CEMENTS BASED ON APPLICATION (ISO 9917-1:2007):

- Luting
- Bases or lining
- Restoration

1.2 USES OF CEMENTS:

- Used for final cementation: Zinc phosphate, zinc silicophosphate, EBA cement, zinc polycarboxylate, glass ionomer cement.
- Used for temporary cementation: Zinc oxide eugenol, noneugenol zinc oxide. Zinc phosphate, reinforced zinc oxide eugenol, zinc polycarboxylate, glass ionomer, zinc oxide eugenol, calcium hydroxide
- Used for long term restorations: Glass ionomer, compomer, metal modified GIC.
- Temporary and intermediate restorations: Zinc oxide eugenol, reinforced zinc oxide eugenol, zinc polycarboxylate, glass ionomer.
- **Pulp therapy**: Calcium hydroxide
- Obtundant (pain relief): Zinc oxide eugenol.
- Liners: Calcium hydroxide in suspension
- Root canal sealer: Zinc oxide eugenol, zinc polycarboxylate.



2. PLANT PROFILE:

2.1 ACMELLA PANICULATA:

Acmella paniculata, commonly known as Toothache Plant or Paracress, is a medicinal plant native to tropical regions of South America and parts of Asia. Here's a detailed plant profile:



Fig: 1 Acmella paniculata

2.2 SCIENTIFIC CLASSIFICATION:



Kingdom: Plantae Order: Asterales Family: Asteraceae



Subfamily: Asteroideae
Tribe: Heliantheae
Subtribe: Spilanthinae



Genus: Acmella

Species: A. paniculata

Common Name: Toothache plant

Fig: 2 Scientific Classification

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2.3 DESCRIPTION:

Acmella paniculata is an herbaceous perennial plant that can grow up to 50 cm (20 inches) tall. It has oval, dark green leaves and produces bright yellow, button-like flowers, which are its most distinctive feature. These flowers are often arranged in dense clusters and are surrounded by small, bract-like leaves.

- Leaves: Simple, oval-shaped, and deeply veined.
- Flowers: Small, yellow, with a distinct conical central disk surrounded by a ring of shorter, yellowish petals.
- Stem: Erect and somewhat fleshy, with a characteristic green or purplish color.
- **Root**: Fibrous root system.

2.4 CHEMICAL CONSTITUENTS STRUCTURE:

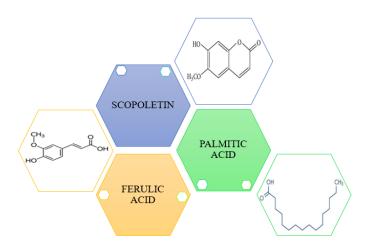


Fig: 3 Chemical Constituents Structure

Fig: 4 Chemical Structure Of Spilanthol

2.5 MEDICINAL USES:

Acmella paniculata has been used traditionally in indigenous medicine for its various health benefits. The plant contains an active compound called spilanthol, which is responsible for its characteristic numbing or tingling sensation when chewed. Some of the medicinal uses include:

- Pain Relief: Especially for toothaches and oral infections. The numbing effect makes it an effective remedy.
- Anti-inflammatory: Often used in folk medicine to treat swelling, pain, and certain inflammatory conditions.
- Antibacterial & Antifungal: Spilanthol and other compounds in the plant have shown potential in combating bacteria and fungi.



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- **Oral Health**: Used as a mouthwash or in toothpaste formulations.
- 3 MATERIALS AND METHODS:
- 3.1 MOLECULAR DOCKING:

3.1.1 PROTEIN PROFILE:

PHOSPHOLIPASE A2: (PLA2): Phospholipase A2 receptor (PLA2R) is a type of receptor that plays a critical role in cellular processes, particularly in the regulation of the immune system and inflammation. PLA2R is a membrane-bound protein that acts as a receptor for the enzyme phospholipase A2 (PLA2). PLA2 is involved in the hydrolysis of phospholipids, releasing arachidonic acid, a precursor to various signaling molecules like prostaglandins and leukotrienes, which are involved in inflammation and immune responses.

PENICILLIN – **BINDING PROTEINS:** (**PBPs**): Penicillin-binding proteins (PBPs) are a group of proteins found in the cell membrane of bacteria, and they play a crucial role in the synthesis of the bacterial cell wall. They are called "penicillin-binding" because they can bind to β-lactam antibiotics like penicillin and other similar drugs, which inhibit their activity.

POTENTIAL VANILLOIDS 1: (TRPV1): TRPV1 (Transient Receptor Potential Vanilloid 1) is a receptor and ion channel found primarily in sensory neurons. It plays a crucial role in the perception of pain, heat, and inflammation, as well as in a variety of physiological and pathological processes. TRPV1 is one of the most studied receptors in the Transient Receptor Potential (TRP) channel family, which is involved in the detection of physical stimuli such as temperature, pressure, and chemicals.

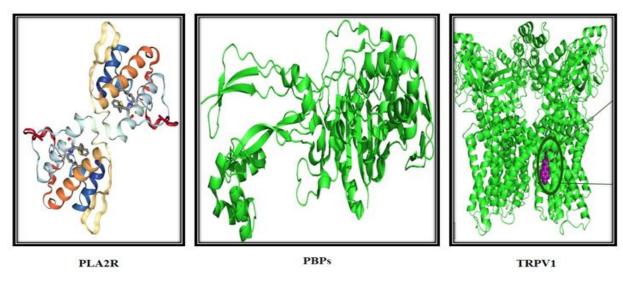


Fig: 5 Protein

3.1.2 PROCEDURE:

Energy minimization of all 3D structure of proteins by Chimera 1.6.1.

CHIMERA 1.6.1 is an extensible programme for visualization and analysis of molecular structure and related data including density maps, supramolecular associations, sequence alignments, docking results, routes and conformational ensembles. One of the best features is the structural editing job. It can minimize the energy of molecules providing them high stability.

- i. Chimera window was opened.
- ii. From the option file, the 3D structure of protein was retrieved.
- iii. The total residues were selected.
- iv. From the tool option, by the structure editing option, minimized structure option was clicked.



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v. The minimized structure was saved in .pdb format.

Preparation of ligand structures:

Marvin sketch is a tool for drawing chemical structures, adding or deleting functional group or atoms, queries and reactions. Assigning stereochemistry, charge, valence, radicals and isotopes to each atom can be done and moreover single, double, triple bonds and aromatic forms can also be created (Table No.1).

- i. Marvin sketch window was opened.
- ii. The ligand .pdb format was retrieved.
- iii. Addition, deletion of functional group changes were made keeping in mind to increase solubility.
- iv. The new molecules were saved in .pdb format

Ligands Used For Docking:

Table: 1 Ligand Profile

S.No	Compound	Structure	IUPAC Name	Mol. formula (Mol. Wt.)
1.	Spilanthol	CH ₃	(2E,6Z,8E)-N-(2-methylpropyl)deca-2,6,8-trienamide.	C ₁₄ H ₂₃ NO (221.34)

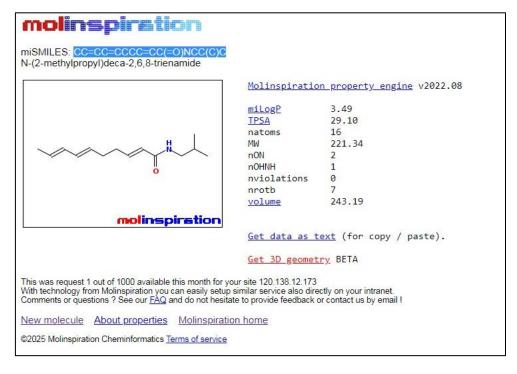


Fig: 6 Ligand

3.2 COLLECTION AND AUTHENTICATION OF PLANT:

The seed of Acmella paniculata were collected from the natural habitat in and local area, Tamilnadu and the plant material were authentified by Dr.KN Sunil kumar., research officer/Sci-II HOD, Department of Pharmacognosy and by Dr. A.Kanagarajan., research officer [siddha], Sci-IV/Incharge, SIDDHA CENTRAL RESEARCH INSTITUTE [central council for research in siddha ministry of AYUSH, Government of India], Arumbakkam, Chennai-601106.

3.3 EXTRACTION:

The seed from Acmella paniculata were shade dried for a week. The dried plant material was powdered, and 50g of Acmella paniculata powder mixed well and subjected to different methods of extraction. 99% of ethanol were macerated for 72 hours.



Fig: 7 Maceration

3.4 PHYTOCHEMICAL TEST:

The Ethanolic extracts of Acmella paniculata were subjected to the following preliminary phytochemical analysis.

- Test for Carbohydrates (Molisch Test)
- Test for Alkaloids (Mayer's Test, Dragendroff's reagents)
- Test for Steroids and Sterols (Salkowski test)
- Test for Glycosides (Legal's test)
- Test for Saponins (Foam test)
- Test for Flavonoids
- Test for Tri-terpenoids
- Test for Terpenoids (Copper acetate test)
- Tests for Tannins
- Tests for Phenolic Compounds (Phenol litmus test)
- Test for Gums and Mucilage (Ruthenium red test)



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- Test for Proteins and Amino acids (Biuret test, Ninhydrin test, Millon's test)
- Test for Fixed Oils and Fatty acids (Saponification test, Litmus test)

3.5 METHODOLOGY:

3.5.1 List Of Ingredients Used In The Formulation Of Zinc Phosphate Dental Cement:

Table: 2 Zinc Phosphate Dental Cement

Zinc Phosphate Dental Cement							
Solid Ingredients			Liquid	Liquid Ingredients			
S.No	Ingredients	Weight %	S.No Ingredients		Weight %		
1	Zinc phosphate	90.2	1	Extract	2		
2	Magnesium oxide	8.2	2	Phosporic acid	38.2		
3	Bismuth trioxide	0.2	3	Water	34		
4 Silica 1.4		4	Aluminium phosphate	18.7			
			5	Zinc	7.1		

3.5.2 List Of Ingredients Used In The Formulation Of Zinc Oxide Dental Cement:

Table: 3 Zinc Oxide Dental Cement

Zinc O	Zinc Oxide Dental Cement					
Solid Ingredients			Liquid Ingredients			
S.No	Ingredients	Weight %	S.No	Ingredients	Weight %	
1	Zinc oxide	40-60	1	Extract	2	
2	Zinc sulphate -1-hydrate	1-20	2	Phosporic acid	38.2	
3	Calcium sulphate hemihydrate	15-35	3	Water	34	
4	Ethylene bis oxyethylene	15-35	4	Aluminium phosphate	18.7	
	diacetate					
5	Barium sulphate	0-20				
6	Poly vinyl acetate	Q.S	5	Zinc	7.1	
7	Diatomaceous earth	Q.S				

3.5.3 Procedure:

Preparation Of Phosporic Acid: The typical concentration of phosporic acid used in the preparation of dental cement is 50-60%. At this concentration the pH of the phosporic acid.

Procedure: Measurement of concentrated phosphoric acid: Measure the desired amount of concentrated phosphoric acid (85% or 90%) using a pipette or a measuring cylinder. Measurement of distilled water: Measure the desired amount of distilled water using a pipette or a measuring cylinder. Mix the acid and water: Slowly add the measured distilled water to the measured concentrated phosphoric acid while stirring with a glass rod or a spatula. Stir and cool: Continue stirring the mixture until it is fully dissolved and cooled to room temperature. Verify the concentration: Verify the concentration of the prepared phosphoric acid solution using a pH meter or a titration method.

Preparation Of Zinc Solution: Zinc salt such as zinc chloride is dissolved in water to prepare a solution. The pH of this solution is 4-6.

Preparation Of Aluminium Phosphate Solution: The solution of aluminium phosphate is prepared by dissolving the aluminium phosphate powder in water. The pH of this solution is 2-4.

3.5.4 Preparation Of Zinc Phosphate And Zinc Oxide Dental Cement:



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Step 1: Measurement of Powders: Measure out the correct amount of zinc phosphate and other powders by using a measuring cup or spoon. The typical ratio is 1 part powder to 0.5-1 part liquid.

Step 2: Measurement of Liquids: Measure out the correct amount of phosphoric acid and other liquids by using a measuring cup or spoon.

Step 3: Mixing of Powder and Liquid: Place the measured powders on the mixing slab or glass plate. Gradually add the measured liquids one by one to the powder while mixing with a spatula. Mix in a circular motion, starting from the center and working your way outwards.

Step 4: Mix to the Correct Consistency: Continue mixing until the cement reaches the correct consistency. The cement should be smooth creamy, free of lumps. The mixing time is around 30-60seconds.

Step 5: Check the cement: Check the cement for the correct consistency by lifting some of the cement with the spatula. If it forms a smooth rounded peak it is ready to use. If it is too runny add small quantity of powder and mix again.

Step. 6: Use cement: Use the prepared cement immediately as it will start to set within a few minutes.

Step. 7: Application of dental cement on teeth: Wash the teeth surface with water then place a thin layer of cement.



Fig: 8 Preparation Of Zinc Phosphate & Zinc Oxide Dental Cement

3.6 EVALUATION PARAMETERS:

3.6.1 pH: The samples were designed using stainless steel molds with a diameter of 15 mm and a thickness of 1.5 mm (n ½ 30). Each specimen was then immersed in 15 mL of deionized water and stored in an incubator at 37 _C for 24 hours. The pH of the deionized water was measured using a pH meter.

3.6.2 Antimicrobial assay: (Antibacterial): Antimicrobial analysis was followed using standard agar well diffusion method to study the antimicrobial activity of compounds (Perez *et al.*, 1990; Erdemoglu *et al.*, 2003; Bagamboula *et al.*, 2004). Each bacterial isolate was suspended in Brain Heart Infusion (BHI) broth and diluted to approximately 10⁵ colony forming unit (CFU) per mL. They were flood-inoculated onto the surface of Media (Mueller Hinton Agar for Bacteria) and then dried. Five-millimeter diameter wells were cut from the agar using a sterile cork-borer and 30 μL (50μg compound in 500 μL DMSO) of the sample solution were poured into the wells. The plates were incubated for 18 h at 37°C for bacteria. Antimicrobial activity was evaluated by measuring the diameter of the zone of inhibition in mm against the test microorganisms and the solvent. DMSO was used as solvent control. Ciprofloxacin was used as reference antibacterial agent. The tests were carried out triplicates.

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3.6.3 Anti-Inflammatory: Effect on Protein Denaturation: Protein denaturation assay was done according to the method described by Gambhire et al. with some modifications as described in Gunathilake et al. The reaction mixture (5 mL) consisted of 0.2 mL of 1% bovine albumin, 4.78 mL of phosphate buffered saline (PBS, pH 6.4), and 0.02 mL of extract, and the mixture was mixed, and was incubated in a water bath (37 _C) for 15 min, and then the reaction mixture was heated at 70 _C for 5 min. After cooling, the turbidity was measured at 660 nm using a UV/VIS spectrometer (Optima, SP-3000, Tokyo, Japan). Phosphate buffer solution was used as the control. The percentage inhibition of protein denaturation was calculated by using the following formula:

% Inhibition of denaturation = $100 \times (1 - A2/A1)$,

Where,

A1 = absorption of the control sample, and

A2 = absorption of the test sample.

3.6.4 Setting Time: Time taken for the cement to set and become rigid. Both initial and final setting times are critical for handling and placement in dental procedures.

3.6.5 Solubility: The amount of cement that dissolves when exposed to oral fluids. Lower solubility indicates better long-term stability.

3.6.6 Flow: Measures how easily the cement spreads. Good flow ensures proper adaptation to the tooth and restoration.

3.6.7 Adhesion to Tooth Structure: Bond Strength: The strength of the bond between the cement and tooth structure is essential for the long-term success of restorations. While zinc phosphate has traditionally been used for mechanical retention, modern zinc oxide cements (with Spilanthol or other additives) may offer better adhesion when used with bonding agents.

3.6.8 Chemical Properties:

Acidity: Zinc phosphate cements are acidic when mixed, which can cause irritation to the dental pulp if not properly handled. Zinc oxide Spilanthol cements are generally less acidic and more neutral, which can make them more compatible with pulp tissue.

Reaction to Water: Zinc phosphate cements are sensitive to moisture during setting. Zinc oxide Spilanthol cements, however, show better resistance to moisture exposure and environmental factors.

3.6.9 Aesthetic Considerations:

Color Stability: Zinc oxide Spilanthol cements are often more translucent, while zinc phosphate can be less aesthetically pleasing due to its opacity. Color stability over time is important, especially in anterior restorations.

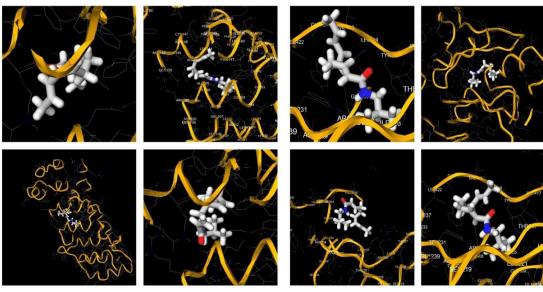
4 RESULTS AND DISCUSSION:

4.1 MOLECULAR DOCKING ANALYSIS:

Table: 4 Docking Analysis

S.NO	COMPOUND CODE	SPILANTHOL			
		Binding Energy	Mode	RMSD lower	RMSD upper
		(kJ mol ⁻¹)		bound	bound
1.	PLA2R	-6.3	0	0.0	0.0
2.	PBPs	-6.2	1	4.204	8.077
3.	TRPV1	-6.0	2	9.087	11.22

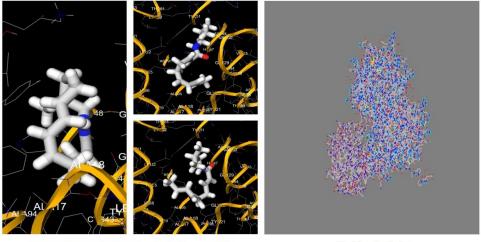
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Compound Spilanthol Docked At The Receptor Of Transient

Receptor Potential Vanilloid 1 (TRPV1)

Compound Spilanthol Docked At The Receptor Of Penicillin-Binding Proteins (PBPs)



Compound Spilanthol Docked At The Receptor Of Penicillin-Binding Proteins (PBPs)

Docking Analysis

Fig: 9 Docking Analysis

4.2 APPEARANCE AND PERCENTAGE YIELD OF ACMELLA PANICULATA:

Table: 5 Appearance and Percentage Yield

Drug	Acmella paniculata
Solvent	Ethanol 99%
Color	Light green
Consistency	Liquid
Percentage yield	60% w/w

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4.3 PRELIMINARY PHYTOCHEMICAL SCREENING:

The *Acmella paniculata* extract were macerated. The residue were collected and the chemical test was conducted separately. Various phytoconstituents were demonstrated and result were obtained. The results of this phytochemical analysis is listed below.

Table: 6 Preliminary Phytochemical Screening

S.NO.	CONSTITUENTS	ETHANOLIC EXTRACT
1.	Alkaloids	+
2.	Carbohydrates	-
3.	Protein and amino acids	+
4.	Terpenoids	+
5.	Phenols	+
6.	Tannins	+
7.	Flavonoids	+
8.	Glycoside	+
9.	Saponins	-
10.	Gum and mucilage	-
11.	Phytosterols	+

(+) indicate the presence. (-) indicate the absence.

4.4 UV ANALYSIS:

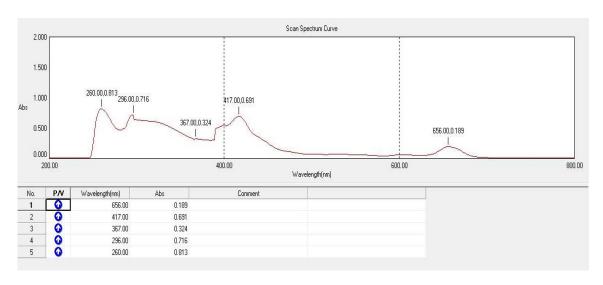


Fig: 10 UV Spectrum Of Extract



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4.5 FT-IR:

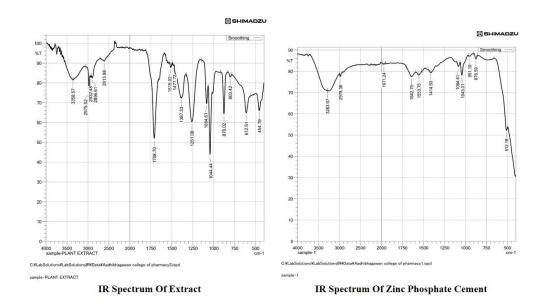


Fig: 11 IR Spectrum Of Extract & Cements

IR Spectrum Of Zinc Oxide Cement

rig. 11 ik Spectrum Of Extract & Cem

Table: 7 Dental Cement Evaluation

4.6 DENTAL CEMENT EVALUATION:

S.NO	PROPERTY	ZINC PHOSPHATE CEMENT	ZINC OXIDE CEMENT
1	Setting Time (Initial)	$2-3 \min$	1 – 2 min
2	Setting Time (Final)	5 – 9 min	4 – 7 min
3	Solubility	0.06 – 0.1 %	0.04-0.08~%
4	Flow	15 – 30 mm	20 – 35 mm
5	Bond Strength	4 – 6 MPa	2 – 4 MPa
6	Acidity	pH 3.5	pH 6.5
7	Reaction Of Water	Slightly expansion	Slightly expansion
8	Color Stability	Good	Excellent

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Fig: 12 Dental Cement Evaluation

4.7 MICROSCOPY ANALYSIS:



Fig: 13 Dental Cement Microscopy Analysis

4.8 ANTIMICROBIAL STUDIES:

Table: 8 Anti-microbial Study

S.No.	Microorganisms	Control	ZNO	ZnPO4	E	Ciprofloxacin
		Zone of inhibition	n in mm			
1.	Staphylococcus mutant	-	02	08	15	28



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Fig: 14 Anti-microbial Study

4.9 ANTI INFLAMMATORY ACTIVITY:

Table: 9 Anti Inflammatory Activity

S.NO	NAME OF THE CONTENT	OD VALUE AT 660 nm	% OF INHIBITION
1.	BLANK	0.00	
2.	CONTROL	0.33	91.35%
3.	TEST	0.43	

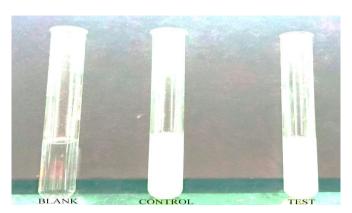


Fig: 15 Anti Inflammatory Activity

DISCUSSION:

The docking analysis data provide valuable insights into the potential interactions of *Acmella paniculata* compounds with specific receptors, with binding energies ranging from -6.3 to -6.0 kJ/mol, indicating moderate binding strength. The preliminary phytochemical screening confirmed the presence of bioactive compounds such as alkaloids, phenols, and flavonoids, which are known to exhibit antimicrobial and anti-inflammatory properties. The UV and FT-IR analyses further characterized the chemical constituents, confirming the presence of functional groups that may contribute to the therapeutic activities of the plant. The antimicrobial study demonstrated that zinc oxide and zinc phosphate dental cements showed varying inhibition zones against *Staphylococcus mutans*, suggesting their effectiveness as dental materials. Additionally, the anti-inflammatory activity with a 91.35% inhibition supports the potential use of the extract in inflammation-related conditions.

In the dental cement evaluation, zinc phosphate cement showed better acidity and bond strength, while zinc oxide cement exhibited superior color stability. The setting time for both cements was within the acceptable range, making them suitable for dental applications. The results also highlight the overall effectiveness of *Acmella paniculata* as a promising plant with multiple pharmacological properties beneficial for dental health.

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5. CONCLUSION:

This research explores the therapeutic potentials of *Acmella paniculata*, focusing on its chemical composition, antimicrobial activity, anti-inflammatory effects, and its suitability in dental applications. The compound docking analysis showed moderate binding energies with various receptors, while the phytochemical screening revealed essential bioactive compounds. The antimicrobial study suggested the effectiveness of zinc-based dental cements, and the anti-inflammatory test confirmed significant inhibition. Furthermore, the dental cement evaluation illustrated the differences in properties between zinc phosphate and zinc oxide cements, offering insights for their potential use in dentistry. The findings demonstrate that *Acmella paniculata* holds significant potential for use in dental and medical applications due to its diverse bioactive constituents and favorable pharmacological properties. The compound's antimicrobial and anti-inflammatory effects, along with its potential to enhance dental cement formulations, position it as a valuable plant for future research and application in therapeutic and dental fields.

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