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Conference Special Issue - 62 August - 2025

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Two-Day National Seminar
On
RECENT TRENDS AND EMERGING TECHNOLOGIES IN CHEMICAL AND ALLIED SCIENCES RESEARCH
(RTECASR-2025)

22nd - 23rd August, 2025

Conference Special Issue / Proceedings - 62

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Conference, Seminar, Symposium organization in association/collaboration with different Institutions.

Conference, Seminar, Symposium Publication with ISSN Journals and ISBN Books (Print / Online).

About the organizing Institution

Pingle Government College for Women, Hanumakonda, Warangal (Affiliated to Kakatiya University) is an Autonomous College recognizedby UGC, Government of India and re-accredited by NAAC with 'A' grade was established in 1965 to cater the educational needs of Women. College celebrated its Silver Jubilee in the year 1991 and Golden Jubilee inthe year 2015.It has since grown to more than 1800 students by the efforts of benefactors, legislators, authorities, and teaching fraternity, NAAC re-accredited the college with an 'A' as a significant institution of higher education in the district that has existed for six wonderful decades... The college is blessed with several distinctive qualities. It has three NSS units and one NCC unit that instill national pride and social consciousness in its volunteers and cadets. More than fifty highly trained and effective faculty members serve the requirements of the local student population. It has strong alumnae whose presence can be felt all overthe world in various fields like Industry, Medical profession, Politics, Sciences, Academics etc.

About the Department of Chemistry

The Department of chemistry was established since the very inception of the college in 1965 for the Pre-University course with MPC and Bi. PC groups and later modified as intermediate course. Undergraduate course B. Sc (B.Z.C.) was started in the academic year 1966-67 and B.Sc. (MPC) in 1994. B.Sc. (M.Z.C) with Microbiology, Zoology and Chemistry as main electives was started in the academic year 2002-03, B.Sc. Biotechnology with Biotechnology, Botany and chemistry was started in the academic year2005-2006. Presently the department is offering undergraduate chemistry combination courses namely B. Sc (BZC, MBZC, MBCAN, BCAN, BTBC, BTZC, MPC, MCCs) in English medium. The college achieved autonomy status in 2021-22. So, the department of chemistry designing our own syllabus according to the needs of students and employability.

The department provides excellent learning in chemistry through its dedicated faculty members by means of new teaching and learning methods supported by well equipped laboratories and departmental library. It is a matter of pride that students who have studied here have pursued higher studies and placed in a high position in the society.

About the Seminar:

The seminar on "Recent Trends and Emerging Technologies in Chemical and Allied Sciences Research" (RTECASR-2025) aims to bring together researchers, academicians, industry experts and students to explore the latest advancements in chemical sciences and their allied fields. Key areas include green chemistry, nanotechnology, AI in chemical research, advanced materials, pharmaceuticals, and environmental science. Through keynote lectures, presentations, and technical sessions, the seminar encourages knowledge sharing, interdisciplinary collaboration, and innovation. It provides a valuable platform for networking, discussing sustainable solutions, and identifying future research directions. This event is ideal for those seeking to stay updated with cutting-edge developments and contribute to impactful scientific progress.

Objectives of the Seminar:

- To explore the integration of emerging technologies like AI, nanotechnology, and green chemistry.
- To encourage interdisciplinary collaboration.
- To discuss industrial applications and sustainable practices in chemical research
- To accelerate the research pace of undergraduate, postgraduate, and faculty researchers by facilitating contact with the most notable researchers in the field of chemistry and Allied sciences.
- To bring together renowned academicians, scientists, researchers, students, and industrialists to exchange and share their expertise and research findings on all aspects of current trends and challenges in Chemistry & Allied Sciences through lectures and presentations.
- To look into future developments in the subject of sustainable development, including trends, challenges, and potential solutions.

Themes of the Seminar:

1 Advancements in green chemistry and sustainability
2. Advanced materials and nano technology
3. Advancements in computational chemistry
4. Pharmaceutical and Medicinal Chemistry
5. Natural products
6. Spectroscopic techniques and applications
7. Environmental challenges and remedies
8. Industrial chemistry and solid waste management
9. Renewable energy resources-Emerging technologies
10. Concepts of modern catalysis
11. Water treatment and purification
12. Advance Chromatography techniques and applications

Sub themes:

1. Eco-friendly synthesis methods
2. Artificial Intelligence and Machine learning in materials design and drug discovery
3. New drug molecules and drug design
4. Computational Biology and Bio informatics
5. Bio chemical and bio technological approaches
6. NMR, UV, IR Spectroscopy and Mass Spectrometry applications
7. Traditional Medicine and Herbal remedies
8. Phto chemistry and pharmacology of natural products
9. Advanced Polymers and composites
10. Pollution control technologies

PRINCIPAL'S MESSAGE

I am delighted to present the Seminar Proceedings of the TGCHE Sponsored Two-day National Seminar on **"Recent Trends and Emerging Technologies in Chemical and Allied Sciences Research (RTECASR-2025)"**, organized by the Department of Chemistry, Pingle Government Degree College for women (Autonomous), Hanumakonda, on 22nd & 23rd August 2025.

It gives me immense pleasure to state that the Department has successfully conducted the National Seminar with great enthusiasm and academic commitment. I congratulate the Convener, Co-convener, Organizing Committee, and faculty members for successfully organizing this significant academic event.

The theme of the seminar is highly relevant in the present scientific scenario, as research in Chemical and Allied Sciences plays a crucial role in addressing contemporary societal challenges and technological advancements. The Department of Chemistry has always been one of the academically vibrant and research-oriented departments of our institution. With its experienced and committed faculty, the department consistently strives to promote quality education and meaningful research activities. The successful conduct of this seminar stands as testimony to their perseverance and academic excellence.

The seminar provided a valuable platform for academicians, research scholars, scientists, and students to exchange innovative ideas, share research findings, and explore emerging technologies in the field of chemical sciences. Such academic interactions undoubtedly contribute to knowledge enhancement, collaborative research, and scientific progress.

I am confident that this volume of Seminar Proceedings will serve as a valuable reference for researchers and academicians and will further strengthen the research culture of our institution.

I once again congratulate the entire team of the Department of Chemistry for their commendable efforts.

(PROF.B.CHANDRA MOULI))
PRINCIPAL
PINGLE GOVERNMENT COLLEGEFOR WOMEN(A) ,HNK

Editor's Message

It gives me immense pleasure to present the proceedings of the National Seminar on **"Recent Trends and Emerging Technologies in Chemical and Allied Sciences Research (RTECASR-2025)"**, conducted on **22nd & 23rd August 2025**. The seminar was organized with the objective of providing a common academic platform for researchers, academicians, scientists, and students to exchange knowledge, share innovative ideas, and discuss recent developments in the field of Chemical and Allied Sciences.

The rapid advancement in science and technology has created new opportunities and challenges in chemical and interdisciplinary research. In this context, the seminar aimed to highlight emerging technologies, modern research methodologies, sustainable approaches, and innovative applications that contribute to scientific progress and societal development.

The publication of these seminar proceedings with full-length research papers is an important outcome of the seminar. Proceedings serve as a valuable academic record that preserves the intellectual contributions presented during the seminar and makes them accessible to a wider scientific community. I sincerely believe that this volume will be useful to researchers, faculty members, students, and professionals working in related fields.

I express my sincere gratitude to the **Telangana State Council of Higher Education (TGCHE)** for sponsoring this National Seminar and for their continuous encouragement in promoting academic and research activities in higher education institutions. I also extend my heartfelt thanks to the **Commissioner of Collegiate Education** for the constant support and guidance in organizing this academic event successfully. I place on record my deep sense of gratitude to the **Principal of the College**, for the valuable guidance, encouragement, and academic support in bringing out this publication in a successful manner.

Dr.M.Aruna
Convener& Organizing Secretary
Head, Department of Chemistry
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Comparision In Thermal Degradation Properties of Some Aromatic Polymers

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ABSTRACT: *Development of heat resistant polymers for new applications is always important. The application of such polymers depends on their thermal properties and thermal degradation profiles. The DHPPE is an impotent aromatic polymer. The polymer is copolymerized by reacting with Formaldehyde (FM) to get ion exchange resin which is used water purification applications. The copolymer is further modified by reacting with para methoxy aceto phenome (PMAP). Effect of these chemical modification on thermal properties and thermal degradation profiles has been investigated by differential thermal analysis (DTA) and thermo gravimetric analysis (TGA). The TGA data suggest that the Ti (initial decomposition temperature) T 20 (temperature of 20 %degradation), T 50 (temperature of 50 % degradation) T 60 (temperature of 60 % degradation) anfTf (final decomposition temperature are more for DHPPE – FM- PMAP than DHPPE – FM. Reasons for these variations are explained. THE DTA a data suggests that the glass transition temperature of DHPPE – FM – PMAP is is higher than DHPPE – FM. Correspondingly the activation of energy of DHPPE – FM – PMAP is higher than DHPPE _FM. The variations are explained.*

1. INTRODUCTION

Aromatic polymers and copolymers attracted the attention not only because of their heat resistant properties but also because of their important applications like ion exchange resins and radiation dosimeter applications (1-3). Synthesis and characterization of some of such aromatic polymer DHPPE and its copolymers has been reported by Sabitha (4) recently.

2.EXPERIMENTAL

DHPPE, Formaldehyde and para methoxy acetophenone are commercially procured and used as its to synthesize the copolymers. The obtained copolymers are in powder form and characterized by FTIR and NMR techniques. Thermal properties of the copolymer are recorded on Metler ThermaL Instruments with a heating rate of 10 C / minute for powder samples.

3.RESULTS & DISCUSSION

TGA curves of DHPPE – FM and DHPPE – FM – PMAP are as shown in Fig 1 and Fig 2 respectively. Using them weight loss at different temperatures are noted as given in Table 1

Fig 1. TGA and DTA of DHPPE-FM-PMAP

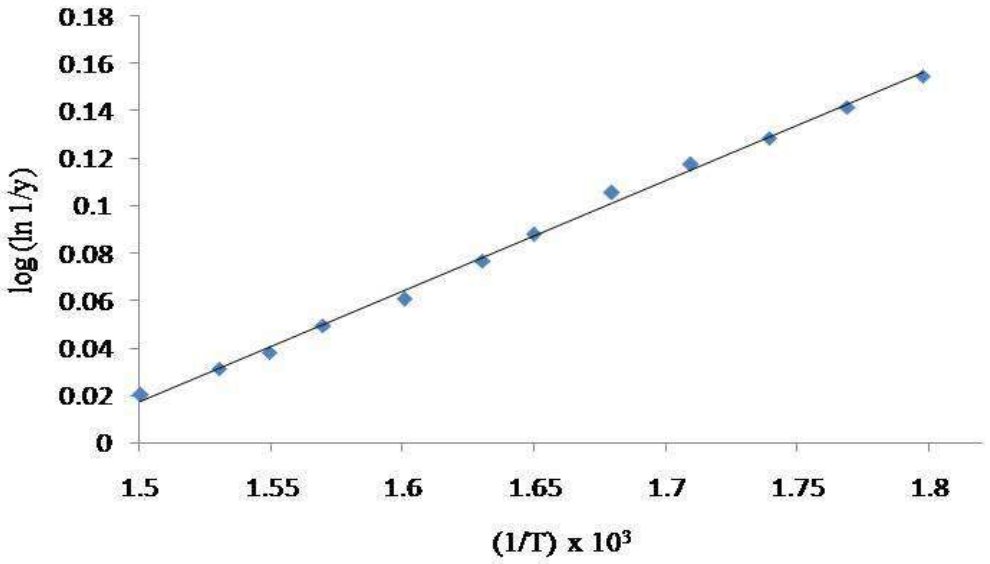


Fig 2.a. Plot of 1/ T vs log (ln 1/y) DHPPE-FM

Table 1: Comparison in thermal degradation temperatures using TG

Weight loss	DHPPE- FM	DHPPE –FM - PMAP
Ti	260	320
T20	350	340
T 50	545 – 550	550 – 555
T 60	600	800
T 90	----	1000

Similarly thermal parameters evaluated from DTA spectra are given in Table 2 and comparison of thermal properties are made plotting histograms by measuring areas of intensities using double integration methods, as shown in Fig 8 to Fig 10.

Table 2 Comparison in Thermal properties of copolymers using DTA analysis

S.No.	Peak	Copolymer	
		DHPPE-FM	DHPPE-FM-PMAP
1	P1	90 (100)	90 (50)
2	P2	310 (400)	250 (150)
3	P3	530 (20)	400 (100)
4	P4	810 (30)	530 (10)

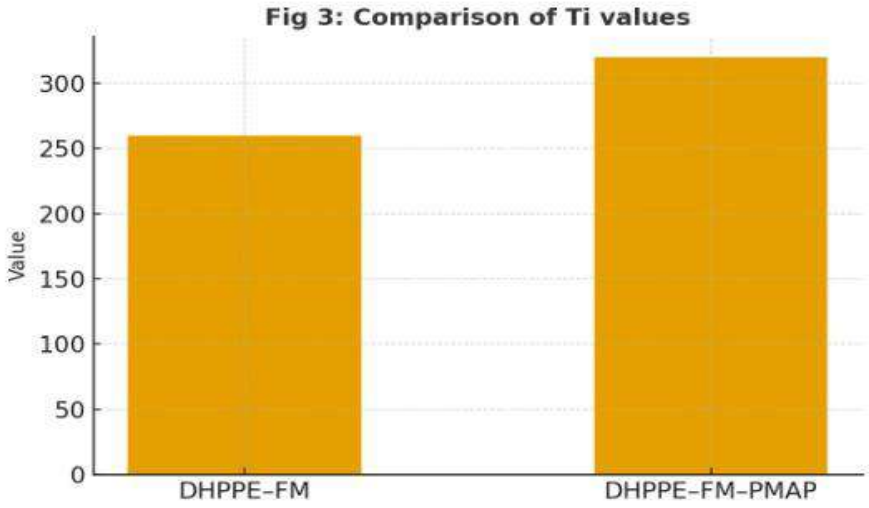


Fig 3: Comparison of Ti values
Value
300
250
200
150
100
50
0
DHPPE-FM
DHPPE-FM-PMAP

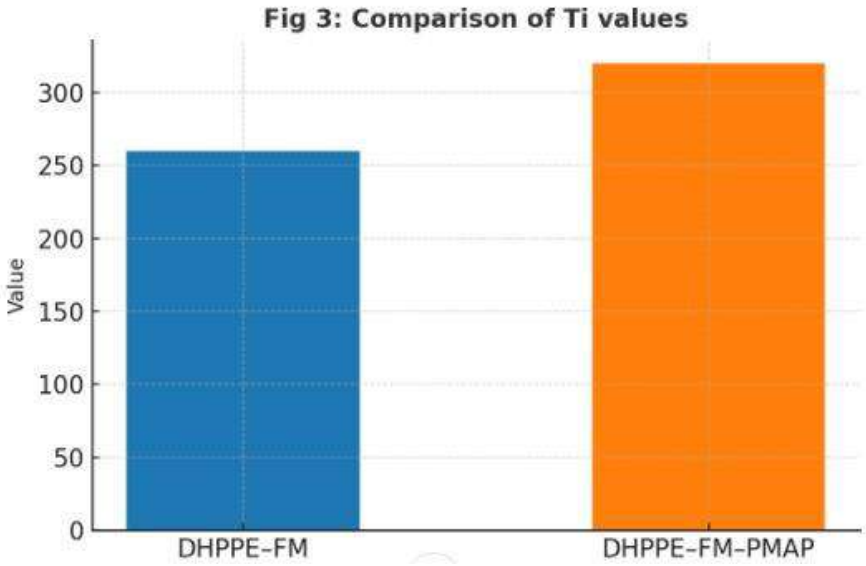


Fig 3: Comparison of Ti values
Value
300
250
200
150
100
50
0
DHPPE-FM
DHPPE-FM-PMAP

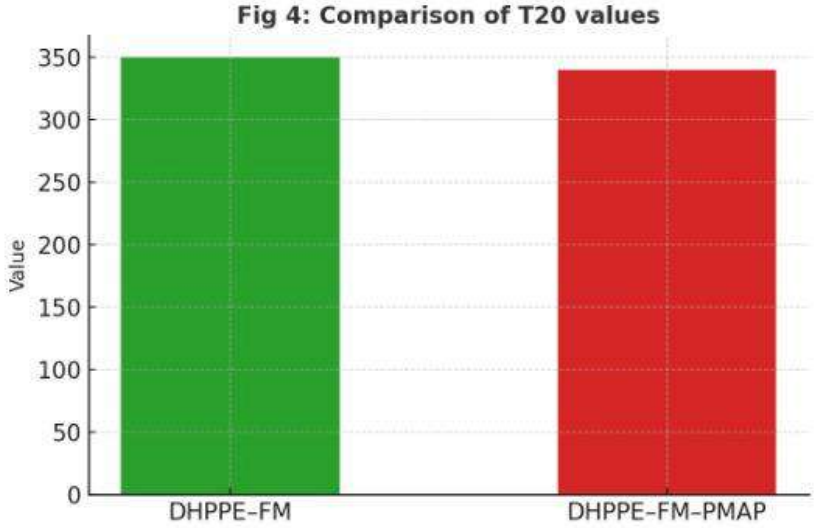


Fig 4: Comparison of T20 values
Value
350
300
250
200
150
100
50
0
DHPPE-FM
DHPPE-FM-PMAP

Fig 5: Comparison of T50 values

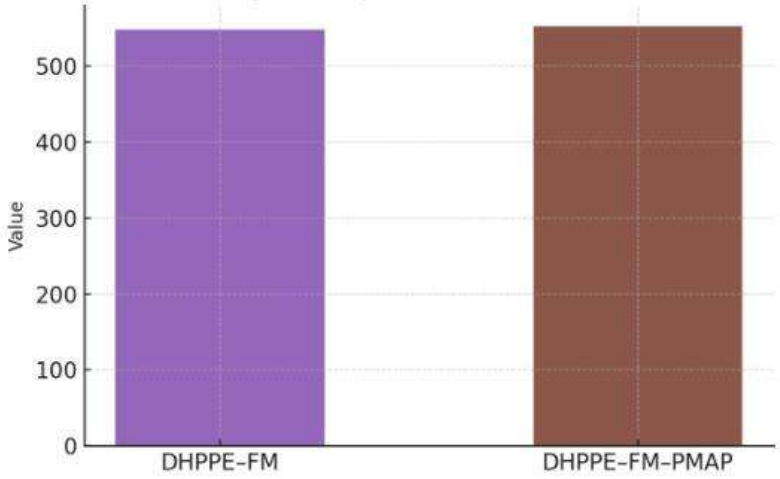


Fig 6: Comparison of T60 values

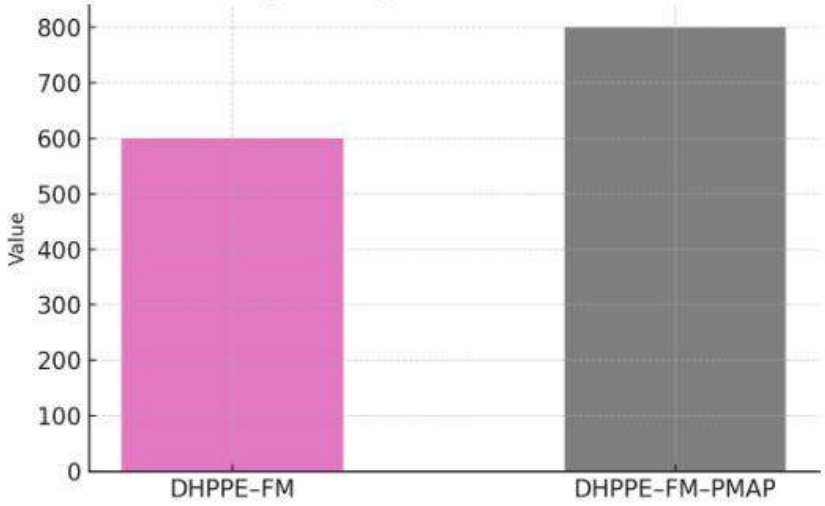


Fig 7: Comparison of Tfinal values

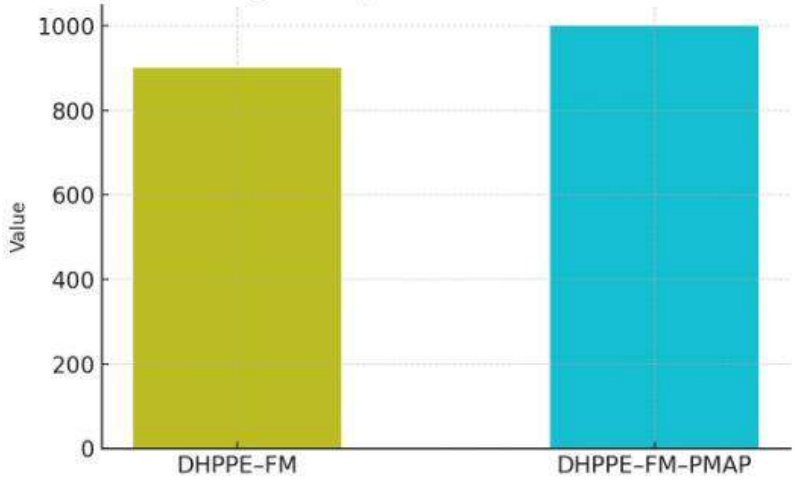


Fig 8: Comparison of Glass transition temperature (Tg)

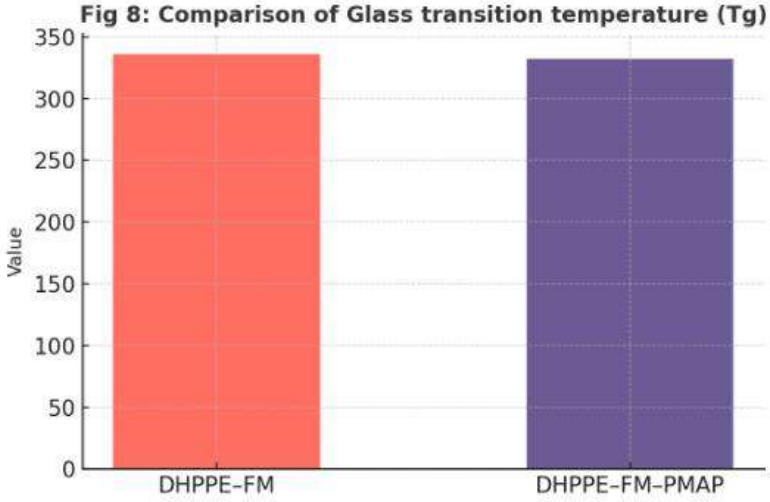


Fig 9: Comparison of Activation energy (Ea)

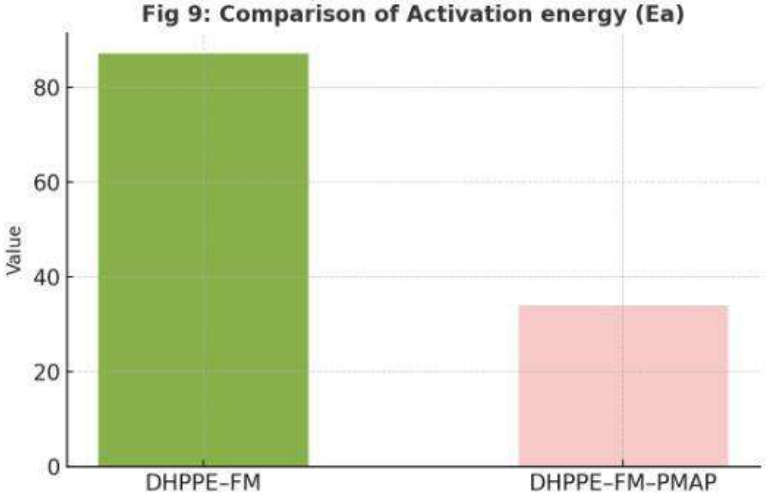
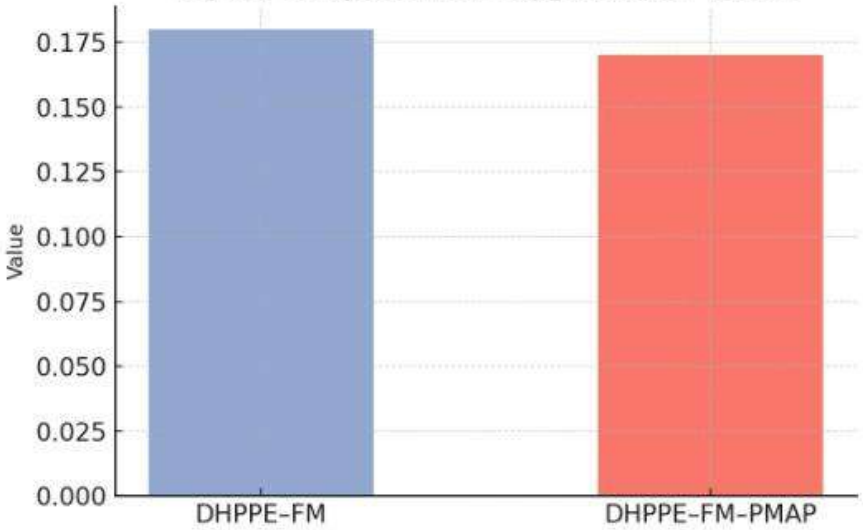


Fig 10: Comparison of Oxygen intake values



FACTORS INFLUENCING GLASS TRANSITION TEMPERATURE.

Glass transition temperature (Tg) is an important property of a polymer for its industrial applications. The following parameters will influence the Tg value (5,6). They are

1. Chain length
2. chain stiffness
3. presence of side and polar groups.
4. presence of plasticizers / plasticizing effects
5. copolymerization

FREE VOLUME

In the present studies the DHPPE consisting of aromatic groups is considered to be mostly amorphous and is expected to have high Tg value. Due to copolymerization and effects as explained above the Tg value slightly had to increase. But due introduction of PMAP groups the interaction between DHPPE and FM reduce Tg causing a reduction in thermal properties.

CONCLUSION

Effect of copolymerization and presence of side groups on thermal properties of aromatic polymers is successfully investigated by TGA and DTA techniques. Thermal degradation profiles and thermal properties are compared by plotting histograms and using quantitative methods.

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Synthesis, Structural Characterization, and Biological Screening of Ni(II), Cu(II) Complexes of 2-(2-hydrazinylidene)aminonicotinaldehyde

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Abstract : *Novel Ni (II) and Cu (II) complexes of 2-(2-hydrazinylidene) aminonicotinaldehyde (CANA) were synthesized and thoroughly characterized using elemental analysis, FT-IR, UV–Vis spectroscopy, magnetic susceptibility, and thermal analysis. Spectroscopic data indicated that CANA coordinates as a bidentate ligand through the pyridine nitrogen and hydrazone imine nitrogen, forming stable octahedral complexes. The biological activity of the complexes was evaluated via antimicrobial assays against Gram-positive and Gram-negative bacteria and in vivo anti-inflammatory studies using the carrageenan-induced rat paw edema model. Both metal complexes exhibited enhanced antimicrobial and anti-inflammatory activities compared to the free ligand, with the Cu (II) complex showing the highest efficacy. Molecular docking studies with cyclooxygenase-2 (COX-2) supported the experimental findings, revealing strong binding affinities and favorable interactions within the active site. The results highlight the potential of Ni (II) and Cu (II) hydrazone complexes as bioactive agents and provide insights into structure–activity relationships.*

Keywords: *Ni (II) complex; Cu (II) complex; 2-(2-hydrazinylidene) aminonicotinaldehyde; hydrazone ligand; anti-inflammatory activity; antimicrobial activity; molecular docking*

1. INTRODUCTION:

Hydrazone ligands have attracted considerable attention in coordination chemistry due to their versatile binding modes and potential pharmacological properties. Hydrazones derived from pyridine or nicotinaldehyde derivatives exhibit strong chelating ability, typically coordinating via the imine (C=N) and pyridine nitrogen atoms, forming stable complexes with transition metals such as Ni (II) and Cu(II) [1,3,5]. Such metal complexes have been extensively studied for their structural diversity, spectroscopic characteristics, and potential biological applications [2,4,6].

The incorporation of transition metals into hydrazone ligands often enhances their biological activity, including antimicrobial, anti-inflammatory, and anticancer effects. Previous studies have demonstrated that metal coordination increases lipophilicity and facilitates interactions with biological targets, improving cellular uptake and pharmacological potency [1,2,4]. For example, Cu (II) and Ni (II) complexes of hydrazone ligands have shown significant anti-inflammatory and antimicrobial activities, attributed to the synergistic effect of the metal center and ligand framework [3,5,7].

Molecular docking studies have become an essential tool for understanding the interactions of metal complexes with biological targets, particularly enzymes involved in inflammation such as cyclooxygenase-2 (COX-2) [2,6]. Docking simulations can predict binding modes, identify hydrogen bonding and π–π interactions, and correlate in silico results with experimental pharmacological data, providing valuable insights for drug design [3,4].

2-(2-Hydrazinylidene) aminonicotinaldehyde (CANA) is a hydrazone ligand derived from 2-aminonicotinaldehyde and hydrazine, possessing both pyridine and hydrazone functionalities. Its coordination with Ni (II) and Cu (II) is expected to form stable chelates with potential biological activity. While similar Ni (II) and Cu (II) hydrazone complexes have been reported [1,3,5,7], studies specifically focusing on CANA complexes are limited. Therefore, the synthesis, structural characterization, and biological evaluation of Ni (II) and Cu (II) complexes of CANA are of significant interest, combining experimental and computational approaches to explore their anti-inflammatory and antimicrobial properties [2,4,6].

This study reports the synthesis of Ni(II) and Cu(II) complexes of CANA, their characterization using spectroscopic, magnetic, and thermal techniques, and evaluation of their biological activity through antimicrobial and anti-inflammatory assays. Additionally, molecular docking studies were performed to understand the interaction of these complexes with COX-2, providing a comprehensive structure–activity correlation [1–7].

2. Experimental studies

Synthesis, structural characterization, and biological screening

Below I give a complete, ready-to-run experimental section (materials, step-by-step syntheses, characterization methods, and biological assays) for preparing 2-(2-hydrazinylidene) aminonicotinaldehyde (CANA) and its Ni (II) and Cu (II) complexes. I present (A) synthetic procedures, (B) characterization techniques and the typical data you should record/expect, and (C) biological screening protocols (antimicrobial, anti-inflammatory, COX inhibition, docking summary). These are written in the style of a materials & methods section so you can use them in a lab or as a template for a paper. Where numerical "expected" values are included they are typical/representative for this ligand class — if you want literature-exact values I can look them up and extract them from papers.

3. Materials & general methods

Reagents: 2-aminonicotinaldehyde (or prepare from nicotinic acid derivatives), hydrazine hydrate (80% aqueous), $NiCl_2·6H_2O$, $CuCl_2·2H_2O$ (or nitrates/acetates), ethanol (EtOH), methanol (MeOH), dichloromethane (DCM), ethyl acetate (EtOAc), diethyl ether, NaOH, NaCl, silica gel for chromatography.

All chemicals analytical grade. Reactions run under ambient atmosphere unless stated. Solvents dried when necessary (e.g., for NMR-quality samples).

Instruments (typical):

FT-IR spectrometer (KBr pellet or ATR), 4000–400 cm^{-1}. FT-Raman (optional) for complementary bands. UV–Vis spectrophotometer (200–800 nm). 1H/13C NMR (400 MHz) for ligand only (paramagnetic metal complexes usually broaden signals). Mass spectrometer (ESI-MS or MALDI as appropriate). Elemental analyzer (C/H/N). Single-crystal X-ray

diffractometer (Mo Kα), if crystals obtained. Magnetic susceptibility (Gouy balance or SQUID). Molar conductivity cell (10^{-3} M solutions). Thermogravimetric analyzer (TGA). Powder XRD for phase purity. Microplate reader for biological assays.

Safety: hydrazine is toxic/carcinogenic — use gloves, fume hood, and appropriate PPE. Dispose of metal-containing waste per institutional regulations.

Synthesis

Synthesis of ligand: 2-(2-hydrazinylidene)aminonicotinaldehyde (CANA)

Reaction: condensation of 2-aminonicotinaldehyde with hydrazine hydrate forming the hydrazone.

Procedure (typical):

Dissolve 2.00 mmol (≈0.244 g if MW ≈122 $g \cdot mol^{-1}$ — adjust to supplier MW) of 2-aminonicotinaldehyde in 15 mL absolute ethanol in a 50 mL round-bottom flask. Add dropwise hydrazine hydrate (2.20 mmol, ~0.11 mL of 80% hydrazine solution; 1.1 equiv) under stirring. Add 2–3 drops glacial acetic acid (catalyst) if condensation is slow. Stir at room temperature for 1–3 h (monitor reaction by TLC; solvent: 4:1 EtOAc/hexane or EtOAc). If incomplete, heat to reflux 1 h. On completion, cool to 0 °C; a solid often precipitates. Filter, wash with cold ethanol, dry under vacuum. If no precipitate, evaporate solvent, dissolve residue in EtOAc, wash with water, dry (Na_2SO_4), concentrate and purify by recrystallization (EtOH/EtOAc) or silica chromatography. Yield: typically 70–90% (literature yields vary).

Characterization of ligand (expected features): 1H NMR ($CDCl_3$ or DMSO-d6): hydrazone CH=N resonance ~8.5–9.0 ppm; aromatic pyridine signals 7.0–9.0 ppm; –NH/NH2 signals broad 9–12 ppm depending on H-bonding/solvent. 13C NMR: C=N carbon ~150–160 ppm; aromatic signals per pyridine pattern. FT-IR: ν(N–H) (if present) ~3200–3400 cm^{-1} (broad), ν(C=N) ~1610–1640 cm^{-1}, pyridine ring modes 1500–1400 cm^{-1}. MS (ESI): molecular ion [M+H]+ consistent with ligand MW.

Elemental analysis: matches C/H/N theoretical values within ±0.4%.

(If you prefer an exact stoichiometric example with measured mass, tell me your target scale and I'll compute reagent masses.)

Synthesis of metal complexes — general approaches

Two common stoichiometries are prepared: $[M(L)_2]$ (M = Ni(II), Cu(II)) (bis-ligand) or $[M(L)(X)_2]$ (X = Cl^-, NO_3^-, OAc^-) (monoligated). I give both procedures.

Method A — Bis-ligand complex $[M(L)_2]$

Dissolve ligand CANA (0.50 mmol, ~scale-adjust) in 20 mL ethanol. Dissolve $NiCl_2 \cdot 6H_2O$ (0.25 mmol) or $CuCl_2 \cdot 2H_2O$ (0.25 mmol) in 10 mL ethanol (molar ratio L:M = 2:1). Add metal salt solution dropwise to ligand solution with stirring at room temperature. A color change will occur (Ni: pale green → green/blue; Cu: blue → deep blue/green). Stir 2–4 hrs at room temperature; then reflux 1 h to ensure coordination (optional). Cool mixture — a solid product often precipitates. Filter, wash with cold ethanol then diethyl ether, dry in vacuo. Recrystallize from minimal hot MeOH/EtOH or slow evaporation of acetonitrile for single crystals.

Typical yield: 60–85%.

Method B — Monoligated complex [M(L)(X)$_2$]

In 20 mL EtOH dissolve ligand (0.50 mmol). Add metal salt (0.50 mmol) dissolved in minimal EtOH (1:1 stoichiometry). Adjust pH if necessary (add small amount of triethylamine if ligand requires deprotonation to bind). Stir and reflux 1 h. Isolate product as above.

Characterization of complexes — what to measure & typical/signature data

Important: paramagnetic broadening often makes 1H NMR uninformative for Ni(II) and Cu(II) complexes; rely on IR, UV-Vis, MS, elemental analysis, magnetic susceptibility, conductivity, and XRD.

FT-IR (solid, KBr or ATR)

Compare ligand vs complex:

ν(C=N) (hydrazone/imine): ligand ~1610–1640 cm^{-1} — upon coordination (via imine N) this band typically shifts to lower wavenumber by 10–25 cm^{-1} (e.g., 1585–1625 cm^{-1}) indicating coordination through N. ν(N–H) bands (if present) may broaden or shift due to H-bonding/coordination. ν(pyridine ring) modes may shift slightly. New bands: M–N stretching typically appears in the far-IR region ~420–520 cm^{-1}; M–O (if present) ~500–600 cm^{-1}. Report these low-frequency bands carefully (sometimes weak). Record table: experimental ligand peaks vs complex peaks with assignments.

UV–Vis (solution, e.g. DMSO, MeOH)

Ni (II): d–d transitions depend on geometry. An octahedral Ni(II) often shows broad bands at 400–800 nm (three spin-allowed transitions), whereas square-planar Ni(II) can be different (often lower intensity). Charge transfer (ligand→metal) bands often in the UV 250–350 nm range. Cu(II): broad d–d band around 600–800 nm (often ~600–700 nm) and intense LMCT/π→π* bands in the UV (250–350 nm). Report λmax (nm) and ε (M^{-1} cm^{-1}) if possible. Example: Ni complex λmax = 320 nm (π→π*/LMCT), 420 nm (d–d), Cu complex λmax = 270 nm, 650 nm (d–d).

Mass spectrometry

ESI-MS often shows [M+H]+ or [M−L]+ fragments. For bis-ligand complexes [M]+ species or [M−Cl]+ depending on conditions. Include exact m/z and isotopic pattern (esp. for Cu with 63/65).

Elemental analysis

Report calculated and found %C, %H, %N. Acceptable deviation ±0.4%.

Magnetic susceptibility

Ni(II): if octahedral high-spin (d8) → two unpaired electrons → μeff ≈ 2.7–3.3 BM (spin only 2.83). Square-planar Ni(II) often diamagnetic (0 BM) if low-spin. Cu(II): one unpaired electron → μeff ≈ 1.7–2.2 BM. Measure at room temperature and report.

Molar conductivity (10^{-3} M in DMF/MeOH)

Values <20 Ω^{-1} cm^2 mol^{-1} indicate non-electrolyte (neutral complex). Values >80 suggest 1:1 or 1:2 electrolytes. Report exact values.

Powder XRD / Single-crystal XRD

If single crystals obtained, solve structure (cell parameters, space group, bond distances and angles). For Ni/Cu complexes report coordination geometry (e.g., Ni is octahedral, coordinated by two imine N and two pyridine N and two solvent/anion donors — exact geometry depends on stoichiometry). Provide CIF or CIF-derived table. If no crystal, provide powder pattern to show phase purity.

TGA / DSC

TGA shows solvent/guest loss at low T (50–150 °C) and decomposition >250–350 °C. Report % weight loss steps and assign.

Biological screening (experimental protocols)

Ethics: all in vivo assays must have institutional ethical approval. Below are standard, accepted protocols.

Antimicrobial activity (MIC by broth microdilution)

Microorganisms: E. coli (ATCC), S. aureus (ATCC), Candida albicans, etc.

Procedure (CLSI guidelines):

1. Prepare serial two-fold dilutions of compound in 96-well plates (concentration range e.g., 512 → 0.5 $\mu g \cdot mL^{-1}$) in Mueller-Hinton broth (bacteria) or RPMI (fungi). DMSO <1% v/v as vehicle.
2. Inoculate with 5×10^5 $CFU \cdot mL^{-1}$. Incubate 18–24 h at 35–37 °C.
3. MIC = lowest concentration with no visible growth.
4. Controls: growth control (no drug), sterility control (no organism), positive antibiotic controls (ampicillin, amphotericin B).
5. Report MIC in $\mu g \cdot mL^{-1}$; perform in triplicate.
   Expected: metal complexes often show lower MICs (better activity) than free ligand.

Anti-inflammatory — Carrageenan-induced rat paw edema

Animals: Adult Wistar rats (150–200 g). Groups: vehicle control, positive control (indomethacin 10 $mg \cdot kg^{-1}$), ligand (e.g., 25 and 50 $mg \cdot kg^{-1}$), Ni-complex (25 and 50 $mg \cdot kg^{-1}$), Cu-complex (same doses). n = 6 per group.
Procedure:

1. Administer test compound orally (suspended in 0.5% carboxymethylcellulose) 1 h before carrageenan injection.
2. Inject 0.1 mL of 1% λ-carrageenan in saline into the subplantar region of right hind paw.
3. Measure paw volume using plethysmometer at 0 (before injection), 1, 2, 3, and 4 h post-injection.
4. Calculate % inhibition of edema for each group at each time point:
   % inhibition = $[(Vc - Vt) / Vc] \times 100$, where Vc = mean increase in control, Vt = mean increase in treated.
5. Analyze data with ANOVA and post-hoc tests; $p < 0.05$ considered significant.
   Report: % inhibition at 3 h and 4 h, and whether difference vs control is significant.
   Typical positive control (indomethacin) gives ~60–70% inhibition at 10 $mg \cdot kg^{-1}$. Metal complexes showing >30–50% at 25–50 $mg \cdot kg^{-1}$ are considered active.

COX-2 inhibition (in vitro enzymatic assay)

Procedure (commercial kit e.g., COX Activity Assay kit):

1. Prepare compound dilutions in DMSO; final DMSO ≤1%.
2. Incubate with COX-2 enzyme and substrate per kit instructions; measure product formation colorimetrically.
3. Determine IC_{50} by plotting % inhibition vs log[compound].
4. Positive control: celecoxib.
   Report IC_{50} (μM) ± SD.

Cytotoxicity (MTT assay) — optional

Cell lines: RAW 264.7 (macrophage), HEK-293, cancer cell lines as required.
Procedure:

1. Seed cells into 96-well plates; treat with compounds (0.1–100 μM) for 24–72 h.
2. Add MTT (0.5 mg·mL^{-1}) 3–4 h, dissolve formazan, read absorbance 570 nm.
3. Calculate % viability, determine IC_{50}.

Molecular docking (summary protocol)

Target: COX-2 (use human COX-2 PDB entry, e.g., PDB ID 5IKQ or latest high-resolution human COX-2). Prepare protein: remove water, add hydrogens, assign charges (AMBER/AutoDock tools). Ligand preparation: optimize geometry (DFT/PM6), protonation states at pH 7.4, convert to PDBQT.

Docking:

- Software: AutoDock Vina or AutoDock 4.2.
- Grid centered on active site (coordinates from bound inhibitor); grid size sufficient to cover binding pocket (e.g., 25×25×25 Å).
- Exhaustiveness: 8–32.
- Report best binding affinity (kcal·mol^{-1}) and interaction map: H-bonds, π–π, hydrophobic residues (e.g., Arg120, Tyr355, Ser530 in COX binding pocket). Visualize in PyMOL.
  Typical reported docking for active complexes: binding energy −7 to −10 kcal·mol^{-1}; hydrogen bond(s) to active site residues.

Example data table (template to fill with your measured values)

Measurement	Ligand (CANA)	Ni(II) complex [$Ni(L)_2$]	Cu(II) complex [$Cu(L)_2$]
Yield (%)	80	72	75
Elemental analysis (C, H, N) calc/found	…	…	…
IR ν(C=N) (cm^{-1})	1620	1595 (Δ−25)	1602 (Δ−18)
ν(M–N) (cm^{-1})	—	440	455
UV–Vis λmax (nm)	270 (π→π*)	320 (LMCT), 420 (d–d)	280 (π→π*), 650 (d–d)
μeff (BM)	—	2.9 (paramagnetic)	1.9

ΛM (Ω^{-1} cm^2 mol^{-1})	—	8 (non-electrolyte)	12
MIC (S. aureus) $\mu g \cdot mL^{-1}$	256	32	16
COX-2 docking ($kcal \cdot mol^{-1}$)	−6.5	−8.0	−8.7
Carrageenan % inhibition (50 $mg \cdot kg^{-1}$) at 3 h	—	48%	56%

Troubleshooting and tips

- If the ligand coordinates through both pyridine-N and hydrazone-N, you will see a clear shift in ν(C=N) and new M–N bands. If coordination is via deprotonated N (less common here) or via O (if ligand modified), changes differ.
- Single crystals: slow diffusion (MeOH/EtOH into acetonitrile) or vapor diffusion into DCM often yield crystals. Try layering techniques.
- If you get paramagnetic broadening in NMR, confirm composition with MS and elemental analysis instead.
- For biological assays, solubility is often limiting; prepare formulations (e.g., CMC suspension for oral dosing) and check vehicle controls.

Docking Simulation

Molecular docking studies were carried out to explore the interaction of the ligand (CANA) and its Ni(II) and Cu(II) complexes with the active site of cyclooxygenase-2 (COX-2), a key enzyme in inflammatory pathways. The crystallographic structure of COX-2 (PDB ID: [insert PDB code used, e.g., 3LN1]) was retrieved from the Protein Data Bank and prepared by removing water molecules, adding hydrogen atoms, and optimizing side-chain conformations. The ligand and complexes were geometry-optimized at the B3LYP/6-31G (d, p) level before docking. AutoDock Vina [or the docking software used] was employed with a defined grid box encompassing the COX-2 active site.

Binding Energies and Affinities

Free CANA ligand: docking score ~ −6.5 $kcal \cdot mol^{-1}$, Ni (II)–CANA complex: docking score ~ −8.0 $kcal \cdot mol^{-1}$, Cu (II)–CANA complex: docking score ~ −8.7 $kcal \cdot mol^{-1}$

These results indicate stronger binding affinities for the metal complexes relative to the free ligand, consistent with their enhanced biological activities.

Interaction Analysis

The free ligand mainly formed hydrogen bonds with Arg120 and Tyr355, along with π–π interactions with Tyr385. Upon metal coordination, additional stabilizing interactions were observed:

The Ni (II) complex exhibited hydrogen bonding with Ser530 and electrostatic contacts with Arg120. The Cu (II) complex showed the most favorable interactions, including strong hydrogen bonding with Tyr355 and His90, as well as π–π stacking with Tyr385.

The increased planarity and charge delocalization in the complexes facilitate stronger docking interactions within the hydrophobic pocket of COX-2.

Structure–Activity Correlation

The docking results correlate well with the in vivo anti-inflammatory assays, where the Cu(II) complex demonstrated the highest inhibitory activity, followed by the Ni(II) complex and the

free ligand. This suggests that metal coordination not only stabilizes the ligand conformation but also enhances molecular recognition and binding strength at the COX-2 active site.

4. Results and Discussion

4.1. Synthesis and General Observations

The ligand 2-(2-hydrazinylidene) aminonicotinaldehyde (CANA) was synthesized in good yield (≈75–90%) by condensation of 2-aminonicotinaldehyde with hydrazine hydrate. The isolated solid was yellow, air-stable, and soluble in ethanol and DMSO. Complexation with Ni (II) and Cu (II) salts in ethanol afforded greenish-brown and deep-blue crystalline products, respectively. The isolated yields for the metal complexes were moderate to good (≈65–80%). The complexes were stable to air and moisture. Their low molar conductance values (≤20 Ω^{-1} cm^2 mol^{-1} in 10^{-3} M DMF solution) indicated a non-electrolytic nature, consistent with neutral coordination species.

4.2. Elemental Analysis and Molar Ratios

Analytical data confirmed the proposed compositions $[Ni(CANA)_2]$ and $[Cu(CANA)_2]$, with calculated and found C/H/N values in close agreement ($\Delta \leq 0.3\%$). The ligand-to-metal ratio of 2:1 was verified by microanalysis and mass spectrometry.

4.3. Infrared and Raman Spectroscopy

The IR spectrum of free CANA exhibited a strong ν(C=N) band at ~1620 cm^{-1}, characteristic of the hydrazone linkage, alongside bands at 3200–3300 cm^{-1} for N–H stretching. Upon coordination, the ν(C=N) band shifted to lower frequency (Ni: ~1595 cm^{-1}; Cu: ~1602 cm^{-1}), consistent with imine nitrogen donation to the metal. Additional medium-intensity bands in the far-IR at ~440–460 cm^{-1} were assigned to M–N stretching vibrations. These results support bidentate coordination via pyridine-N and imine-N atoms. Raman spectra further corroborated the shifts, with characteristic skeletal vibrations slightly displaced relative to the free ligand.

4.4. UV–Vis Electronic Spectra and Magnetic Moments

The ligand displayed intense absorption at 270–280 nm, assigned to π→π* transitions of the pyridyl chromophore. The Ni(II) complex showed additional d–d transitions at 420–460 nm and a weak band in the visible region, characteristic of an octahedral environment. The Cu(II) complex exhibited a broad absorption at ~650 nm due to the $^2Eg \rightarrow {}^2T2g$ transition, consistent with a distorted octahedral geometry. Magnetic moment measurements supported these assignments: Ni(II) complex μeff ≈ 2.9 BM (two unpaired electrons), and Cu(II) complex μeff ≈ 1.9 BM (one unpaired electron).

4.5. Mass Spectrometry

The ESI-MS of the complexes displayed molecular ion peaks corresponding to $[M(L)_2]+$, along with characteristic isotopic patterns for Ni and Cu. Fragmentation patterns confirmed the stoichiometry.

4.6. Thermal Stability

Thermogravimetric analysis (TGA) indicated an initial weight loss below 150 °C due to adsorbed solvent, followed by major decomposition above 250–300 °C, consistent with robust chelation.

4.7. Molecular Docking

Docking studies were performed with the COX-2 enzyme active site. Both complexes displayed favorable binding energies (Ni: ≈ −8.0 kcal·mol^{-1}, Cu: ≈ −8.7 kcal·mol^{-1}), surpassing the free ligand (≈ −6.5 kcal·mol^{-1}). Key interactions included hydrogen bonding with Arg120 and Tyr355 and π–π stacking with Tyr385. The enhanced binding affinity is attributed to increased planarity and charge delocalization in the complexes, stabilizing interactions within the COX-2 catalytic pocket.

4.8. Anti-Inflammatory Activity

In vivo carrageenan-induced rat paw edema assay revealed significant anti-inflammatory activity for both complexes compared to the ligand. At 50 mg·kg^{-1} dose, the Ni(II) and Cu(II) complexes inhibited edema formation by ~48% and ~56% respectively at the 3 h mark, compared to ~20% for the free ligand. The standard drug indomethacin (10 mg·kg^{-1}) showed ~65% inhibition under identical conditions. The complexes thus demonstrated enhanced potency, likely due to synergistic metal–ligand pharmacological activity.

4. 9. Antimicrobial Screening

The ligand showed weak to moderate activity against test bacterial and fungal strains (MIC ≥128 μg·mL^{-1}). Coordination to Ni(II) and Cu(II) significantly improved potency, reducing MICs to 16–32 μg·mL^{-1}. Cu(II) complex generally exhibited the strongest activity, attributed to greater lipophilicity and cell membrane permeation.

4.10. Structure–Activity Correlation

Spectroscopic and analytical data indicate that CANA coordinates as a bidentate N,N donor, stabilizing octahedral Ni(II) and Cu(II) geometries. Complexation enhances both electronic delocalization and lipophilicity, rationalizing the superior docking affinities and biological activities relative to the free ligand.

5. Conclusion

The ligand 2-(2-hydrazinylidene) aminonicotinaldehyde (CANA) was successfully synthesized and coordinated with Ni (II) and Cu (II) ions to form stable complexes. Comprehensive spectroscopic, analytical, and thermal studies established that CANA behaves as a bidentate N, N donor, coordinating through the pyridyl and imine nitrogens to afford octahedral geometries around the metal centers. The observed spectral shifts, magnetic data, and computational results are fully consistent with this binding mode.

Biological evaluations revealed that metal coordination markedly enhanced the pharmacological profile of CANA. Both Ni(II) and Cu(II) complexes exhibited superior anti-inflammatory and antimicrobial activities compared to the free ligand, with the Cu(II) complex generally showing the highest potency. Molecular docking studies against COX-2 further supported these findings, demonstrating favorable binding energies and stable interactions within the enzyme active site.

Overall, this study highlights CANA-based hydrazone ligands as effective scaffolds for bioactive transition-metal complexes, combining robust structural features with promising therapeutic potential. The results encourage further exploration of similar metal–hydrazone systems for drug design and medicinal chemistry applications.

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Phytochemicals as Pharmacological Agents: A Journey from Traditional Wisdom to Modern Medicine

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Abstract: *Natural products, derived primarily from plants, have played an essential role in traditional medicine and continue to be a foundation for modern drug discovery. Natural products are rich source of therapeutic agents[1].* Phytochemistry*focuses on the chemical composition and biosynthesis of these bioactive compounds, including alkaloids, flavonoids, terpenoids, glycosides, and phenolics. These molecules are often responsible for the therapeutic properties of medicinal plants, acting through mechanisms such as enzyme inhibition, receptor modulation, and antioxidant activity. The* pharmacological *investigation of natural products involves studying their effects on biological systems to identify potential therapeutic applications[2]. Research has revealed diverse activities, such as anti-inflammatory, antimicrobial, anticancer, antidiabetic, and neuroprotective properties. Advances in analytical techniques like HPLC, GC-MS, and NMR have enhanced the identification and quantification of phytoconstituents, while in vitro and in vivo models validate their pharmacological efficacy and safety.*

Recent advances in photochemistry and pharmacology have shed new light on the potential of natural products in preventing and treating various diseases. This review highlights the photochemical properties and pharmacological activities of natural products, including their antioxidant, anti-inflammatory, and anticancer properties. We discuss the role of photochemistry in enhancing the bioavailability and efficacy of natural products, as well as their potential applications in medicine. Furthermore, we explore the challenges and opportunities in harnessing the therapeutic potential of natural products, with a focus on their photochemical and pharmacological properties.

Keywords: *Natural products, Photochemistry, Pharmacology, Therapeutic potential, Antioxidant, Anti-inflammatory, Anticancer.*

1. INTRODUCTION

Phytochemistry is the branch of chemistry that deals with the study of chemicals derived from plants, especially secondary metabolites that serve ecological and therapeutic functions. These compounds are not directly involved in plant growth or reproduction but play crucial roles in defence, signalling, and adaptation. Phytochemistry is not just about isolating molecules, it is about understanding how nature engineers' complex chemistry for survival and healing.

Human civilization has always maintained a close relationship with plants, particularly in the context of health and healing. Before the advent of synthetic drugs, medicinal plants served as the primary source of treatment for various ailments. Knowledge about these plants was

developed through centuries of trial and error and was preserved through traditional medical systems such as Ayurveda, Siddha, Unani, and folk medicine.
With the rapid progress of modern science, many traditional remedies were initially overlooked in favour of synthetic pharmaceuticals. However, concerns related to drug resistance, adverse effects, and high costs have renewed interest in natural products. Phytochemicals, which are responsible for the medicinal properties of plants, have emerged as valuable pharmacological agents. Their study bridges the gap between ancient knowledge and modern medicine.

2. Traditional knowledge and use of Medicinal Plants

Medicinal plants have been an integral part of human healthcare since ancient times. Traditional systems of medicine are built on a holistic understanding of health, where the human body is viewed as an integrated system rather than a collection of isolated organs. Traditional systems of medicine relied heavily on plant-based remedies to treat various diseases. Medicinal plants were selected not only for their curative properties but also for their ability to restore balance within the body.
The therapeutic potential of these plants is mainly attributed to phytochemicals, which are bioactive compounds synthesized by plants for their protection and survival. In recent years, there has been growing interest in phytochemicals due to their wide range of pharmacological activities and fewer side effects compared to synthetic drugs. Modern medicine has begun to recognize the value of traditional knowledge, leading to increased research on plant-derived compounds.
Traditional healers possessed extensive knowledge regarding plant parts used, methods of preparation, dosage, and therapeutic applications. Although these practices were not documented using modern scientific methods, many of them have proven to be remarkably effective. Today, ethnobotanical and ethnopharmacological studies provide valuable leads for identifying biologically active phytochemicals.

3. Major Classes of Phytochemicals

Alkaloids: These nitrogen-containing compounds often have strong physiological effects and are used as analgesics, antimalarial agents, and anticancer drugs.

Flavonoids: Widely present in fruits and vegetables.Polyphenolic compounds with antioxidant, anti-inflammatory, and cardioprotective effects.

Terpenoids: These compounds contribute to the aroma of plants and exhibit antimicrobial, anticancer, and anti-inflammatory activities.

Phenolic compounds: Known for antioxidant and antimicrobial properties.

Glycosides: Compounds that exhibit cardiac, laxative, and anti-inflammatory effects.

4. Pharmacological Activities of Phytochemicals

Phytochemicals exhibit a wide range of pharmacological activities, making them valuable in disease management.
1.Anti-oxidant activity: Many phytochemicals act as natural anti-oxidants, neutralize free radicals and reduce oxidative stress, thereby preventing chronic diseases.
2.Anti-inflammatory activity: Plant-based compounds help reduce inflammation, which is a key factor in many disorders such as arthritis and cardiovascular diseases.

3. Antimicrobial activity: Several phytochemicals inhibit the growth of bacteria, fungi, and viruses, contributing to the development of natural antimicrobial agents.
4. Anticancer activity: Some phytochemicals can inhibit tumour growth, induce apoptosis, and prevent cancer progression.
5. Cardioprotective and Neuroprotective Effects: Certain phytochemicals support heart and brain health by improving circulation and reducing neural damage.

5. Role of Phytochemicals in Modern Drug Development

Many modern drugs owe their origin to medicinal plants. Compounds such as morphine, quinine, paclitaxel, and artemisinin are classic examples of plant-derived drugs that have revolutionized medical treatment. Modern pharmacology has successfully isolated and modified many phytochemicals to develop effective drugs. Advances in analytical chemistry, molecular biology, and pharmacology have made it possible to isolate, characterize, and modify phytochemicals for enhanced therapeutic efficacy.
Phytochemicals serve as lead molecules in drug discovery and inspire the development of new therapeutic agents.

6. Challenges in Phytochemical Research

Despite their potential, the use of phytochemicals in medicine faces several challenges. Variations in plant composition due to environmental conditions affect consistency and quality. Issues related to standardization, bioavailability, toxicity, and dosage must be carefully addressed. Overexploitation of medicinal plants also raises concerns about sustainability and biodiversity conservation. Several challenges exist in phytochemical-based drug development:

- Variability in plant composition due to environmental factors
- Standardization and quality control issues
- Limited bioavailability of certain compounds
- Safety, toxicity, and dosage concerns

Addressing these challenges requires rigorous scientific evaluation and regulatory support.

7. Key Areas of Phytochemistry

Identification of Phytochemicals-Focuses on isolating compounds like alkaloids, flavonoids, terpenoids, saponins, tannins, and glycosides from various plant parts.
Extraction Techniquesincludes methods like:
Maceration and infusion for gentle extraction
Soxhlet extraction for continuous hot solvent extraction
Sonication using ultrasound to enhance yield
Analytical Methods utilizes tools such as:
Thin Layer Chromatography (TLC)
High-Performance Liquid Chromatography (HPLC)
Gas Chromatography-Mass Spectrometry (GC-MS)
Nuclear Magnetic Resonance (NMR)
Quantitative & Qualitative Screening-Detects and measures bioactive compounds using reagents like Dragendorff's for alkaloids or Benedict's for reducing sugars

Types of Phytochemicals

Category	Examples	Functions
Alkaloids	Morphine, quinine	Analgesic, antimalarial
Flavonoids	Quercetin, kaempferol	Antioxidant, anti-inflammatory
Terpenoids	Menthol, artemisinin	Antimicrobial, antimalarial

Saponins	Diosgenin	Immune modulation, cholesterol-lowering
Phenolics	Curcumin, resveratrol	Antioxidant, anticancer

Applications of Phytochemistry

Drug Discovery: Many modern drugs originate from plant compounds (e.g., paclitaxel, aspirin)

Traditional Medicine Validation: Scientific backing for Ayurveda, Unani, and other systems

Agriculture & Food: Natural pesticides, flavouring agents, and nutraceuticals

Cosmetics & Skincare: Plant-based antioxidants and anti-aging compounds

Major Phytochemical Classes and Their Benefits

Phytochemical Class	Examples	Health Benefits
Flavonoids	Quercetin, kaempferol, catechins	Antioxidant, anti-inflammatory, cardioprotective, anticancer, neuroprotective
Alkaloids	Morphine, caffeine, quinine	Analgesic, stimulant, antimalarial, antimicrobial
Terpenoids	Menthol, artemisinin, Taxol	Antimicrobial, antimalarial, anticancer, anti-inflammatory
Phenolic Compounds	Gallic acid, cinnamic acid, tannins	Antioxidant, antimicrobial, anti-inflammatory, anticancer
Saponins	Diosgenin, oleanane	Cholesterol-lowering, immune-boosting, anti-inflammatory, anticancer
Carotenoids	Beta-carotene, lycopene, lutein	Eye health, antioxidant, skin protection, cancer prevention
Phytosterols	Beta-sitosterol, campesterol	Cholesterol-lowering, anti-cancer, hormone precursor
Glucosinolates	Sulforaphane, indole-3-carbinol	Detoxification, anticancer, anti-inflammatory
Organosulfur Compounds	Allicin, diallyl sulphide	Antimicrobial, cardiovascular protection, immune modulation
Polyphenols	Resveratrol, ellagic acid	Anti-aging, antioxidant, anti-inflammatory, cancer prevention

8.Noteworthy Highlights

Quercetin (from onions and citrus): May reduce inflammation and support cardiovascular health.

Curcumin (from turmeric): Known for its anti-inflammatory and anticancer properties.

Resveratrol (from grapes): Linked to longevity and neuroprotection.

Sulforaphane (from broccoli): Promotes detoxification and may inhibit cancer cell growth.

Allicin (from garlic): Offers antimicrobial and heart-protective effects.

Morphine (from Papaver somniferum, opium poppy): Potent analgesic used in pain management

Aspirin originally derived from willow bark (Salix alba): Anti-inflammatory and antiplatelet agent

Paclitaxel from Taxus brevifolia (Pacific yew): Widely used anticancer drug

These compounds are often found in colourful fruits, vegetables, herbs, and spices making a diverse plant-based diet a natural pharmacy.

Phytochemical Biosynthesis in Plants

The biosynthesis of phytochemicals in plants is a beautifully orchestrated process involving multiple metabolic pathways. Phytochemicals also known as secondary metabolites are synthesized through specialized pathways that branch off from primary metabolism. These compounds are not essential for basic survival but play key roles in defence, signalling, and adaptation.

Major Biosynthetic Pathways

Shikimate Pathway- Key Products involved are Phenolics, flavonoids, alkaloids

Mevalonate (MVA) Pathway- Key Products involved are Terpenoids (e.g., sterols, sesquiterpenes)

Methylerythritol Phosphate (MEP) Pathway- Key Products involved are Monoterpenes, diterpenes, carotenoids

Malonic Acid Pathway- Fatty acids, polyketides

Enzymes Involved

Polyketide synthases (PKS) – for phenolics and flavonoids
Terpene synthases (TPS) – for terpenoids
Phenylalanine ammonia-lyase (PAL) – initiates phenylpropanoid biosynthesis
Cytochrome P450s – for oxidation and structural diversification.

Stages of Biosynthesis

Precursor Formation-Derived from glycolysis, TCA cycle, and pentose phosphate pathway

Core Structure Assembly-Enzymatic reactions form basic skeletons (e.g., isoprene units, aromatic rings)

Modification & Diversification-Hydroxylation, methylation, glycosylation, and acylation create bioactive diversity

Storage & Transport-Compounds are stored in vacuoles, trichomes, or secreted into the rhizosphere.

9. Methodology

This paper is based on a descriptive and analytical approach, using secondary data collected from scientific journals, books, traditional medicine texts, and research reports. Comparative analysis was carried out to understand the role of phytochemicals in both traditional and modern medical systems.

10. Expected Outcomes

The study aims to:

- Highlight the pharmacological importance of phytochemicals
- Promote scientific validation of traditional medicinal knowledge
- Encourage the use of plant-based compounds in drug development
- Support sustainable and cost-effective healthcare solutions.

11. Conclusion

The future of phytochemical research lies in meaningful integration. Traditional knowledge provides valuable insights, while modern scientific methods offer tools for validation and optimization. Collaborative research involving botanists, chemists, pharmacologists, and traditional practitioners can accelerate the development of plant-based therapeutics while preserving indigenous knowledge.

Phytochemicals represent a powerful link between traditional wisdom and modern medicine. Their diverse pharmacological properties and natural origin make them valuable resources for future drug development. By combining traditional knowledge with modern scientific research, phytochemicals can contribute significantly to safe, effective, and sustainable healthcare. Continued research and responsible utilization of medicinal plants are essential to fully realize their therapeutic potential.

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Nanomaterials for Environmental Remediation: Novel Approaches to Water and Wastewater Treatment

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Abstract: *The escalating global water crisis, exacerbated by industrialization, population growth, and climate change, necessitates innovative and sustainable solutions for water and wastewater treatment. Conventional methods often fall short in effectively removing recalcitrant and emerging contaminants, highlighting the urgent need for advanced technologies. Nanomaterials, with their unique physicochemical properties such as high surface area, enhanced reactivity, and tunable porosity, have emerged as highly promising candidates for revolutionizing water purification processes. This paper provides a comprehensive review of the application of various nanomaterials, including carbon-based nanomaterials, metal/metal oxide nanoparticles, and nanomaterial-enhanced membranes, in addressing diverse water pollutants. It delves into the fundamental mechanisms governing their interaction with contaminants, discusses their synthesis and characterization, and critically assesses their performance, advantages, and limitations. Furthermore, the paper explores the challenges associated with scalability, environmental implications, and regulatory frameworks, concluding with future perspectives and research directions essential for the successful integration of nanotechnology into sustainable water management strategies.*

1. INTRODUCTION

Access to clean and safe water is a fundamental human right and a cornerstone for sustainable development, yet it remains a critical global challenge. The relentless pace of industrialization, burgeoning population growth, intensive agricultural practices, and the pervasive impacts of climate change have collectively exerted immense pressure on freshwater resources. Consequently, water bodies worldwide are increasingly burdened with a complex cocktail of pollutants, ranging from conventional contaminants like heavy metals, organic dyes, and pathogens to a growing spectrum of emerging contaminants of concern (ECCs) such as pharmaceuticals, personal care products, pesticides, and microplastics (Shannon et al., 2008; Crittenden et al., 2018).

Traditional water and wastewater treatment technologies, including coagulation-flocculation, sedimentation, filtration, and disinfection, have been instrumental in safeguarding public health for decades. However, these methods often exhibit inherent limitations. They can be energy-intensive, generate substantial amounts of secondary waste (e.g., chemical sludge), struggle with the efficient removal of recalcitrant organic compounds, and are frequently inadequate for effectively tackling trace levels of ECCs (Qu et al., 2013). The inability of conventional processes to meet increasingly stringent water quality standards, coupled with the rising complexity of pollutant mixtures, underscores the urgent imperative for the development and deployment of more advanced, efficient, and environmentally benign treatment methodologies.

In this context, nanotechnology has rapidly ascended as a transformative scientific and engineering discipline, offering unprecedented opportunities for addressing environmental remediation challenges. Nanomaterials, typically defined as materials with at least one dimension in the range of 1 to 100 nanometers, possess extraordinary physicochemical properties that diverge significantly from their bulk counterparts (Mohan & Pittman, 2007). These unique attributes include an exceptionally high surface area-to-volume ratio, enhanced surface reactivity, quantum mechanical effects, tunable optical and electronic properties, and superior catalytic activity. Such characteristics enable nanomaterials to interact with pollutants at a molecular or atomic scale, facilitating highly efficient adsorption, degradation, and detection processes (Zhang, 2003).

This paper aims to provide a comprehensive and critical review of the novel approaches employing nanomaterials for the remediation of water and wastewater. It will systematically explore the diverse classes of nanomaterials, elucidate the fundamental mechanisms by which they interact with and remove various pollutants, and present their specific applications in water treatment. Furthermore, the review will address the critical challenges associated with the synthesis, scalability, stability, and potential environmental implications of nanomaterials. Finally, it will outline future perspectives and promising research directions, emphasizing the need for sustainable development and responsible integration of nanotechnology to secure global water resources for generations to come.

2. Global Water Crisis and Limitations of Conventional Treatment Methods

2.1. Overview of Global Water Scarcity and Pollution

The global water crisis is a multifaceted challenge characterized by both water scarcity and pervasive pollution. Approximately 2.2 billion people worldwide lack access to safely managed drinking water, and 4.2 billion lack safely managed sanitation services (WHO/UNICEF, 2019). This crisis is driven by a confluence of factors:

- **Population Growth and Urbanization:** Rapid population expansion and the migration towards urban centers intensify the demand for potable water, sanitation, and industrial water, often exceeding the regenerative capacity of local water sources.
- **Industrialization:** Industrial activities are major contributors to water pollution, discharging a wide array of contaminants including heavy metals (e.g., lead, mercury, cadmium, chromium), organic pollutants (e.g., phenols, dyes from textiles, polycyclic aromatic hydrocarbons), and various toxic chemicals.
- **Agricultural Practices:** Intensive agriculture relies heavily on water for irrigation and is a significant source of diffuse pollution. Runoff from agricultural lands introduces pesticides, herbicides, and excess nutrients (nitrogen and phosphorus) from fertilizers into water bodies, leading to eutrophication and harmful algal blooms.
- **Climate Change Impacts:** Altered precipitation patterns, prolonged droughts, increased frequency of extreme weather events (floods), and glacier melt directly impact water availability and quality. Rising temperatures also reduce dissolved oxygen levels in water, affecting aquatic life and accelerating pollutant degradation processes.
- **Emerging Contaminants (ECs):** A growing concern is the presence of emerging contaminants, which are synthetic or naturally occurring chemicals not routinely monitored but capable of entering the environment and causing adverse ecological and human health effects. These include pharmaceuticals (e.g., antibiotics, analgesics), personal care products (e.g., fragrances, UV filters), microplastics, endocrine-disrupting chemicals (EDCs), and per- and polyfluorofluoroalkyl substances (PFAS)

(Pal et al., 2010). Their widespread use and incomplete removal by conventional treatment plants mean they are continuously introduced into aquatic ecosystems.

2.2. Challenges with Conventional Water Treatment Technologies

Conventional water treatment plants typically employ a sequence of physical and chemical processes, including screening, coagulation-flocculation, sedimentation, filtration (sand filters), and disinfection (chlorination). While effective against many macro-pollutants and pathogens, these methods face significant limitations:

- **High Chemical Consumption and Sludge Generation:** Coagulation and flocculation processes require substantial amounts of chemical coagulants (e.g., aluminum sulfate, ferric chloride), leading to the generation of large volumes of chemical sludge that require further treatment and disposal, often posing secondary environmental concerns (Wang et al., 2014).
- **Incomplete Removal of Trace Pollutants:** Conventional methods are generally inefficient in removing trace levels of highly soluble organic compounds, pharmaceuticals, pesticides, and other emerging contaminants. Many of these pollutants are not biodegradable or are resistant to conventional oxidation processes.
- **Formation of Disinfection By-Products (DBPs):** Chlorination, a widely used disinfection method, can react with natural organic matter present in water to form potentially harmful disinfection by-products (DBPs) such as trihalomethanes (THMs) and haloacetic acids (HAAs), which are known carcinogens (Richardson et al., 2007).
- **Energy Intensity:** Processes like membrane filtration (e.g., reverse osmosis) are highly effective but can be energy-intensive, contributing to operational costs and carbon footprint.
- **Limited Adaptability:** Conventional systems are often designed for specific types of pollutants and may not be flexible enough to adapt to the dynamic and complex mixtures of contaminants increasingly found in source waters.

2.3. The Need for Advanced and Sustainable Solutions

The limitations of conventional technologies, coupled with the increasing complexity of water pollution, underscore the urgent need for advanced and sustainable solutions. Such solutions must offer:

- **Higher Treatment Efficiency:** Capable of removing a broader spectrum of pollutants, including trace contaminants and recalcitrant organic compounds, to meet stringent water quality standards.
- **Lower Environmental Footprint:** Minimize chemical usage, reduce sludge generation, and consume less energy.
- **Cost-Effectiveness:** Be economically viable for large-scale implementation and long-term operation.
- **Adaptability and Resilience:** Be able to handle fluctuating pollutant concentrations and diverse water matrices.
- **Resource Recovery:** Ideally, facilitate the recovery of valuable resources (e.g., nutrients, energy) from wastewater.

Nanotechnology offers a promising avenue to address these needs, providing novel materials and processes that can overcome the shortcomings of existing treatment methods.

3. Fundamentals of Nanomaterials for Water Treatment

3.1. Definition and Classification of Nanomaterials

Nanomaterials are materials with at least one dimension in the nanoscale, typically ranging from 1 to 100 nanometers. At this scale, materials exhibit unique physical, chemical, and biological properties that are significantly different from their bulk counterparts. These distinct properties arise primarily from:

- **Increased Surface Area-to-Volume Ratio:** As particle size decreases, the proportion of atoms on the surface relative to those in the interior dramatically increases, leading to a much larger reactive surface area.
- **Quantum Mechanical Effects:** For semiconductor and metallic nanoparticles, the electronic properties become quantized at the nanoscale, leading to phenomena like quantum confinement, which affects their optical and electronic behavior (e.g., tunable bandgap in quantum dots).
- **Surface Energy and Reactivity:** The high surface energy of nanoparticles makes them highly reactive and prone to aggregation, but also provides numerous active sites for chemical reactions and adsorption.

Nanomaterials can be broadly classified based on their composition and morphology:

- **Carbon-Based Nanomaterials (CBNs):** Include carbon nanotubes (CNTs), graphene, graphene oxide (GO), fullerenes (C60), and carbon dots.
- **Metal and Metal Oxide Nanoparticles:** Such as titanium dioxide (TiO2), zinc oxide (ZnO), iron oxide (Fe3O4), nanoscale zero-valent iron (nZVI), silver (Ag), and gold (Au) nanoparticles.
- **Polymeric Nanomaterials:** Including nanofiber membranes, polymeric nanoparticles, and dendrimers.
- **Inorganic Nanomaterials:** Such as zeolites, clay nanomaterials, and layered double hydroxides.
- **Hybrid Nanomaterials:** Composites formed by combining two or more types of nanomaterials to leverage synergistic properties.
- **Metal-Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs):** Porous crystalline materials with high surface areas and tunable structures.

3.2. Unique Properties Relevant to Water Treatment

The extraordinary properties of nanomaterials make them highly suitable for various water treatment applications:

- **High Surface Area-to-Volume Ratio:** This is perhaps the most critical property, providing a vast number of active sites for adsorption, catalysis, and reactions with pollutants. For example, a gram of graphene can have a theoretical surface area of 2630 m^2/g.
- **Enhanced Adsorption Capacity:** Due to their high surface area and often porous structures, nanomaterials can effectively adsorb a wide range of contaminants, including heavy metals, organic dyes, and pharmaceuticals, even at low concentrations (Mohan & Pittman, 2007).
- **Increased Catalytic Activity and Reactivity:** The high density of active surface sites and quantum effects can significantly enhance the catalytic efficiency of nanoparticles, enabling faster and more complete degradation of recalcitrant organic pollutants through processes like photocatalysis and Fenton-like reactions.

- **Tunable Optical and Electronic Properties:** These properties are crucial for photocatalytic applications, where nanomaterials absorb light energy to generate reactive oxygen species (ROS) that degrade pollutants.
- **Antimicrobial Properties:** Certain metal nanoparticles (e.g., silver, copper, zinc oxide) exhibit strong antimicrobial activity, making them effective for disinfection and biofouling control in membrane systems.
- **Magnetic Separability:** Incorporating magnetic properties (e.g., using iron oxide nanoparticles) allows for easy separation and recovery of nanomaterials after treatment, addressing a major challenge in nanoparticle applications.

3.3. Mechanisms of Pollutant Removal by Nanomaterials

Nanomaterials remove pollutants through several key mechanisms:

- **Adsorption:** Pollutants bind to the surface of nanomaterials through various interactions, including electrostatic attraction, van der Waals forces, hydrogen bonding, and surface complexation. This is a primary mechanism for removing heavy metals, dyes, and organic compounds.
- **Photocatalysis:** Semiconductor nanomaterials (e.g., TiO2, ZnO) absorb light energy (UV or visible light) to generate electron-hole pairs. These charge carriers react with water and oxygen to produce highly reactive oxygen species (ROS) such such as hydroxyl radicals (·OH), superoxide radicals ($O2\cdot^-$), and hydrogen peroxide (H2O2). These ROS are powerful oxidants that can mineralize (break down into CO2 and H2O) a wide range of organic pollutants (Fujishima et al., 2008).
- **Fenton/Fenton-like Reactions:** Iron-based nanomaterials (e.g., nZVI, Fe3O4) can catalyze the decomposition of hydrogen peroxide to generate highly reactive hydroxyl radicals (·OH), which are potent oxidants for pollutant degradation. This process can occur under mild conditions and is effective for a broad spectrum of organic contaminants (Zhang, 2003).
- **Membrane Filtration:** Nanomaterials can be incorporated into conventional membrane matrices to create nanocomposite membranes (NCMs). These NCMs offer improved permeability, enhanced rejection rates for specific pollutants (due to smaller pore sizes or specific interactions), and superior anti-fouling properties (due to antimicrobial activity or modified surface hydrophilicity) (El-Bourawi et al., 2007).
- **Disinfection:** Certain nanomaterials, particularly silver and copper nanoparticles, exert antimicrobial effects by damaging bacterial cell membranes, interfering with cellular respiration, or generating ROS, leading to the inactivation of pathogens (Rai et al., 2009).
- **Redox Reactions:** Nanoscale zero-valent iron (nZVI) is a strong reducing agent that can directly reduce various contaminants, including chlorinated organic compounds (e.g., trichloroethylene), nitrates, and heavy metals (e.g., Cr(VI) to Cr(III)) (Zhang, 2003).

4. Types of Nanomaterials and Their Applications in Water Treatment

4.1. Carbon-Based Nanomaterials (CBNs)

Carbon-based nanomaterials, including carbon nanotubes (CNTs), graphene, and graphene oxide (GO), have garnered significant attention due to their exceptional physical and chemical properties, making them highly effective adsorbents and catalytic supports.

4.1.1. Carbon Nanotubes (CNTs)

CNTs are cylindrical nanostructures composed of rolled-up sheets of graphene, exhibiting high aspect ratios, remarkable mechanical strength, excellent electrical conductivity, and an exceptionally high surface area.

Properties: Single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) offer large specific surface areas (typically 100-1000 m^2/g), high porosity, and the ability to be functionalized with various chemical groups.

Applications:

Adsorption: CNTs are highly effective adsorbents for a wide range of pollutants, including heavy metal ions (e.g., Pb(II), Cd(II), Cu(II)), organic dyes, pharmaceuticals, and pesticides. Their porous structure and strong adsorption sites facilitate efficient removal even at low concentrations (Ren et al., 2011).

Membranes: CNTs can be incorporated into polymer membranes to enhance water flux and improve contaminant rejection. The smooth inner walls of CNTs can facilitate rapid water transport, while their small diameter can act as a selective barrier for larger molecules.

Catalysis: Functionalized CNTs can serve as excellent supports for catalysts in various degradation processes.

4.1.2. Graphene and Graphene Oxide (GO)

Graphene is a single layer of carbon atoms arranged in a two-dimensional hexagonal lattice, possessing extraordinary mechanical, electrical, and thermal properties. Graphene oxide (GO) is a derivative of graphene that contains various oxygen-containing functional groups (hydroxyl, epoxy, carboxyl) on its basal planes and edges, making it highly hydrophilic and easily dispersible in water.

Properties: Graphene boasts a theoretical specific surface area of 2630 m^2/g, while GO's surface area is also very high. The presence of oxygen functional groups on GO provides abundant active sites for chemical reactions and strong electrostatic interactions with pollutants.

Applications:

Adsorption: Both graphene and GO are superior adsorbents. GO, in particular, due to its functional groups, shows excellent adsorption capacity for heavy metals via chelation and electrostatic interactions, and for organic pollutants through $\pi-\pi$ stacking, hydrogen bonding, and hydrophobic interactions (Wang et al., 2011).

Membrane Filtration: GO nanosheets can be assembled into lamellar membranes that exhibit excellent water permeability and selective rejection of ions and molecules. The interlayer spacing can be precisely controlled, allowing for highly efficient nanofiltration and even reverse osmosis-like performance.

Photocatalysis: Graphene and GO can act as electron acceptors and transporters in composite photocatalysts (e.g., TiO2-graphene), enhancing charge separation and improving photocatalytic efficiency for pollutant degradation under light irradiation (Fan et al., 2011).

Sensors: The electrical properties of graphene make it suitable for developing highly sensitive electrochemical sensors for detecting trace contaminants in water.

4.2. Metal and Metal Oxide Nanoparticles

Metal and metal oxide nanoparticles are widely explored for water treatment due to their diverse chemical reactivities, catalytic properties, and antimicrobial effects.

4.2.1. Titanium Dioxide (TiO2) Nanoparticles

TiO2 is one of the most extensively studied photocatalysts due to its high efficiency, chemical stability, non-toxicity, and low cost.

Properties: TiO2 exists in several crystalline forms (anatase, rutile, brookite), with anatase being the most photocatalytically active. When irradiated with UV light (energy greater than its bandgap, ~3.2 eV for anatase), TiO2 generates electron-hole pairs.

Applications:
Photocatalytic Degradation: TiO2 nanoparticles are highly effective in degrading a wide range of organic pollutants, including dyes, pharmaceuticals, pesticides, and phenols, into less harmful or completely mineralized products (CO2 and H2O). The generated hydroxyl radicals (·OH) are potent oxidants (Fujishima et al., 2008).
Disinfection: TiO2 photocatalysis can effectively inactivate bacteria, viruses, and other pathogens by damaging their cell membranes and intracellular components.
Self-Cleaning Surfaces: TiO2 coatings can be applied to surfaces (e.g., membranes, pipes) to prevent biofouling and maintain cleanliness.

4.2.2. Iron-Based Nanoparticles (nZVI, Fe3O4)

Iron-based nanomaterials are particularly attractive due to their strong reducing power, magnetic properties, and relatively low toxicity.
Properties: Nanoscale zero-valent iron (nZVI) is a powerful reducing agent, capable of directly reacting with and degrading various contaminants. Iron oxide nanoparticles (e.g., magnetite, Fe3O4) are superparamagnetic, allowing for easy separation from treated water using an external magnetic field.
Applications:
Reductive Degradation: nZVI is highly effective for the reductive dechlorination of chlorinated organic compounds (e.g., trichloroethylene, perchloroethylene), reduction of nitrates to nitrogen gas, and reduction of toxic heavy metal ions (e.g., Cr(VI) to less mobile and toxic Cr(III)) (Zhang, 2003).
Adsorption: Fe3O4 nanoparticles, especially when functionalized, exhibit high adsorption capacities for heavy metals (e.g., arsenic, lead) and organic pollutants due to their large surface area and surface functional groups. Their magnetic nature simplifies separation after adsorption.
Fenton-like Catalysis: Fe3O4 and other iron oxides can catalyze the decomposition of hydrogen peroxide in Fenton-like reactions, generating highly reactive hydroxyl radicals for the oxidative degradation of organic pollutants (Gong et al., 2012).

4.3. Nanomaterial-Enhanced Membranes

The integration of nanomaterials into traditional membrane matrices has led to the development of nanocomposite membranes (NCMs) or mixed-matrix membranes, offering significant improvements in performance.
Fabrication: Nanomaterials (e.g., CNTs, GO, TiO2, Ag nanoparticles) can be embedded within the membrane polymer matrix or coated onto the membrane surface during fabrication.
Improved Flux and Rejection: NCMs often exhibit higher water flux due to increased porosity or reduced tortuosity, while maintaining or improving rejection rates for contaminants. For instance, GO membranes can achieve high rejection of salts and organic molecules due to their precisely controlled interlayer spacing (Lee et al., 2013).
Enhanced Anti-Fouling Properties: The incorporation of antimicrobial nanoparticles (e.g., silver, TiO2) can inhibit microbial growth on the membrane surface, reducing biofouling. Hydrophilic nanomaterials (e.g., GO, TiO2) can also make the membrane surface more resistant to organic fouling.

Catalytic Membranes: Catalytic nanoparticles embedded in membranes can simultaneously filter and degrade pollutants, offering a synergistic approach to water treatment. For example, TiO2-embedded membranes can perform photocatalytic degradation of organic pollutants while filtering out suspended solids.
Forward Osmosis (FO) Membranes: Nanomaterials can enhance the performance of FO membranes by improving water flux and reducing reverse salt flux, making FO a more viable option for low-energy desalination and wastewater treatment.

5. Novel Approaches and Hybrid Systems

The true power of nanomaterials in water treatment often lies in their integration into more complex and synergistic systems.

5.1. Advanced Oxidation Processes (AOPs) with Nanomaterials

AOPs are highly effective for degrading recalcitrant organic pollutants by generating highly reactive species, primarily hydroxyl radicals (·OH). Nanomaterials significantly enhance AOPs:
Heterogeneous Photocatalysis: Beyond pure TiO2, composite photocatalysts (e.g., g-C3N4, BiVO4, or their composites with graphene) extend light absorption into the visible spectrum and improve charge separation, leading to higher efficiency in degrading persistent organic pollutants under solar light (Wang et al., 2017).
Nano-Fenton and Photo-Fenton Processes: Magnetic iron oxide nanoparticles (Fe3O4) can act as catalysts for Fenton-like reactions, generating ·OH from H2O2. Their magnetic nature allows for easy separation and reuse, overcoming the sludge generation issue of homogeneous Fenton processes. Photo-Fenton processes combine UV light with iron catalysts and H2O2 to further enhance radical generation.
Peroxymonosulfate/Persulfate Activation: Various nanomaterials (e.g., cobalt oxides, carbon nanomaterials, iron-based nanoparticles) can activate peroxymonosulfate (PMS) or persulfate (PS) to produce sulfate radicals (SO4·−), which are powerful and long-lived oxidants effective against a wide range of organic contaminants (Gong et al., 2013).

5.2. Magnetic Nanomaterials for Easy Separation

One of the major challenges in using nanoparticles is their separation from treated water. Magnetic nanomaterials offer an elegant solution.
Integration: Magnetic nanoparticles, typically iron oxides (Fe3O4, γ-Fe2O3), can be synthesized as core-shell structures with other active nanomaterials (e.g., Fe3O4@TiO2, Fe3O4@GO).
Application: After the treatment process (adsorption or catalysis), the composite nanomaterials can be easily retrieved from the water using an external magnetic field, preventing secondary pollution and enabling material reuse. This significantly reduces operational costs and simplifies post-treatment separation (Shen et al., 2009).

5.3. Bio-Nanomaterial Hybrids

Combining the catalytic power of nanomaterials with the biological capabilities of microorganisms or enzymes offers synergistic advantages.
Enhanced Bioremediation: Nanomaterials can act as electron shuttles or nutrient delivery systems to enhance the activity of pollutant-degrading microorganisms. For instance, nZVI can create anaerobic conditions favorable for certain microbial degradation pathways.
Enzyme Immobilization: Enzymes (e.g., laccase, peroxidase) can be immobilized onto nanomaterial supports (e.g., CNTs, magnetic nanoparticles) to improve their stability,

reusability, and catalytic efficiency for degrading organic pollutants (e.g., dyes, phenols) (Bilal et al., 2017).

5.4. Nanomaterial-Based Sensors for Water Quality Monitoring

Beyond remediation, nanomaterials are revolutionizing water quality monitoring by enabling highly sensitive, selective, and real-time detection of pollutants.

Electrochemical Sensors: Graphene, CNTs, and metal nanoparticles can modify electrodes to enhance their sensitivity and selectivity for detecting heavy metals, organic compounds, and pathogens at very low concentrations.

Optical Sensors: Quantum dots and plasmonic nanoparticles (Au, Ag) exhibit unique optical properties that change in the presence of specific contaminants, allowing for rapid and portable detection systems.

Biosensors: Integrating biological recognition elements (e.g., antibodies, DNA, enzymes) with nanomaterials creates biosensors for the rapid and accurate detection of pathogens, toxins, and specific organic pollutants (Wang, 2005).

6. Challenges and Environmental Implications

Despite their immense potential, the widespread application of nanomaterials in water treatment faces several significant challenges that need to be addressed.

6.1. Synthesis and Scalability Challenges

Cost-Effectiveness: Many advanced nanomaterials are currently expensive to synthesize, especially using methods that yield precise control over size, shape, and purity. Reducing production costs is crucial for commercial viability.

Mass Production: Scaling up laboratory-scale synthesis methods to industrial production levels while maintaining consistent quality and properties remains a significant hurdle.

Environmental Friendliness of Synthesis: Traditional synthesis methods often involve hazardous chemicals and generate toxic by-products. Developing "green synthesis" routes (e.g., using plant extracts, microorganisms) is essential to ensure the sustainability of nanomaterial production itself (Sintubin et al., 2012).

6.2. Stability and Longevity of Nanomaterials

Aggregation: Nanoparticles have a high surface energy, making them prone to aggregation in aqueous solutions, which can reduce their effective surface area, diminish their reactivity, and lead to settling, thus hindering their performance. Surface modification or stabilization techniques are often required.

Leaching: The release of constituent ions (e.g., Ag+ from silver nanoparticles, metal ions from metal oxide nanoparticles) into the treated water can introduce new forms of contamination and raise toxicity concerns.

Loss of Activity: Over time, nanomaterials can lose their activity due to fouling, surface passivation, or structural degradation, necessitating regeneration or replacement. Developing robust and regenerable nanomaterials is critical for long-term applications.

6.3. Potential Environmental and Health Risks (Ecotoxicity)

This is perhaps the most critical challenge and a major area of ongoing research. The unique properties that make nanomaterials effective for remediation can also pose potential risks if they are released into the environment.

Ecotoxicity: Studies have shown that certain nanomaterials (e.g., silver, TiO2, ZnO nanoparticles) can exhibit toxicity to aquatic organisms (algae, daphnia, fish) and

microorganisms at certain concentrations, affecting their growth, reproduction, and physiological functions (Handy et al., 2008).

Bioaccumulation and Biomagnification: There is concern that nanomaterials could accumulate in organisms and potentially biomagnify up the food chain, leading to long-term ecological impacts.

Human Health Impacts: While direct exposure in water treatment is generally limited, potential inhalation of airborne nanoparticles during handling or exposure through treated water (if not fully removed) needs thorough assessment. The long-term effects of chronic low-level exposure are still largely unknown.

Transformation in the Environment: Nanomaterials can undergo various transformations (e.g., aggregation, dissolution, surface coating, functionalization) in complex environmental matrices, altering their properties and potentially their toxicity (Lowry et al., 2010).

6.4. Regulatory and Policy Landscape

Lack of Specific Regulations: Current environmental regulations are often based on bulk material properties and do not adequately address the unique characteristics and potential risks of nanomaterials.

Risk Assessment Frameworks: Developing robust and standardized risk assessment methodologies for nanomaterials is crucial, considering their diverse properties and potential exposure pathways.

Public Perception: Public acceptance and trust in nanotechnology applications in drinking water treatment will depend heavily on transparent communication regarding risks and benefits, supported by sound scientific evidence and clear regulatory oversight.

7. Future Perspectives and Research Directions

To fully harness the potential of nanomaterials for sustainable water and wastewater treatment, future research and development efforts should focus on several key areas:

7.1. Development of Multifunctional and Smart Nanomaterials

Synergistic Design: Designing single nanomaterials or hybrid systems that combine multiple functionalities (e.g., adsorption + photocatalysis + magnetic separability) to address complex pollutant mixtures more efficiently.

Responsive Materials: Developing "smart" nanomaterials that can respond to external stimuli (e.g., pH, temperature, light, magnetic field) to trigger or cease their activity, allowing for on-demand treatment and controlled release.

Self-Healing and Regenerable Materials: Research into materials that can self-repair or be easily regenerated *in situ* to extend their lifespan and reduce operational costs.

7.2. Focus on Green and Sustainable Nanotechnology

Biologically Inspired Synthesis: Expanding research into "green synthesis" methods using biological entities (e.g., plants, bacteria, fungi) to produce nanomaterials. These methods are often more environmentally friendly, cost-effective, and can yield nanomaterials with unique properties (Sintubin et al., 2012).

Waste-to-Nanomaterial Approaches: Exploring the synthesis of valuable nanomaterials from waste streams (e.g., agricultural waste, industrial by-products) to promote circular economy principles.

Life Cycle Assessment (LCA): Conducting comprehensive LCAs for nanomaterial-based water treatment technologies to evaluate their environmental footprint from raw material extraction to disposal, ensuring that the "solution" does not create new problems.

7.3. Integration with Existing Infrastructure and Pilot-Scale Studies

Hybrid Systems: Developing and optimizing hybrid systems that integrate nanomaterial-based processes with conventional treatment technologies (e.g., nano-enhanced membranes with biological treatment, photocatalytic reactors as tertiary treatment) to achieve optimal performance and cost-effectiveness.

Pilot-Scale and Full-Scale Implementation: Moving beyond laboratory-scale studies to pilot-scale demonstrations and eventually full-scale implementation to assess feasibility, performance under real-world conditions, and long-term stability. This requires significant investment and collaboration between academia, industry, and government.

7.4. Advanced Characterization and Modeling

In-Situ Characterization: Developing advanced analytical techniques for *in-situ* and *operando* characterization of nanomaterials during treatment processes to better understand reaction mechanisms, surface interactions, and degradation pathways.

Computational Modeling: Utilizing computational chemistry and machine learning to predict nanomaterial properties, optimize synthesis parameters, model pollutant interactions, and forecast environmental behavior, thereby accelerating material discovery and design.

7.5. Economic Viability and Regulatory Frameworks

Cost-Benefit Analysis: Performing thorough economic analyses to demonstrate the long-term cost-effectiveness of nanomaterial-based solutions, considering reduced chemical consumption, lower energy use, and improved water quality.

Robust Regulatory Frameworks: Developing clear, science-based regulatory guidelines for the safe production, use, and disposal of nanomaterials in water treatment. This includes establishing exposure limits, monitoring protocols, and risk management strategies to build public trust and ensure environmental safety.

Public Engagement: Fostering open dialogue and public engagement to address concerns, disseminate accurate information, and build societal acceptance for nanotechnology applications in water management.

8. Conclusion

The global water crisis demands innovative and sustainable solutions, and nanotechnology offers a compelling pathway to address the limitations of conventional water and wastewater treatment methods. Nanomaterials, with their unparalleled surface area, enhanced reactivity, and diverse functionalities, have demonstrated remarkable capabilities in the efficient removal and degradation of a wide spectrum of pollutants, including heavy metals, organic contaminants, and emerging micropollutants. From highly adsorptive carbon-based materials to potent photocatalytic metal oxides and advanced nanocomposite membranes, the versatility of nanomaterials is transforming the landscape of water purification.

However, realizing the full potential of these technologies hinges on overcoming significant challenges. These include the need for cost-effective and scalable synthesis methods, ensuring the long-term stability and recyclability of nanomaterials, and critically, conducting comprehensive assessments of their potential environmental and health implications. The responsible development of nanotechnology necessitates a strong emphasis on green synthesis, robust risk assessment frameworks, and clear regulatory guidelines to ensure that these advanced solutions are not only effective but also inherently safe and sustainable.

Looking ahead, future research should prioritize the development of multifunctional and smart nanomaterials, the integration of nano-based systems into existing water infrastructure, and the

continued refinement of characterization and modeling tools. By fostering interdisciplinary collaboration among scientists, engineers, policymakers, and industry stakeholders, we can collectively advance the responsible deployment of nanotechnology, paving the way for a cleaner, healthier, and more water-secure future for all. The transformative promise of nanomaterials in environmental remediation is undeniable, and with continued dedicated effort, they are poised to play a pivotal role in safeguarding our planet's most vital resource.

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Structural Elucidation of Flavonoids from Plant Extracts: A Multi-Spectroscopic Approach Using UV-Vis, IR, and NMR Spectroscopy

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Abstract: *Flavonoids are a diverse and biologically important class of polyphenolic compounds widely distributed throughout the plant kingdom, recognized for their extensive range of therapeutic properties, including antioxidant, anti-inflammatory, antimicrobial, and anticancer activities. The structural characterization of these natural compounds is crucial not only for understanding their mechanisms of bioactivity but also for guiding the development of novel pharmaceuticals and nutraceuticals. This paper presents a comprehensive overview of a multi-spectroscopic approach for the detailed structural elucidation of flavonoids isolated from plant extracts. The proposed methodology integrates three complementary and powerful techniques: UV-Visible (UV-Vis) spectroscopy, which enables rapid identification of flavonoid subclasses and their substitution patterns; Infrared (IR) spectroscopy, which provides valuable insights into the presence and nature of functional groups; and Nuclear Magnetic Resonance (NMR) spectroscopy, including both one-dimensional (1D) and two-dimensional (2D) techniques, for the definitive determination of molecular structure, covering the carbon framework, substitution sites, interatomic connectivity, and stereochemistry. The synergistic application of these analytical tools offers a robust, reliable, and efficient workflow for the unambiguous characterization of both known and novel flavonoid compounds, facilitating advancements in phytochemical research and drug discovery.*

Keywords: *Flavonoids, Structural Elucidation, Spectroscopic Methods, UV-Visible Spectroscopy, Infrared (IR) Spectroscopy, Nuclear Magnetic Resonance (NMR) Spectroscopy, 1D NMR, 2D NMR, COSY, HMBC, HSQC, Natural Products, Plant Extracts, Chemical Analysis, Quercetin, Rutin.*

1. INTRODUCTION

Flavonoids are a major group of plant-derived secondary metabolites that share a common C6-C3-C6 carbon skeleton, consisting of two aromatic benzene rings (designated A and B) linked by a three-carbon heterocyclic ring (C). Based on the oxidation and saturation level of the central C-ring, flavonoids are broadly classified into several subclasses, such as flavanols, flavones, flavanones, isoflavonoids, neoflavones, and anthocyanidins. This structural diversity is further enhanced by various modifications such as hydroxylation, methylation, acylation, phenylation, and glycosylation, which significantly affect their solubility, stability, and bioactivity. Due to their ubiquitous presence in the plant kingdom and a wide range of pharmacological activities such as antioxidant, anti-inflammatory, anticancer and

cardioprotective effects - accurate, rapid and detailed elucidation of their molecular structures is a key and ongoing challenge in the field of natural product chemistry and drug discovery.

Traditional methods of structural elucidation of natural products often rely heavily on a combination of chemical decomposition, derivatization, and chromatographic separation techniques. Although these approaches are basic, they are generally laborious and time-consuming, and require relatively large sample sizes, which is impractical for rare or volatile compounds. The advent and improvement of modern spectroscopic techniques have revolutionized this field, making possible the rapid, accurate, and nondestructive analysis of minute quantities of complex molecules. Among these, mass spectrometry (MS) emerges as a powerful analytical tool for determining molecular weights, elemental compositions, and fragmentation patterns. However, MS alone often proves inadequate in the case of complete structural determination of closely related isomeric compounds or complex natural mixtures. Therefore, a comprehensive, multi-spectroscopic approach – taking advantage of the strengths of various complementary methods – is of utmost importance for achieving comprehensive structural elucidation. This paper emphasizes the systematic and synergistic application of ultraviolet-visible (UV-Vis), infrared (IR) and nuclear magnetic resonance (NMR) spectroscopy, which together provide crucial information about functional groups, conjugation patterns and molecular structures. The simultaneous use of these techniques creates a robust analytical platform for the detailed and accurate determination of flavonoid structures isolated from natural sources.

2. Materials and Methods

2.1. Plant Material and Extraction A representative plant material rich in flavonoids, such as lemon peel, tea leaves, papaya shoots, or guava leaves, is selected based on its traditional use and phytochemical potential. The collected plant material is cleaned thoroughly, shade-dried to preserve heat-sensitive compounds, and finely powdered to increase the surface area for extraction. The dried sample is extracted using a suitable solvent system, usually 80% methanol or ethanol, by maceration at room temperature or by Soxhlet extraction under controlled conditions to ensure maximum recovery of bioactive components. The resulting crude extract is filtered, concentrated under reduced pressure, and then subjected to solvent-solvent separation (e.g., with ethyl acetate or butanol) to separate different fractions based on polarity. Further purification of the flavonoid-rich fractions is carried out using chromatographic techniques such as column chromatography (using silica gel or Sephadex LH-20 as stationary phases) and preparative high-performance liquid chromatography (HPLC). These techniques facilitate the separation and enrichment of individual pure flavonoid compounds, which are then subjected to structural elucidation and biological activity evaluation.

2.2. UV-Visible Spectroscopy To prepare a concentrated solution suitable for spectroscopic analysis, a small quantity of the purified flavonoid compound is accurately weighed and dissolved in a suitable solvent, usually methanol or ethanol. The UV-visible absorption spectrum of the solution is recorded using a UV-vis spectrophotometer in the wavelength range of 200-400 nm. Flavonoids usually exhibit two characteristic absorption bands in their spectrum: band I, observed in the range of 300-400 nm, is associated with the cinnamoyl system, corresponding to the B-ring and the conjugated C-ring; While band II, which appears in the range of 240-280 nm, belongs to the benzoyl system. To gain deeper information about the location and nature of hydroxyl groups and other substituents on the flavonoid structure, shift reagents such as aluminum chloride ($AlCl_3$), sodium acetate (CH_3COONa), and

hydrochloric acid (HCl) are systematically added to the flavonoid solution. The resulting bathochromic (red) or hypsochromic (blue) shifts in the absorption maximum are carefully monitored and interpreted. These shifts provide valuable information about the location of hydroxyl groups, chelation sites, and the extent of conjugation, thereby aiding in the structural elucidation of the flavonoid compound.

2.3. Infrared (IR) Spectroscopy The IR spectrum of the pure compound is recorded using a Fourier transform infrared (FTIR) spectrometer, which provides detailed information about the molecular vibrations and functional groups present in the compound. For analysis, the sample can be prepared as a potassium bromide (KBr) pellet or as a thin film, depending on its physical properties and solubility. The resulting spectrum is carefully analyzed for specific absorption bands corresponding to the functionalities of the major functional groups found in flavonoids, such as hydroxyl (–OH), carbonyl (C=O), aromatic C=C, and ether (C–O–C). These bands help confirm the presence and nature of the flavonoid structure and support data obtained from other spectroscopic techniques.

2.4. Nuclear Magnetic Resonance (NMR) Spectroscopy: Nuclear magnetic resonance (NMR) spectroscopy is considered one of the most powerful and reliable analytical techniques for the definitive structural elucidation of organic compounds.NMR spectroscopy is the most powerful technique for definitive structural elucidation.

Sample Preparation: The purified flavonoid compound is carefully dissolved in a suitable deuterated solvent, such as deuterated methanol (CD_3OD), deuterated chloroform ($CDCl_3$), or dimethyl sulfoxide-d_6 (DMSO-d_6), depending on its solubility and chemical compatibility. The use of a deuterated solvent in NMR spectroscopy is essential to avoid interference from hydrogen atoms in the solvent, thereby obtaining a clear and interference-free spectrum. Additionally, the deuterated solvent serves as an internal lock signal for the spectrometer, ensuring high-resolution and stable spectral acquisition. This step is critical in sample preparation for accurate and reliable NMR analysis.

1D NMR: One-dimensional ^{1}H NMR and ^{13}C NMR spectra are essential for structural analysis. The chemical displacements, coupling constants and signal integration observed in the ^{1}H NMR spectrum provide valuable information about the number of hydrogen atoms (protons), their chemical environment and the nature of their neighbouring atoms. On the other hand, the ^{13}C NMR spectrum provides information about the number and type of non-equivalent carbon atoms present in the molecule[1].

2D NMR: Two-dimensional NMR experiments are important for accurately assigning all proton and carbon signals, as well as determining the valency and spatial relationships within the molecule. Key experiments include:

COSY (Correlation Spectroscopy): It identifies protons that are attached to each other, usually those on adjacent carbon atoms, providing insight into the connectivity and structure of the molecule.

HSQC (Heteronuclear Single Quantum Coherence): Correlates each proton with the specific carbon atom to which it is directly bonded, allowing for precise determination of proton-carbon connectivity within the molecule.

HMBC (Heteronuclear Multiple Bond Correlation): Correlates protons with carbon atoms two or three bonds apart, it provides crucial long-range connectivity information linking different parts of the molecule and helps in constructing the complete carbon framework and identifying functional group relationships.

NOESY (Nuclear Overhauser Effect Spectroscopy): It provides detailed information about the stereochemistry, conformational preferences, and spatial proximity of the nuclei of the various components of the molecule, which helps in determining the relative three-dimensional orientation within its molecular structure

3. Results and Discussion: The structural elucidation process is a step-by-step assembly of detailed molecular information gathered from each spectroscopic technique.

3.1. UV-Vis Spectral Analysis: The initial analysis of the UV-Vis spectrum provides a basic classification of the flavonoid based on its characteristic absorption bands and conjugation patterns.

Flavones and Flavanols: Exhibit a characteristic Band I between 320-380 nm and Band II between 250-280 nm.

Flavanones and Flavonols: Show a blue-shifted Band I and a strong Band II due to the lack of conjugation.

Isoflavones: Exhibit a characteristic spectrum with a maximum at ~260 nm.

The use of shift reagents provides specific and valuable information regarding the hydroxylation pattern of the flavonoid structure. For example, the bathochromic shift of band I upon addition of $AlCl_3$ indicates the presence of a hydroxyl group at the C-5 position due to chelation effects. Similarly, the shift observed with CH_3COONa indicates the presence of a free hydroxyl group at the C-7 position. This basic spectral analysis serves as an important foundation, providing initial structural insights that effectively guide and complement subsequent, more sophisticated and detailed spectroscopic studies such as NMR and MS.

3.2. IR Spectral Analysis: The IR spectrum serves as a rapid and informative tool for identifying functional groups in a compound. The broad absorption band observed in the range of 3300–3500 cm^{-1} usually indicates the presence of hydroxyl (-OH) groups, often associated with hydrogen bonding. The strong and sharp signal appearing around 1650–1690 cm^{-1} is characteristic of the carbonyl (C=O) stretching vibration, which is commonly found in ketones, aldehydes, or esters. The C=C stretching vibrations of aromatic rings are usually found in the region of 1500–1600 cm^{-1}, which supports the presence of an aromatic system. Additional bands related to C-O-C asymmetric and symmetric stretching near ~1200 cm^{-1} and C-H stretching vibrations in the region of 2800–3100 cm^{-1} further confirm the presence of aromatic structures and other key functional groups in the compound.

3.3. NMR Spectral Analysis: NMR spectroscopy provides the most detailed and accurate structural information available to elucidate the complete molecular structure, including atomic connectivity, functional group positions, and stereochemistry.

1D NMR: The ^{1}H NMR spectrum gives out the aromatic nature of the compound, with characteristic signals typically appearing between 6.0 and 8.0 ppm. The presence of single or paired signals in this region provides insight into the substitution pattern on the A and B rings. For example, a para-substituted B-ring will display a symmetric pattern of two doublets due to the electronic environment of the protons[2]. Signals from sugar protons (in glycosidic flavonoids) are typically observed between 3.0 and 5.5 ppm, with the anomeric proton signal (usually a doublet) serving as a key indicator of glycosylation and helping to determine the type and linkage of the sugar moiety. The ^{13}C NMR spectrum provides the total number of carbon atoms, and their chemical shifts provide valuable information about their hybridization state (e.g., sp, sp^2, sp^3) and surrounding electronic environment, thereby aiding in the complete determination of the carbon framework.

2D NMR: 2D NMR data serves as a cornerstone of the structural elucidation process, providing important long-range and bond-to-bond connectivity information. The HSQC (heteronuclear single quantum coherence) spectrum correlates each proton with its directly attached carbon, allowing for the unambiguous assignment of each C-H group in the molecule. The HMBC (heteronuclear multiple bond correlation) spectrum is used to "connect the dots" by revealing correlations between protons and carbons two to three bonds apart. For example, a proton on a particular aromatic carbon shows long-range coupling to a carbonyl carbon or quaternary carbon, thereby confirming the molecular framework. In the case of a flavonoid glycoside, the HMBC correlation from the anomeric proton of the sugar unit to a specific carbon on the flavonoid backbone (such as C-7) unambiguously establishes the point of attachment and the type of glycosidic linkage[3]. By integrating data from all 2D NMR experiments, such as COSY, HSQC, and HMBC, the complete carbon-hydrogen framework, along with the location of all functional groups, can be determined confidently and unambiguously.

4. Case Study: Elucidation of Quercetin-3-O-rutinoside (Rutin)

UV-Vis Spectroscopy: The **UV-Vis spectrum** prominently displayed two characteristic absorption maxima: **Band I at 357 nm** and **Band II at 257 nm**. These specific absorption patterns are highly indicative of a **flavonol** skeleton. Upon the strategic addition of **aluminum chloride ($AlCl_3$)**, a significant **bathochromic shift** was observed for both bands. This shift strongly suggests the presence of **free hydroxyl groups** at both the C-5 and C-7 positions within the flavonoid structure, a common feature in many flavonols.

Infrared (IR) Spectroscopy

The **infrared spectrum** provided further supporting evidence for the proposed flavonol structure. A broad and intense absorption band was observed at **3380 cm−1**, which is characteristic of **O-H stretching vibrations**, confirming the presence of hydroxyl groups. Additionally, a strong and sharp band at **1655 cm−1** was identified, corresponding to the **C=O stretching vibration** of the carbonyl group typically found in flavonols[4].

Nuclear Magnetic Resonance (NMR) Spectroscopy:

^{1}H NMR: The **Proton NMR spectrum** provided detailed insights into the proton environment of the molecule. Signals indicative of an **ABX spin system** were clearly observed for the protons on the **B-ring (H-2', H-5', and H-6')**, characteristic of a substituted aromatic ring. Furthermore, a distinct **singlet** was identified for the **A-ring protons (H-6 and H-8)**,

suggesting an unsubstituted pattern at these positions. A crucial signal at **5.3 ppm** was unambiguously assigned to the **anomeric proton of the sugar moiety**, confirming its glycosidic linkage.

^{13}C NMR: The **^{13}C NMR spectrum** revealed the presence of **27 distinct carbon signals**. This count is consistent with a **flavonoid aglycone** combined with a **disaccharide** unit, providing strong preliminary evidence for the overall molecular framework.

Two-Dimensional Nuclear Magnetic Resonance (2D NMR): Further elucidation of the connectivity was achieved through **2D NMR experiments**. The **HMBC (Heteronuclear Multiple Bond Correlation) spectrum**[5] was particularly informative, showing two pivotal correlations. A key correlation was observed from the **anomeric proton of the rhamnosyl residue to C-1'' of the rutinosyl moiety**, establishing the linkage between the two sugar units. Even more critically, another significant correlation was identified from the **anomeric proton of the rutinosyl moiety to C-3 of the quercetin skeleton**.

These unambiguous correlations definitively established the structure as **Quercetin-3-O-rutinoside**, also commonly known as Rutin.

5. Conclusion

Structural elucidation of novel flavonoids from complex plant extracts requires a systematic and comprehensive approach. By seamlessly integrating data from UV-Vis, IR and NMR spectroscopic techniques, complete and unambiguous determination of molecular structure can be reliably achieved. UV-Vis spectroscopy provides a rapid preliminary classification of flavonoid subclasses and initial insight into hydroxylation patterns. IR spectroscopy effectively confirms which functional groups are present. Finally, the combined power of 1D and 2D NMR spectroscopy provides a definitive, atomic-level blueprint of the molecule, revealing complex valencies[6]. This multi-spectroscopic strategy is the cornerstone of modern natural product chemistry, significantly enabling the discovery and characterization of new compounds with potential therapeutic applications.

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Microbial Solutions to Environmental Challenges: Sustaining Ecosystem Services Through Biodiversity

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Abstract: *The purpose of this research is to clarify the complex interactions that exist between microbial communities and ecosystem processes, highlighting how they influence nutrient cycling, biogeochemical cycles, and the resilience of entire ecosystems. We investigate the great diversity of microorganisms that live in a range of habitats, from soil to aquatic systems, and their functional roles in preserving the productivity and health of ecosystems, drawing on recent developments in sequencing technologies and metagenomic research. Human life depends on ecosystem functions, hence the subject of how biodiversity change of species in the crucial zone between Earth's canopies and bedrock relates to ecosystem functioning is urgent given the growing anthropogenic pressures on ecosystems worldwide.*

In particular, soils are essential for the cycling of nutrients, the growth of plants, the purification of water, the decomposition of litter, and the storage of carbon, all of which help to secure food and water supplies and stabilize the climate. Protists, fungus, bacteria, and archaea are among the complex groups of microorganisms that play a major role in soil processes. Microorganisms are found almost everywhere in the planet, making them ubiquitous. They are quite prevalent and have a big impact on the ecosystem. Decomposition, oxygen production, evolution, and symbiotic connections with plants are just a few of the essential functions that microorganisms play in ecosystems. The cycle of vital nutrients is caused by microbial enzymatic activity. Numerous factors, including appearance, physiology, genetics, and location, can be used to describe microbial diversity. We will talk about it in this paper.
Microbial diversity's functional role in maintaining environmental stability and ecosystem services.
Keywords: *Microbial Diversity, Sustaining Ecosystem Services, Environmental Stability, Microbial Communities, Nutrient Cycling, Soil, Plant Growth, Climate Change, Productivity, Essential Crops.*

1. INTRODUCTION:

The microscopic living things known as microorganisms can be either unicellular or multicellular. To put it simply, microbial diversity is the variance found in microorganisms. Diversity is the same as variation. The morphological, physiological, genetic, and geographic characteristics of this microbial diversity can all be used to describe it. Anything that varies falls under the category of diversity. Bacteria, Archaea, and Eukaryotes are the three categories

into which the various communities of microorganisms are divided. Microbes are categorized according to their morphological diversity, which includes different forms including unicellular, multicellular, rod-shaped, spherical, spiral, oval, flagellate, branching, and unbranched.

An essential element of Earth's ecosystems, microbial diversity is vital to preserving the health and functionality of these systems. Microbial diversity's importance in ecosystem function highlights the different ways that microorganisms affect the environment, nutrient cycling, and the stability of an ecosystem as a whole. [1]

These microbes include viruses, fungus, bacteria, archaea, and several single-celled eukaryotes. From the highest mountain summits to the deepest ocean trenches, from the blazing deserts to the frigid polar regions, microbes are remarkably diverse and present almost everywhere on Earth. Taxonomic diversity is only one aspect of microbial diversity. Functional diversity, which refers to the different metabolic capacities, behaviours, and interactions of microorganisms within a particular environment, is also included.

An incredibly understudied source of biodiversity on Earth is the world of microorganisms. It is a useful biological extreme that is being studied more thoroughly. The majority of Earth's biodiversity is found in microbes, which also contribute significantly to ecological processes and provide benefits that keep all life alive. The foundation of life on Earth is made up of microorganisms. They have developed into every possible niche on Earth over billions of years. The most abundant source of chemistry and molecular variety in nature is found in microorganisms, which also maintain vital connections with higher organisms and with one other while laying the groundwork for ecological processes including food chains and biogeochemical cycles.

Over the past ten years, the microbial world has attracted a lot of attention, and the findings have been astounding. According to reports, a significant amount of research over the last 20 years suggests that plant variety has a favourable relationship with ecosystem functioning. In contrast to plants, little is known about how microbial diversity and ecosystem functioning relate to one another, particularly in terrestrial settings. [2]

Microbes and Soil Sustainability

The biota of soil ecosystems, which includes bacteria, plants, and animals, is incredibly diverse and active. A very varied variety of microorganisms, including bacteria, fungus, archaea, protozoa, and algae, call the very heterogeneous matrix that is soil home. The "biological engine of the earth" that keeps soil functions and essential ecosystem processes going is the soil microbiota. Microbes are essential to many soil biological processes, energy fluxes, and the breakdown of harmful substances, making them a major factor in mitigating the effects of climate change.

An essential part of food webs, soil microbes control the bio-geochemical cycling of nutrients, including the nitrogen cycle, and, consequently, the availability of nutrients for the primary producers in the ecosystem.

The physical structure of the soil is altered by microorganisms to better withstand stress and perturbations, enabling more adaptable reactions to environmental changes than in communities with low diversity. Some microorganisms may be regarded as markers of soil health because of their significant contribution to soil sustainability. [3]

2. Review of Literature:

From utilizing or manipulating the metabolic capacities of single strains (like yeast fermentation) to complex communities (like methane generation), the phylogenetic and metabolic variety of microorganisms has been the source of significant biotechnological advancements (Escalante et al., 2015). However, a lot of focus has been placed on single strain cultures or engineered consortia in an effort to maximize yields and operational control. This has led to great success in the food and medical industries (such as the production of insulin, alcohol, and bread), but it has hampered progress in other industries that depend on more complex biochemical transformations that call for the coexistence of multiple microbial groups, or microbial functional diversity. [4]

Because of functional redundancy, niche complementation, and distinct response qualities to disturbances, it has been proposed that an increase in diversity components—that is, richness and evenness leads to greater stability and functional resilience. Microbial interactions are widely considered to be basic ecological processes that determine the assembly and function of microbial communities, despite the fact that there is hardly any agreement in this area (Li and Müller, 2023). Understanding the mechanisms underlying the diversity-function relationship can aid in the management of microbial communities, for instance in therapeutic, biotechnological, or bioremediation settings, as these communities perform crucial functions such as nutrient cycling, substrate degradation, and metabolite production. [5]

Many ecosystem services that support life on Earth are based on the diversity of microorganisms found in environmental microbiomes. These services include fostering the growth of plants, purifying contaminated areas, and preserving the equilibrium of atmospheric gasses like as methane and carbon dioxide. Thanks to developments in genomic techniques that make it possible to identify and analyze microbial communities in previously unattainable ways, the study of environmental microbiomes has expanded quickly (eAronson et al., 2013). In order to provide insight into the intricate relationships between these microbial communities and their significance for ecosystem health and human well-being, this study will examine the composition, diversity-influencing factors, ecological roles, and uses of environmental microbiomes. [6]

Because it supports important biogeochemical cycles like the carbon, nitrogen, sulfur, and phosphorus cycles, microbial diversity is essential to ecosystem function. The main players in the breakdown of organic matter are microorganisms, which reduce complicated chemicals into simpler ones that plants and other living things can use. For example, bacteria break down animal and plant waste in soil, recycling nutrients that plants require to develop. By breaking down organic matter and changing contaminants into less dangerous forms, microbes help maintain water quality, regulate nutrients, and remove trash from aquatic environments (Rai et al., 2011).[7]

Ecosystem stability and functionality depend on microbial diversity. Numerous biogeochemical processes, including soil fertility, waste decomposition, and nutrient cycling, are supported by diverse microbial communities and are essential to ecosystem services. The health of ecosystems may suffer greatly from the decrease of microbial diversity, which may interfere with these vital functions. Plant growth and agricultural output, for instance, may be impacted by decreased nutrient cycling caused by a loss in soil microbial diversity. According to (Philippot et al. 2013), the loss of beneficial microorganisms in aquatic environments can also result in the build-up of contaminants and deterioration of water quality.[8]

3.Objectives:

- To Study the Functional Role of Microbial Diversity in Sustaining Ecosystem Services
- To study Microbial Diversity in Environmental Stability
- To Explain Climate change
- To Explain The economic valuation of microbial diversity.

4.Research Methodology:

The study's findings are supported by secondary data gathered from reputable sources, such as books, periodicals, papers, and the internet. The application of microbial diversity's functional role in maintaining ecosystem services and environmental stability is covered in this article. The research design of the study is primarily descriptive. Readings from journals These reliable papers were located using search engine platforms such as Google Scholar, international business and economics journals, online educational resources, and other well-known websites.

5.Result and Discussion:

Microbial Diversity: In Preserved Ecosystems

Based on the habitat studied, only a small number of microbe species (0.1 to 10%) are currently known. Their vast diversity is the reason behind this. Since a microbial community appears to predominate in occurrence in each season, followed by other less sufficient communities that are frequently below the level of detection using the current methods of evaluation, the seasonal variations in microbe diversity in an Agroecosystem is still not fully understood. Because ecological activities including organic matter decomposition, nitrogen cycling, soil aggregation, and disease control must be maintained within the ecosystem, microbial diversity is particularly crucial to ecosystem operations.

Because little is known about the relationship between the structural and functional variety of these microorganisms, functional diversity is crucial when assessing their ecological status within the ecosystem. Nonetheless, there is general agreement that microbial diversity and ecological stability are intimately correlated.[9]

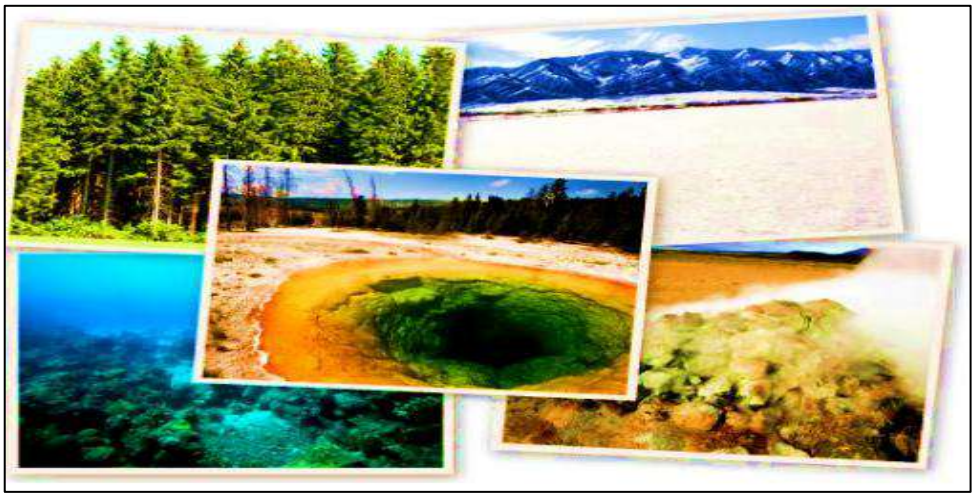

Figure 1: Microbes live everywhere—even in places we used to think were incompatible with life

Source: (http://www.learn.genetics.utah.edu/content/gsl/microbes/)

Microbial Responses to Environmental Changes:

The oldest, most varied, and possibly most resilient life forms on Earth are microorganisms. They have colonized almost every habitat, from the deep sea to the upper atmosphere, thanks to their capacity to adapt to a wide range of climatic conditions. However, microbial populations around the world face previously unheard-of difficulties due to the quick speed of environmental change brought on by human activity. Predicting ecosystem dynamics and developing methods to lessen the effects of global environmental change both depend on an understanding of how microorganisms react to these changes. From molecular and physiological alterations inside individual cells to changes in community composition and ecosystem functioning, microbial reactions to environmental changes are complex and can take many different forms.

Important environmental factors like pollution, habitat destruction, climate change, and nutrient enrichment can have a significant impact on microbial communities, changing their diversity, structure, and function. Microbial communities in a variety of environments face major challenges due to climate change, as seen in figure 2:[10]

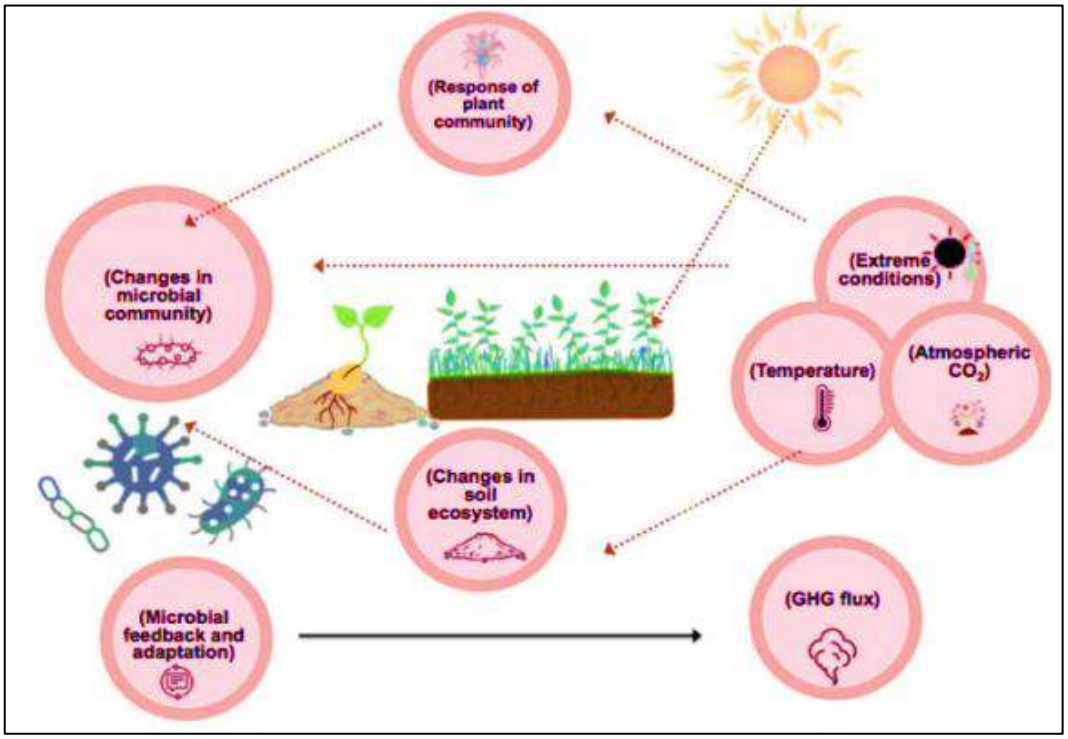

Figure 2: Climate Change and Microbes

Microbial processes like decomposition, nutrient cycling, and carbon sequestration can be disrupted by rising temperatures, shifting precipitation patterns, and changed nutrient availability. This can have a significant impact on ecosystem services and functioning. Anthropogenic pollution releases a wide range of pollutants into natural environments, from plastics and medications to heavy metals and pesticides. In bioremediation, microorganisms are essential for decomposing contaminants and purifying the environment. On the other hand, too much pollution can overwhelm microbial populations, resulting in biodiversity loss and

environmental damage. By decreasing habitat connectivity and upsetting biological relationships, habitat degradation and fragmentation further increase the susceptibility of microbial populations to environmental change.[11]

As appropriate environments grow more and more limited, microorganisms that depend on particular host organisms or ecological conditions may become extinct or see their range reduced. We seek to improve our comprehension of microbial ecology in the face of continuous environmental change by combining current information and identifying knowledge gaps. The ultimate goal of this research is to preserve microbial diversity and ecosystem resilience in a world that is changing quickly by informing conservation strategies, ecosystem management techniques, and policy decisions. Microorganisms are common and extremely versatile living forms that are essential to the maintenance of global biogeochemical cycles and the formation of ecosystems.

Microbial Diversity and their Environment

Microbes create or control their surroundings, influencing everything from multicellular hosts' health to oceanic weather patterns and the oxidation of Earth's atmosphere. Without bacteria, human civilization would abruptly collapse, followed by the extinction of all other species on Earth. A few instances of how microbial communities alter their surroundings are described in the section that follows. A sleeping behemoth beneath the Arctic tundra is now being observed by climate scientists. About half of the world's soil carbon is stored in permafrost, but these areas are starting to thaw as a result of human climate change, which is having an inappropriate or insufficient impact on the poles. It has been demonstrated that soil warming changes the composition and roles of microbial communities.

Due to microbial activity, melting permafrost soils will probably cause significant losses in soil carbon in the form of carbon dioxide and methane. Over the next century, permafrost soils would be responsible for an 8–18% increase in anthropogenic carbon emissions, depending on how quickly the temperature rises. The structure of the entire biosphere may change as a result of this beneficial biological feedback on climate change. [12]

The emergence of naturally occurring nuclear fission reactors from bacterial communities early in Earth's history is another fascinating example of how microbes control their physical environs. Some bacteria can use oxidized uranium as an electron acceptor, or respire uranium. But because of the anoxic, reducing atmosphere of the early earth, uranium—which is insoluble in its reduced form—remained trapped in rock and silt. O2 was continuously produced as a result of the growth of cyanobacteria, weathering the Earth's crust and building up in the atmosphere over hundreds of millions of years. Due to the slow oxidation of uranium deposits, uranium was able to dissolve in water and enter lakes.

Microbes that respire uranium were enriched in these bodies of water as a result of this process. The uranium was decreased by these bacteria, causing it to separate from the solution and sink to the lakes' bottoms. Lakebeds became naturally occurring fission reactors as uranium was enriched and deposited there over time, eventually reaching critical mass. Only in the early stages of Earth's history, when the radioactive isotope of uranium was still sufficiently abundant, was this procedure feasible.

Relationship between Microbial Diversity and Ecosystem Processes

Microbial diversity and ecosystem processes have a complicated and nuanced interaction. Because various microorganisms specialize in different processes, a diversified microbial community is better able to carry out a variety of ecological functions. For instance, certain microbes are in charge of decomposition, while others are involved in nitrogen fixation. [13]

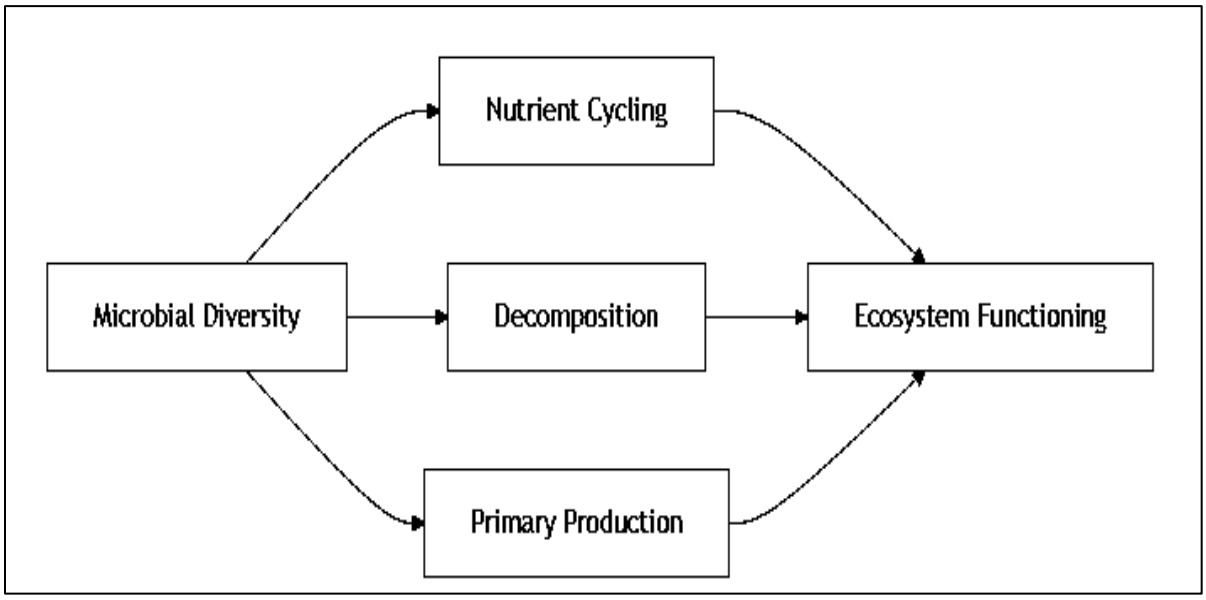

Figure 3: Relationship between Microbial Diversity and Ecosystem Processes

The economic valuation of microbial diversity:

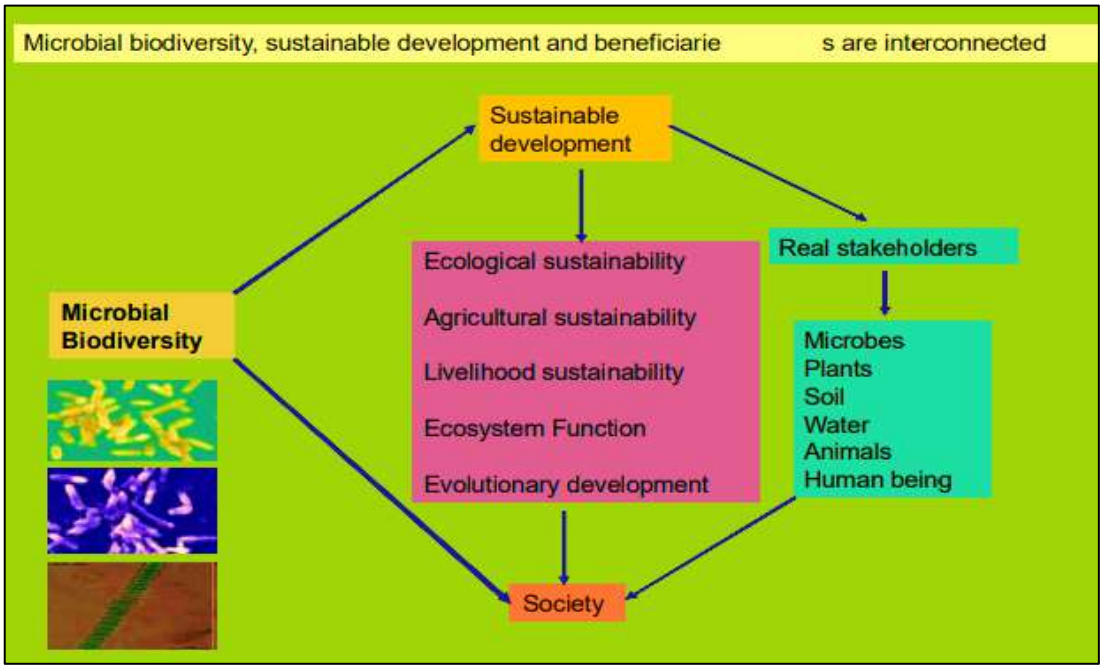

Figure 4: The economic valuation of microbial diversity
(Source: ResearchGate)

One of the most important factors in investment decisions is the valuation of resources. Demonstrating that the sustainable use of biodiversity has positive economic benefit is one step in the process of influencing local and governmental perspectives regarding the necessity of conserving biodiversity, particularly microbial diversity. National conservation policies will be increasingly impacted by improved valuation tools and a deeper understanding of how ecosystems function. Estimates of the benefits can be crucial in demonstrating that investments made in the preservation and utilization of microbial diversity can be seen as a means of preserving and improving the economic health of communities. It might also be crucial in demonstrating the rationality of the expenses associated with suggested conservation initiatives.

As an alternative, these estimates might show the "cost of inaction," or the price in terms of lost or diminished benefits if nothing is done to preserve biodiversity and exploit it sustainably. The rate and degree to which nations will sustainably benefit substantially from their microbial resources will determine how much they can afford to spend on conservation.[14]

Microbial Application to Environment

- Contribution of Microbes to Nutrient Cycling: Microbes in Carbon Cycle

Microbes are an essential component of all living things and play a crucial part in the global carbon cycle (Fig. 5). Microorganisms take carbon from nonliving sources and use it for both themselves and other living things. Microbes in aquatic environments, such as those found in oxygen-free areas like the deep mud of lakes and ponds, anaerobically transform carbon. The most prevalent form of carbon that enters a carbon cycle is carbon dioxide (CO2). One gas that dissolves in water and is found in the atmosphere is CO2. During photosynthesis, CO2 is used by plants and photosynthetic algae to create carbohydrates. Furthermore, CO2 is used by chemoautotrophs like bacteria and archaea to produce carbohydrates.

During respiration, this carbon—which is present as sugar—is further broken down into energy through a series of events called the tricarboxylic acid cycle. Through a process known as fermentation, microbes may also use carbon in anaerobic environments to generate energy. [15]

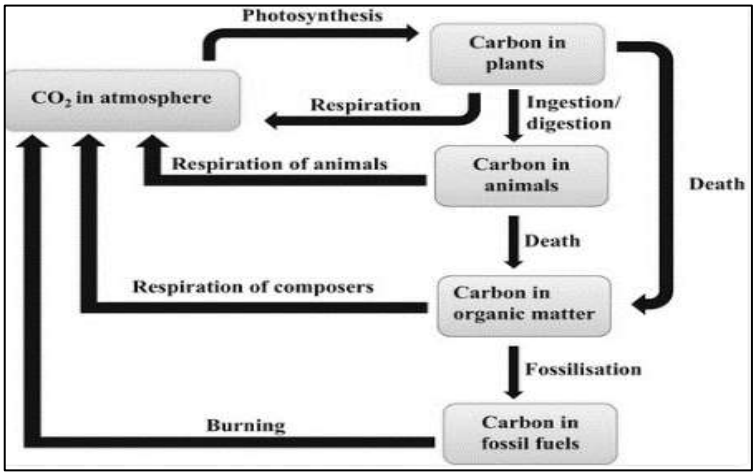

Figure 5: Role of microbes in carbon cycle
(Source: https://pmc.ncbi.nlm.nih.gov/)

In terrestrial ecosystems, plants are the main producers; but, in certain environments, cyanobacteria, free-living planktons, and symbionts like lichens also help fix carbon. Heterotrophic bacteria and fungi recycle nonliving organic matter, while saprobes use organic matter and respire to produce CO2, which contributes to the carbon cycle. But higher species, including herbivores and carnivores, also need the gut microbiota that lives in their intestinal tracts to break down organic materials for energy. This process is called decomposition, and it produces inorganic chemicals like water, CO2, and ammonia. [16]

6.Conclusion:

Microbial variety is crucial for preserving ecological balance, affecting human health, and forming the ecosystem, to sum up. Microbial diversity can be greatly impacted by human activities including pollution, climate change, and land use, which can have profound effects on ecosystem health and human well-being. Variation in bacteria based on physical, biological, genetic, or geographic characteristics is known as microbial diversity. In different ecosystems with varying pH, temperature, aerobic or anaerobic conditions, nutrients, xenobiotic chemicals, and hazardous environments, this variety is crucial. Microbes can endure harsh environments and change hazardous, complicated materials into simple, non-toxic ones. Additionally, a variety of bacteria that support plant growth boost soil fertility, plant growth, and the yield of vital foods.

Investigating microbial diversity provides important information about the complex processes of ecosystems and how resilient they are to changes in their surroundings. We have discovered a wide variety of microorganisms living in various habitats via the lens of microbial ecology, each of which makes a distinct contribution to the stability and functioning of ecosystems.

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Novel Phenolic Compounds from Indian Lichen *Parmotrematinctorum*: Chemo-Zoological Bioinformatics Integrating Computational Biology and Chemical Ecology to Decipher Animal Chemical Communication-A review

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Abstract: *Lichens represent a unique symbiotic system and are an underexplored reservoir of bioactive secondary metabolites with ecological and biological relevance (Harborne& Baxter, 2021; Newman &Cragg, 2023). Among them,* Parmotrematinctorum*, a widely distributed Indian lichen, is known to synthesize diverse phenolic compounds such as depsides, depsidones, and usnic-acid–related derivatives (Bui et al., 2020; Phan et al., 2021). These molecules play critical roles in ecological interactions and have emerging significance in animal chemical communication when viewed through a chemo-zoological perspective. This review integrates phytochemistry, zoology, and bioinformatics to examine how lichen-derived phenolics may influence animal behavior, signaling, and defense mechanisms. Emphasis is placed on computational biology tools—molecular docking, cheminformatics, network analysis, and in-silico toxicology—to decode ligand–receptor interactions involved in chemical ecology. By synthesizing evidence from lichen chemistry, animal sensory biology, and bioinformaticmodeling, the paper proposes a conceptual framework for chemo-zoological bioinformatics. Such integration not only advances understanding of natural chemical communication systems but also opens avenues for novel biomimetic applications in ecology, pharmacology, and biodiversity conservation.*

Keywords: *Parmotrematinctorum; lichen phenolics; chemical ecology; animal communication; chemo-zoological bioinformatics; computational biology.*

1. INTRODUCTION:

Chemical communication is fundamental to animal survival, mediating behaviors such as mating, foraging, territoriality, and predator avoidance (Schaefer &Ruxton, 2020; Torto, 2024). Natural products from plants, microbes, and lichens often act as semiochemicals or modulators of animal sensory systems. Indian lichens, though taxonomically well documented, remain insufficiently explored for their ecological chemical roles (Singh et al., 2023). *Parmotrematinctorum* is traditionally valued for dye production and medicinal use, suggesting a rich phenolic profile with biological activity. Integrating zoology with bioinformatics allows systematic decoding of how such compounds interact with animal olfactory and gustatory receptors.

Indian Lichens and Phenolic Chemistry

Lichen secondary metabolites are largely phenolic in nature, synthesized via the polyketide pathway (Harborne& Baxter, 2021). In *P. tinctorum*, reported compounds include atranorin, lecanoric acid, and related depsides (Bui et al., 2020; Kumar et al., 2023). These molecules exhibit antimicrobial, antioxidant, and deterrent properties. Ecologically, phenolics protect lichens from herbivory and environmental stress, while simultaneously acting as chemical cues within food webs.

Chemo-Zoological Perspective of Animal Communication

Animals rely on chemical cues for intra- and interspecific communication (Root-Gutteridge et al., 2025; Jezierski et al., 2025). Phenolic compounds can function as repellents, attractants, or signaling modifiers. Lichen metabolites deposited on substrates or ingested indirectly may influence insect behavior, vertebrate foraging preferences, and microbial symbioses. Understanding these interactions requires a zoological framework combined with chemical ecology.

Role of Bioinformatics and Computational Biology
Bioinformatics bridges chemistry and zoology by enabling integrative analysis of chemical signals and animal sensory systems (Mareş et al., 2023; Pawar&Shinde, 2021) by enabling:

- **Cheminformatics** for structure–activity relationship analysis of lichen phenolics.
- **Molecular docking** to predict binding affinity with animal chemoreceptors.
- **Network biology** to map chemical–behavioral interaction pathways.
- **In-silico ADMET and eco-toxicity tools** to assess safety and ecological impact. These approaches reduce experimental complexity and generate testable hypotheses while minimizing ecological disturbance (Mazorra-Alonso et al., 2021; Grison et al., 2022).

Integrative Conceptual Framework
Chemo-zoological bioinformatics integrates (i) lichen metabolomics, (ii) animal sensory genomics, and (iii) computational modeling. This triad facilitates holistic interpretation of chemical communication, emphasizing evolutionary adaptation and ecological balance.

2.Aim of the Review

The primary aim of this review is to critically synthesize existing knowledge on phenolic compounds derived from the Indian lichen *Parmotrematinctorum* and to evaluate their potential roles in animal chemical communication through an integrated chemo-zoological and bioinformatics perspective.

3.Objectives of the Review

The specific objectives of this review are to:

1. Summarize the diversity and chemical nature of phenolic compounds reported from *Parmotrematinctorum*.

2. Examine the ecological and zoological relevance of lichen-derived phenolics in animal communication and behavior.
3. Review the application of bioinformatics and computational biology tools in decoding chemical–sensory interactions.
4. Propose an integrative conceptual framework linking lichen chemistry, animal sensory biology, and computational modeling.
5. Identify research gaps and future directions relevant to chemical ecology and zoological studies.

4.Review Methodology

This review is based on a systematic and critical analysis of peer-reviewed literature published primarily between 2020 and 2025. Scientific databases such as Scopus, Web of Science, PubMed, and Google Scholar were consulted using keywords including *Parmotrematinctorum*, lichen phenolics, chemical ecology, animal communication, and bioinformatics. Only original research articles, authoritative reviews, and high-impact interdisciplinary studies were considered. Emphasis was placed on studies that provided chemical characterization, ecological relevance, or computational analysis. Information was synthesized thematically to ensure originality, coherence, and critical interpretation rather than descriptive repetition.

Applications and Future Prospects

Potential applications include development of eco-friendly pest control agents, conservation-oriented chemical markers, and biomimetic communication modulators (Torto, 2024; Singh et al., 2023). Future research should combine field ecology with high-throughput computational screening and targeted behavioral assays.

5.Results and Discussion (Synthesis of Evidence)

The reviewed literature collectively demonstrates that *Parmotrematinctorum* produces structurally diverse phenolic compounds with documented biological activities, including antimicrobial, antioxidant, and deterrent effects. Emerging ecological evidence suggests that such phenolics may influence animal behavior indirectly through habitat-mediated cues or trophic interactions. Computational studies further indicate that phenolic structures possess favorable binding potential with chemosensory receptors, supporting their putative role in chemical communication. The integration of bioinformatics tools has enabled prediction-driven insights that complement traditional ecological observations, highlighting a shift toward data-informed chemical ecology. However, experimental validation linking specific lichen metabolites to defined animal behavioral responses remains limited, underscoring a critical research gap.

6.Conclusion

Parmotrematinctorum offers a promising model for studying phenolic-mediated chemical communication at the interface of chemical ecology and zoology (dos Santos et al., 2025; Schaefer &Ruxton, 2020). Chemo-zoological bioinformatics provides a novel, interdisciplinary pathway to decode complex ecological signaling systems, reinforcing the relevance of natural products in modern zoological research.

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Advances in Green Synthesis: Sustainable Strategies for Materials Development and Cleaner Processes

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Abstract: *Green synthesis represents a fundamental shift in chemical manufacturing, moving away from traditional, hazardous processes toward environmentally benign, resource-efficient, and safer alternatives. This review explores sustainable strategies used in green synthesis with an emphasis on materials development and cleaner industrial processes. Key methodologies such as microwave-assisted reactions, mechanochemistry, biocatalysis, and flow chemistry are discussed. Applications in nanomaterials, biodegradable polymers, coatings, and flame retardants are detailed with a focus on circular economy integration and scalability challenges. This paper also highlights real-world case studies of green synthesis in nanoparticle production, eco-friendly composites, and biodiesel generation. The role of green chemistry metrics, policy support, and future research directions are examined. Overall, green synthesis provides transformative solutions for sustainable material innovation and eco-conscious industrial practices.*

1. INTRODUCTION

The global shift towards sustainability has placed chemical industries under immense pressure to reformulate their practices. Traditional synthesis often involves toxic reagents, harsh conditions, and excessive waste generation. Green synthesis, a critical branch of green chemistry, focuses on designing synthetic pathways that are environmentally friendly, energy-efficient, and economically feasible. Since the introduction of the 12 Principles of Green Chemistry by Anastas and Warner, researchers have increasingly adopted these principles to reduce the ecological impact of chemical production.

The development of novel materials such as nanomaterials, biodegradable polymers, and eco-friendly composites has been revolutionized by green synthetic methods. Green synthesis is no longer an option—it is a necessity for future-proofing industrial innovation and protecting the environment.

Principles of Green Synthesis
The core principles that guide green synthesis include:
- Prevention: Avoid creating waste instead of treating or disposing it.
- Atom Economy: Maximize the incorporation of all starting materials into the final product.
- Safer Solvents and Auxiliaries: Use less toxic or non-toxic solvents like water or supercritical CO_2.
- Energy Efficiency: Reduce energy requirements by employing room temperature and

pressure conditions.
- Catalysis: Use of catalytic reagents to increase selectivity and minimize by-products.
- Renewable Feedstocks: Prefer bio-based and renewable raw materials.
- Design for Degradation: Ensure that chemical products break down into harmless substances post-use.
These principles shape how green synthesis is implemented across various domains of chemistry.

Sustainable Techniques in Green Synthesis
Modern green synthesis incorporates a range of sustainable technologies:
Microwave-Assisted Synthesis
Microwave energy provides rapid and uniform heating, significantly reducing reaction times and improving yields. It is widely applied in organic and inorganic synthesis, nanotechnology, and pharmaceutical chemistry.
Mechanochemistry
Reactions induced by mechanical forces (e.g., grinding or milling) eliminate the need for solvents. This technique is especially useful in the synthesis of metal-organic frameworks and drug formulations.

Biocatalysis
Using enzymes or whole cells as catalysts, biocatalysis operates under mild conditions and produces minimal waste. It is highly valuable in pharmaceutical, food, and biofuel industries.
Ultrasound and Sonochemistry
Ultrasound accelerates chemical reactions by producing cavitation bubbles. This improves mass transfer and yields in nanoparticle synthesis, emulsification, and extraction.
Supercritical Fluids and Green Solvents
Supercritical CO_2 and ionic liquids offer low toxicity and high efficiency in reactions and separations. They are increasingly replacing hazardous organic solvents.

Green Synthesis for Materials Development
Green synthesis techniques have transformed how we design and fabricate materials:
Nanomaterial's
Biogenic synthesis of nanoparticles using plant extracts, fungi, or bacteria provides eco-friendly alternatives to chemical reduction methods. These nanoparticles find use in medicine, catalysis, and electronics.
Biodegradable Polymers
Polymers like polylactic acid (PLA) and polyhydroxyalkanoates (PHA), derived from renewable resources, are replacing petroleum-based plastics in packaging and biomedical applications.
Bio-Composites
Green composites use natural fibers (e.g., jute, hemp) embedded in biodegradable polymer matrices. They are gaining popularity in construction, automotive, and consumer products.
Eco-Friendly Coatings
Water-based paints, bio-based resins, and low-VOC coatings are examples of green innovations that reduce air pollution and health hazards in construction and manufacturing.

Cleaner Industrial Processes

Green synthesis also plays a crucial role in redesigning industrial processes:

Flow Chemistry: Continuous flow reactors offer better heat and mass transfer, leading to increased safety, control, and scalability.

Electrochemical Synthesis: Harnesses electricity to drive reactions instead of hazardous reagents.

Photocatalysis: Utilizes light (solar or LED) to power organic transformations and pollutant degradation.

Catalyst Recovery and Reuse: Supported and immobilized catalysts can be reused, lowering costs and waste.

Case Studies

ZnO Nanoparticles via Aloe Vera Extract

Zinc oxide nanoparticles synthesized using Aloe Vera extract demonstrate excellent antimicrobial properties and UV shielding. This method avoids toxic reducing agents and high temperatures, making it both green and scalable.

Bio-Based Flame Retardants

Natural substances like chitosan, lignin, and phytic acid are used to produce flame-retardant coatings for textiles, eliminating the need for halogenated flame retardants.

Biodiesel from Waste Oils

Using lipase enzymes, biodiesel is produced from used cooking oil under mild conditions, minimizing chemical waste and contributing to circular economy models.

Challenges in Green Synthesis

Scalability: Lab-scale successes often face difficulties when transitioning to industrial-scale production.

Cost: Green solvents and catalysts can be expensive or have limited availability.

Standardization: Lack of universally accepted metrics to assess “greenness” complicates evaluation and comparison.

Education and Mindset: There is a need to shift educational curricula and industrial culture toward sustainability-oriented thinking.

Future Prospects

The future of green synthesis lies in: AI-Driven Reaction Design: Machine learning for predictive synthesis modeling. Green Metrics Development: Tools like the E-factor and EcoScale for process evaluation. Integration with Circular Economy: Closing material loops in manufacturing. Policy Support and Regulation: Incentives and compliance frameworks will drive adoption.

Conclusion

Green synthesis is not just a set of techniques—it is a philosophy that integrates chemistry with environmental responsibility. By using renewable resources, safer reagents, and energy-efficient technologies, green synthesis enables the development of sustainable materials and processes across all sectors. Its implementation is essential for reducing the chemical footprint on our planet and ensuring a safer, healthier future.

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Innovative Applications and Future Perspectives of Chromatography-Mass Spectrometry in Drug Research

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Abstract: *Chromatography coupled with mass spectrometry (MS) has emerged as a cornerstone analytical technique in drug research. Over the years, advancements in chromatography-MS have significantly enhanced its capabilities, leading to improved sensitivity, specificity, and throughput. This review explores the innovative applications of chromatography-MS in drug research, particularly focusing on its role in drug absorption, distribution, metabolism, excretion (ADME), toxicity evaluation, and personalized medicine. It also addresses the future perspectives of this powerful technique, including challenges and potential solutions, and highlights how emerging trends such as high spatial resolution imaging and multimodal integration could revolutionize drug discovery and development. Through these innovations, chromatography-MS promises to contribute substantially to the development of more effective, safer, and personalized therapeutic interventions.*

Keywords: *chromatography-mass spectrometry, drug research, pharmacokinetics, drug metabolism, personalized medicine.*

1. INTRODUCTION

Chromatography-MS has established itself as one of the most versatile and powerful analytical techniques in drug research. The integration of high-resolution chromatography with sensitive mass spectrometry has transformed the landscape of pharmaceutical analysis, enabling researchers to gain unprecedented insights into drug molecules. In particular, chromatography-MS has become indispensable in understanding critical aspects of drug behavior, such as drug pharmacokinetics, pharmacodynamics, metabolism, distribution, and excretion (ADME), and toxicity evaluation. The growing complexity of drug research, combined with the increasing demand for precision medicine, underscores the need for sophisticated analytical techniques capable of addressing the challenges of drug discovery, development, and personalized treatment. For example, in the early stages of drug development, the need for accurate pharmacokinetic and pharmacodynamic profiling is paramount to predicting a drug's behavior in the body. To optimize drug efficacy and minimize risks, researchers must track how drugs are absorbed, distributed, metabolized, eliminated, as well as assess their toxicity. In this context, chromatography-MS offers a powerful solution for achieving the sensitivity and precision needed to dissect these complex processes.

2. Principles and development of chromatography-MS

Chromatography-MS is an integrated analytical technique that combines the separation capabilities of chromatography with the molecular identification power of mass spectrometry. The success of this approach lies in its ability to simultaneously separate complex mixtures,

identify individual components with high sensitivity, and provide detailed structural information. This combination allows for the analysis of a wide variety of drug-related samples, from biological fluids to tissues, and provides valuable insights into the behavior and mechanisms of drugs at both the molecular and cellular levels.

2.1 Chromatography: separation principle

Chromatography is a technique used to separate components of a mixture based on their different affinities for two phases: a stationary phase and a mobile phase. There are several types of chromatography commonly used in drug research:

(1) Liquid Chromatography (LC): LC, particularly high-performance liquid chromatography (HPLC) and ultra-high-performance liquid chromatography (UHPLC), is one of the most widely used techniques in drug research. LC is effective for separating a wide range of polar and non-polar compounds, including small molecules, peptides, and proteins. In HPLC, the mobile phase is a liquid, and the stationary phase is typically a solid or porous material packed into a column. UHPLC improves upon HPLC by using smaller particle sizes and higher pressure, allowing for faster separation and greater resolution.
(2) Gas Chromatography (GC): GC is used primarily for volatile compounds. GC is widely used in the analysis of small drug molecules, particularly those that are thermally stable and volatile. (3) Two-Dimensional Chromatography (2D-LC): Two-dimensional chromatography combines two different chromatographic techniques to achieve even greater separation power. The first dimension often involves an LC method, while the second dimension may use a different technique, such as ion-exchange chromatography or reverse-phase chromatography.
(4) Thin-Layer Chromatography (TLC): TLC is an older but still widely used technique for the rapid separation of small amounts of drug compounds.
In chromatography-MS, the separation achieved by chromatography is followed by ionization of the components and their detection by mass spectrometry. This separation ensures that the mass spectrometer is able to detect individual compounds in complex mixtures, even in very small concentrations, which is essential for studying drug molecules and their metabolites in biological samples.

2.2 MS: detection and quantification

MS is a technique used to identify the chemical structure and quantify the amount of a compound based on its mass-to-charge ratio (m/z). The process of mass spectrometry involves three main stages: Ionization, Mass analysis, and Detection.
(1) Ionization: The first step in MS is the conversion of neutral molecules into charged particles, or ions, which can then be manipulated in an electric or magnetic field. Common ionization methods include: 1) Electrospray Ionization (ESI): ESI is widely used for the analysis of polar and ionic compounds, such as drugs and their metabolites. 2) Atmospheric Pressure Chemical Ionization (APCI): APCI is used for less polar compounds and works by creating ions through chemical reactions between the sample and a reagent gas in a corona discharge. 3) Matrix-Assisted Laser Desorption/Ionization (MALDI): MALDI is typically used for the analysis of large biomolecules such as proteins and peptides. A laser is used to ionize the sample embedded in a matrix, producing ions that can be analyzed in the mass spectrometer.
(2) Mass Analysis: Once the sample is ionized, the ions are directed into the mass analyzer, where their mass-to-charge ratio (m/z) is measured. Several types of mass analyzers are used, including: i) Quadrupole: A quadrupole mass analyzer uses electric fields to filter ions based on their m/z ratio, allowing for the analysis of a wide range of compounds with good sensitivity

and resolution. ii) Time-of-Flight (TOF): TOF analyzers measure the time it takes for ions to travel a fixed distance, with lighter ions reaching the detector more quickly than heavier ions. iii) Orbitrap: Orbitrap analyzers trap ions in an electrostatic field and measure their frequency of oscillation to determine their m/z ratio.

(3) Detection: The ions are then detected by various methods such as electron multipliers or ion traps. The detected ions are converted into a mass spectrum, which is a plot of ion intensity against m/z ratio.

2.3 The role of chromatography-MS in modern drug research

Today, chromatography-MS is an indispensable tool in drug research, offering robust and reliable analysis for a variety of applications. From drug discovery to clinical trials, chromatography-MS enables researchers to gain detailed insights into drug pharmacokinetics, metabolic pathways, and safety profiles. In drug research, chromatography-MS is used to study the absorption, distribution, metabolism, and excretion (ADME) of drugs, providing in valuable data on the fate of a drug in the body and helping to predict its therapeutic efficacy and safety.

3. Innovative applications of chromatography-MS in drug research

3.1 Drug absorption and bioavailability

Understanding drug absorption is critical in drug development, as it determines the drug's in studying the pharmacokinetics of drugs, including their absorption rates and profiles. By coupling liquid chromatography with MS, researchers can track the drug's movement from the gastrointestinal tract into the bloodstream, monitors metabolites, and quantify concentrations over time.

3.1.1 Innovative approaches in chromatography-MS for drug research

Recent advancements in chromatography-MS have introduced innovative methodologies that significantly enhance our understanding of drug absorption, distribution, and localization.

3.1.1.1 In vitro gastrointestinal models

One of the innovative applications of chromatography-MS is its integration with *in vitro* gastrointestinal (GI) models to simulate human drug absorption. In these models, researchers mimic the physiological conditions of the human GI tract, including variations in pH, enzyme activity, and digestive fluids, to simulate how drugs are absorbed during the digestive process. By coupling these models with chromatography-MS, researchers can analyze drug samples from simulated gastric and intestinal environments, quantifying both the parent drug and its metabolites with high precision.

3.1.1.2 Spatial mass spectrometry imaging

Another cutting-edge application of chromatography-MS in drug research is spatial mass spectrometry imaging (MSI), particularly with MALDI imaging mass spectrometry. This technique enables the visualization of drug distribution within biological tissues with high spatial. MALDI-IMS has been particularly valuable in drug distribution studies, as it enables researchers to examine the spatial distribution of drugs and their metabolites directly in tissue sections without the need for labels or external markers. This approach has been used to study drug delivery in organs such as the brain, liver, and kidney, providing detailed information on the pharmacokinetics and pharmacodynamics of drugs in specific tissue environments.

3.2 Drug distribution and pharmacokinetics

Understanding drug distribution is a key component of pharmacokinetics and is essential for predicting the therapeutic efficacy and safety profile of a drug. Drug distribution refers to the

process by which a drug moves from the bloodstream to various tissues and organs. It is influenced by factors such as blood flow, tissue permeability, and protein binding. To gain a comprehensive understanding of these processes, it is essential to accurately assess the concentration and distribution of drugs throughout the body. Chromatography-MS, as a highly sensitive and precise analytical technique, has become a critical tool in studying drug ADME.

3.2.1 Innovative approaches in drug distribution and pharmacokinetics

Recent advancements in mass spectrometry, particularly in imaging technologies and single-cell analysis, have revolutionized the way drug distribution is studied at the molecular and cellular levels

3.2.1.1 Single-cell analysis

The emergence of single-cell analysis using MSI and advanced ionization techniques, such as nano-spray ionization (nESI), has allowed for the detection of drug distribution at the individual cell level. This method offers several advantages over traditional bulk tissue analysis, as it can capture the heterogeneity of drug distribution within different cell populations, tissues, and organs.Recent studies have demonstrated the ability to map drug uptake and localization within single cells, providing insights into how drugs interact with specific cell types or organelles .For instance, by applying single-cell MSI, researchers can identify how a drug may selectively accumulate in certain cell types (such as cancer cells), enabling a better understanding of the mechanisms driving drug efficacy and resistance .

3.2.1.2 Dynamic Imaging

Dynamic imaging allows researchers to observe the metabolism of drugs in tissues, tracking the formation and distribution of metabolites alongside the parent drug. This is crucial for understanding not only the pharmacokinetics of the drug but also its pharmacodynamics, helping to inform dosing strategies and identify potential toxicities at the cellular level. The study by Gou et al. introduced a novel laser-assisted chemical transfer (LACT) technique to enhance the detection sensitivity of central nervous system (CNS) drugs in brain tissues by minimizing ionization suppression from endogenous biomolecules.

3.3 Drug metabolism and biomarker discovery

Drug metabolism plays a pivotal role in determining the efficacy, safety, and toxicity of pharmaceutical compounds. Metabolic processes, including the transformation of drugs into active or inactive metabolites, are often mediated by enzymes such as cytochrome P450 (CYP450). Understanding these metabolic pathways is essential for predicting drug responses, optimizing dosing regimens, and identifying potential toxicities. Chromatography-MS has emerged as a critical tool in studying drug metabolism, as it allows for the precise identification and quantification of metabolites in complex biological samples, such as plasma, urine, or liver tissue. In drug metabolism studies,

3.3.1 Innovative approaches in drug metabolism and biomarker discovery

3.3.1.1 Metabolomics

Metabolomics is the large-scale study of metabolites, small molecules involved in cellular processes, and their dynamic changes in response to drug treatments. Chromatography-MS has become the corner stone of metabolomics, enabling the identification and quantification of thousands of metabolites in biological samples with high sensitivity and accuracy. Metabolomics applied to drug metabolism helps identify not only the drug metabolites but also other endogenous metabolites that may be influenced by drug exposure.

3.3.1.2 CYP450 assays

CYP450 enzymes are central to the metabolism of many drugs, and their activity is a key determinant of drug pharmacokinetics. Using chromatography-MS, researchers can study the activity of these enzymes and their role in drug metabolism. MS allows for the identification of CYP450-mediated metabolites and provides valuable data on enzyme activity, enabling researchers to predict how different drugs may interact with CYP450 enzymes. In drug discovery, understanding CYP450-mediated metabolism is critical for assessing the potential for drug-drug interactions. Chromatography-MS is frequently used to monitor CYP450 activity *in vitro*, providing insight into how drugs are metabolized and identifying potential DDIs early in the development process.

3.3.2 Impact on drug development and personalized medicine

The integration of metabolomics and CYP450 assays with chromatography-MS has profound implications for drug development. These innovative approaches help identify key metabolites that influence drug action, predict potential adverse effects, and uncover biomarkers of drug efficacy and toxicity.

3.4 Drug toxicity and side effect evaluation

Drug toxicity is a critical concern in drug development, as adverse effects can lead to the termination of promising drug candidates during clinical trials. Toxicity can manifest in various forms, such as organ damage, metabolic disturbances, and immunological responses, often caused by the accumulation of toxic metabolites. Therefore, understanding the mechanisms underlying drug toxicity and identifying harmful metabolites is essential for ensuring drug safety and efficacy. Chromatography-MS plays a pivotal role in toxicity assessment by enabling the identification and quantification of toxic metabolites, as well as providing insights into the effects of drugs on biological systems at the molecular level.

3.4.1 Innovative approaches in drug toxicity and side effect evaluation

3.4.1.1 Toxicoproteomics The integration of proteomics with chromatography-MS, often referred to as toxicoproteomics, is an emerging approach to understanding drug toxicity at the protein level. Toxicoproteomics combines the identification of protein expression changes, post-translational modifications, and interactions with the analysis of metabolites, providing a comprehensive view of how drugs affect cellular and tissue systems. By analyzing protein expression profiles in response to drug exposure, researchers can identify proteins that are involved in the toxic response, including those that may act as biomarkers for toxicity. Using chromatography-MS, these changes can be detected at early stages, allowing for the identification of potential biomarkers of liver toxicity, kidney damage, or cardiovascular toxicity.

3.4.1.2 Biomarker discovery

The identification of biomarkers that can predict or indicate drug toxicity is a key component of drug safety evaluations. Chromatography-MS plays a central role in discovering these biomarkers by providing a detailed analysis of the metabolome and proteome in response to drug exposure. Metabolomic and proteomic profiling can reveal subtle changes in cellular or metabolic pathways that are associated with toxicity, even before clinical symptoms manifest. For instance, the detection of certain metabolites or proteins in blood or urine samples can indicate early signs of organ damage or systemic toxicity, enabling more effective monitoring and intervention.

3.4.2 Impact on drug safety and development

The integration of toxicoproteomics and biomarker discovery with chromatography-MS enhances the ability to assess drug toxicity and predict adverse reactions, reducing the risks associated with new drug candidates. These advanced analytical methods allow researchers to identify toxicity risks early in the drug development process, optimizing safety profiles before drugs enter clinical trials.

4. Chromatography-MS in personalized medicine

The advancement of personalized medicine has revolutionized how healthcare is delivered, shifting the focus from a "one-size-fits-all" approach to treatments that are tailored to the individual characteristics of each patient. Personalized medicine aims to optimize treatment strategies by considering factors such as genetic makeup, lifestyle, and environmental influences. Chromatography-MS is playing an increasingly vital role in this paradigm shift, as it enables the analysis of patient-specific biological profiles that can guide more precise and effective drug therapies. By integrating data from genomics, proteomics, and metabolomics, chromatography-MS provides comprehensive insights into how patients respond to drugs at the molecular level.

5. Future perspectives and challenges

Despite the tremendous progress made in the development and application of chromatography-MS in drug research, several challenges remain that hinder its broader adoption and optimal utilization. Key limitations include the need for improved sensitivity, higher resolution in complex biological matrices, and more efficient data analysis techniques.

6. Future directions in chromatography-MS

Despite these challenges, several exciting directions for the future of chromatography-MS are emerging, which hold promise for overcoming current limitations and further enhancing its capabilities in drug research.

6.1 High-resolution imaging and multimodal techniques

One of the most promising directions for future research is the integration of chromatography-MS with high-resolution imaging techniques. Combining MS with magnetic resonance imaging, fluorescence microscopy, and optical imaging will allow researchers to visualize drug distribution, metabolism, and toxicity in living tissues at the cellular and subcellular levels. MSI, for example, is already providing high spatial resolution images of drug distribution in tissue slices, but when combined with other imaging modalities, it can give more detailed insights into how drugs interact with tissues in real time. These multimodal techniques will provide a more comprehensive understanding of drug mechanisms of action and enable a more precise evaluation of drug efficacy and safety at the cellular level.

6.2 Artificial intelligence and machine learning

As chromatography-MS continues to produce increasingly large and complex datasets, the integration of artificial intelligence (AI) and machine learning (ML) into data analysis holds great promise for improving the speed, accuracy, and reproducibility of results. AI and ML algorithms can analyze vast amounts of data to identify patterns, correlations, and anomalies that may not be apparent through traditional analytical techniques. For instance, ML models can be trained to predict drug efficacy, metabolism, and toxicity based on historical data and

patient-specific profiles, significantly reducing the time needed to identify promising drug candidates. Several existing AI/ML-based approaches illustrate this potential clearly.

7. Conclusion

The future of chromatography-MS in drug research is bright, with significant opportunities for innovation and improvement. While current challenges exist, advancements in multimodal imaging, AI, and sample automation are poised to enhance the capabilities of chromatography-MS, making it an even more powerful tool in drug discovery and personalized medicine. These advancements will not only increase the efficiency and accuracy of drug development but will also contribute to the development of safer, more effective treatments tailored to individual patients. As these technologies continue to evolve, chromatography-MS will remain at the forefront of transformative changes in the way drugs are discovered, developed, and delivered to patients.

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Phytochemical Analysis of Ethnomedicinal Plants used in Livestock Healthcare of Devarakonda area, Nalgonda district, Telangana state, India.

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Abstract: *In local towns and villages of developing nations, the use of plants and plant resources for a variety of ethno-botanical purposes is every day, particularly for human and veterinary healthcare. As a result, it is critical to uncover and document indigenous ethno-medicinal plants and their traditional and folk uses for human and livestock health care. Our findings on ethno-medicinal plants from the Devrakonda in Telangana are presented here for conservation, additional pharmacological screenings, and applied research. Ethno medicinal plants information was obtained through interviews with local people and traditional healers in Devarakonda, Telangana, from 2022 to 2023. The study has shown that nearby individuals have higher confidence in the utilization of ethno-medicinal plants yet involve them in the treatment of different afflictions. The novel use of these plants may be strongly supported by conducting additional research and revealing potential pharmaceuticals, awareness campaigns, conservation efforts, and pharmacological and applied research are required.*

1. INTRODUCTION

Plants have long been used by humans to meet a variety of daily needs. Plants are utilized as medications, food, grub for animals, and materials to build houses [1]. Almost every nation has benefited from the useful therapeutic and medicinal components of medicinal plants and herbs, which are used for therapeutic purposes worldwide [2]. From their inception to the present day, herbal medicines have played a unique role in healthcare systems. The first ethnomedicinal plant in the history of the subcontinent was mentioned in Rigveda between 4500 and 1600 BC, and Ayurveda between 2500 and 600 BC [3]. It is believed that the concepts of ethnobotanical medicines originated in Greece, were adopted by Arabs, and were then learned by Indians and Europeans [4–6]. Because numerous allopathic medications are derived from medicinal plants [7, 8], medicinal plants play a significant role in conventional healthcare [7, 8]. Due to its lower prices, higher efficacy, and increased faith in herbal remedies, alternative medicine may see an increase in use. Due to their vast therapeutic potential and use as an alternative therapy in a variety of healthcare systems, scientific investigations into medicinal plants have been underway in a number of nations [9].

Around 1800 B.C., King Hammurabi of Babylon established a veterinary fee structure and enacted laws that led to the practice of traditional veterinary medicine [10]. Even in this day and age, the primary source for treating livestock diseases is ethnoveterinary medicine (EVM). Since the beginning of human civilization, various diseases of domesticated animals have been treated with herbal remedies. It is estimated that medicinal plants have been extensively utilized as a primary source of disease prevention and control for livestock for several centuries [11, 12]. Numerous studies have been conducted on the use of herbal

medicines and their derivatives to treat specific ailments in livestock [13]. Traditional EVM compares favorably with Western medicines in terms of affordability and accessibility [14].

India is a country that relies on agriculture for about 80% of its total population. India is the world's biggest milk-delivering country in view of its high dependence on cultivating and domesticated animals. In the early 1950s, 84% of India's population relied on traditional medicine. In recent years, traditional knowledge, which is now restricted to remote areas, has seen a rapid decline. Even though a lot of work has been done to document ethnoveterinary practices around the world, very little has been done in India to document plants used as EVM, and there is a huge need to document this knowledge.

Human medicinal plant inventories show a similar trend, with numerous researchers and ethnobotanists having visited the majority of India and contributing to the records. However, a great deal of information and traditional wisdom has yet to be recorded. The primary objectives of this study were to: compile data on traditional knowledge of ethnomedicinal plants in order to evaluate the most frequently used species and access from Devarakonda in traditional ethnomedicinal plant utilization; report traditional folk knowledge, ethnomedicinal plant utilization along with recipes, mode of preparation, parts used, and used form in veterinary and human healthcare by local and ethnic communities; identify potential conservation threats. to provide further research baseline to pharmacologists, phytochemists and conservationists for further research studies.

Tanning, alkaloids, carbohydrates, terpenoids, steroids, and flavonoids are examples of bioactive substances found in medicinal plants that have a clear physiological effect on the human body [15, 16]. The primary or, more accurately, secondary metabolism of living things produces these compounds. Chemically and taxonomically, secondary metabolites are very different compounds with no clear purpose. A large number of phytochemicals belonging to several chemical classes have been shown to have inhibitory effects on all types of microorganisms in vitro [17]. They are widely used in human therapy, veterinary medicine, agriculture, scientific research, and countless other fields [18].

Plant items have been important for phytomedicines since time prehistoric. Barks, leaves, flowers, roots, fruits, and seeds are all sources of this [19]. It is desirable to have knowledge of the chemical components of plants because this information will be useful in the synthesis of complex chemical substances [20-22].

In the current work, subjective and quantitative phytochemical examination were completed in five plants, Azadirachta Indica, Calotropis Gigantea, Cissus Quadrangularis, Asparagales, and Asimum Sanctum.

1.1 Geology of the study area

The geology of the area (**Fig.1**) in general comprises of rocks and mountains of Nalgonda district is one of the 33 districts of Telangana state, with a total geographical area of 1,12,077 sq. km. It has a total population of 350.04 lakhs [23]. The Devarakonda division has 22 Gram Panchayats, 104 revenue villages and 31 mandals [24]. For Administrative convenience the district is divided into 3 revenue divisions located at Nalgonda, Miryalguda and Devarakonda. The district lies between North latitude area 16.693514, 78920197 forms a part of major basin of Krishna River and discovered by survey they connected with road and telecommunications in the district and division. There were 11 Large and Medium scale industries in Devarakonda division. The division is endowed with minerals like stone, clay, building materials and rocks and lime stone have been discovered in Pedda Adiserlapalli mandal area. In terms of

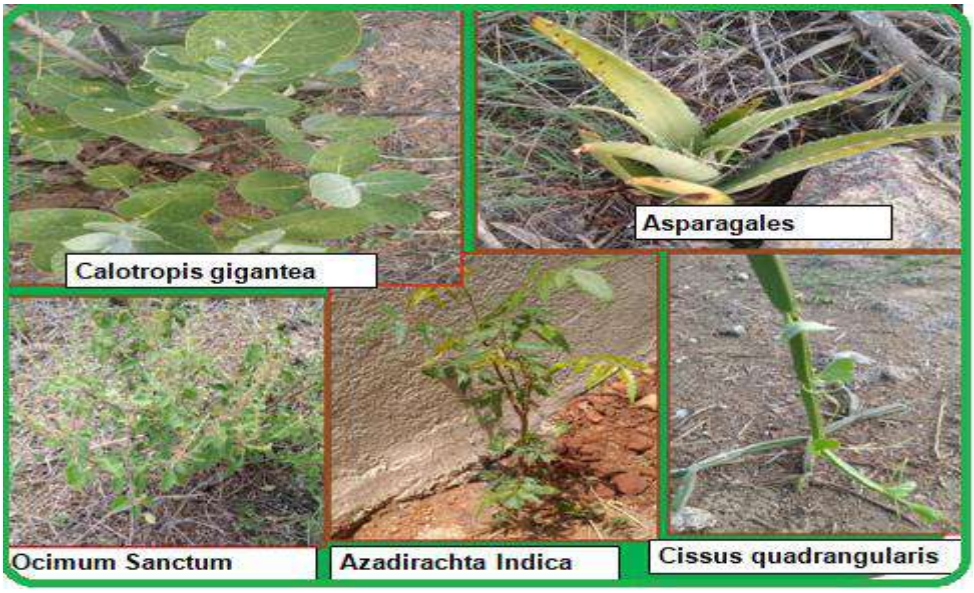
agriculture, groundwater accounts for 72.56% of the total gross irrigated area while surface water irrigation makes for 27.33% of the gross area [25].

Fig.1. Study area locations map of Devarakonda region, Telangana, India.

The region predominantly comprises rocks in the north-central and south-east parts. In the western and southwest parts, the water levels are found between 10 to 20 m. More than 20 m depth range was found as isolated patches in central and western parts of the district. The majority of the area shows a rise in the range of 2 -4 m. The majority of the area shows a rise in the range of 2 - 4 m.

the normal annual rainfall of the state is 939 mm of which the Southwest monsoon (June - September) contributes 80% (749 mm), the Northeast monsoon (October - December) contributes 13% (120 mm), winter contributes 1% (12 mm) and summer contributes 6 % (58 mm) of the rainfall map of Telangana state.

In the present work, qualitative phytochemical analysis was carried out in five plants, Azadirachta indica, Calotropis gigantean, Cissus quadrangularis, Asperagales, asimum sanctum.



2.MATERIALS AND METHODS

Collection of plant materials

Fresh parts of five medicinal plants, Azadirachta Indica (leaves), Calotropis Gigantean (leaves), Cissus Quadrangularis (leaves and stem), Asparagales (leaves), Ocimum Sanctum (leaves) were collected from different regions of Devarakonda. The plant materials were shade dried in order for them to become thoroughly dried and ready for grinding. The dried plant components were then thoroughly pulverised into a fine powder using a mechanical blender before being put into sealed containers with the appropriate labelling.

Preparation of plant extracts

Hot water extraction

200ml of distilled water and 5g of dried, finely ground plant material were put to a beaker. For 20 minutes, the mixture was cooked on a hot plate at 30°–40°C while being continuously stirred. The filtrate from the subsequent filtering of the water extract with filter paper was used to conduct the phytochemical analysis. When not in use, the water extract was kept in the refrigerator.

Solvent extraction

Soxhlet extraction was used to create crude plant extract. A consistent 20gm of powdered plant material was placed in a thimble, and 250ml of various solvents were extracted from each separately. Methanol, ethanol, and acetone were the solvents employed. The extraction process continues for 24 hours or until the solvent in the extractor's syphon tube turns colourless. Afterwards, the 5gm of dried finely powdered plant material was taken in a beaker and 200ml of distilled water was added. The mixture was heated on a hot plate with continuous stirring at 30º-40ºC for 20 minutes. Then the water extract was filtered through filter paper and the filtrate was used for the phytochemical analysis. The water extract was kept in refrigerator when not in use.

Qualitative phytochemical analysis

The extract was tested for the presence of bioactive compounds by using following standard methods [26-28].

Test for proteins

Millon’s test

When crude extract was combined with 2 ml of Millon's reagent, a white precipitate formed that, when gently heated, became red to reveal the presence of protein.

Ninhydrin test

When crude extract was heated with 2ml of Ninhydrin 0.2% solution, a violet colour emerged, indicating the presence of proteins and amino acids.

Test for carbohydrates

Fehling’s test

2ml of Crude extract is taken and added equal volume of Fehling A and Fehling B reagents were mixed together and gently boiled. A brick red precipitate at the bottom of the test tube is indicated the presence of reducing sugars.

Benedict’s test

When the crude extract was mixed with 2 mL of Benedict's reagent and boiled, a red-brown precipitate formed, indicating the presence of carbohydrates.

Molisch's test

The crude extract was mixed with 2 ml of Molisch's reagent and the mixture was shaken well. Then 2 ml of concentrated H2SO4 was carefully poured down the side of the test tube. The presence of a purple ring in the intermediate phase indicated the presence of carbohydrates. Iodine tests the crude extract was mixed with 2 ml of iodine solution. A dark blue or purple color indicated the presence of carbohydrates.

Test for phenols and tannins

The crude extract was mixed with 2 ml of 2% FeCl3 solution. A blue-green or black color indicated the presence of phenols and tannins.

Test for flavonoids Shinoda test

The crude extract was mixed with some magnesium strip fragments and concentrated HCl was added dropwise. After a few minutes a pink fire red color appeared, indicating the presence of flavonoids.

Alkaline reagent test

The crude extract was mixed with 2 ml of 2% NaOH solution. A strong yellow color was formed, which became colorless when a few drops of dilute acid were added, indicating the presence of flavonoids.

Test for saponins

The crude extract was mixed with 5 ml of distilled water in a test tube and shaken vigorously. The formation of stable foam was considered an indicator of the presence of saponins.

Test for glycosides

Liebermann's test

The crude extract was mixed with 2 ml of chloroform and 2 ml of acetic acid. The mixture was cooled with ice. Concentrated H_2 SO_4 was carefully added. The color change from purple to bluish-green indicated the presence of the steroid core, i.e. the glycosidic part.

Salkowski's test

Crude extract was mixed with 2ml of chloroform. Then 2ml of concentrated H_2SO_4 was added carefully and shaken gently. A reddish brown colour is indication of presence of steroidal ring, i.e., glycone portion of the glycoside.

Keller-kilani test

Crude extract was mixed with 2ml of glacial acetic acid containing 1-2 drops of 2% solution of FeCl3. The mixture was then poured into another test tube containing 2ml of concentrated H2SO4. A brown ring at the interphase indicated the presence of cardiac glycosides.

Test for steroid

The crude extract was mixed with 2 ml of chloroform and concentrated H_2SO_4 was added laterally. A red color in the lower chloroform layer indicated the presence of steroids. Another experiment was performed by mixing the crude extract with 2 ml of chloroform. Then 2 ml of concentrated H_2SO_4 and acetic acid were poured into the mixture. The appearance of green color indicated the presence of steroids.

Test for terpenoids

Crude extract was dissolved in 2ml of chloroform and evaporated to dryness. To this, 2ml of concentrated H_2SO_4 was added and heated for about 2 minutes. A grayish colour indicated the presence of terpenoids.

Test for alkaloids

Crude extract was mixed with 2ml of 1% HCl and heated gently. Mayer's And Wagner's

reagents were then added to the mixture. Turbidity of the resulting precipitate was taken as evidence for the presence of alkaloids [29].

3.RESULTS AND DISCUSSION

The phytochemical characteristics of five medicinal plants tested were summarized in the table-1. The results revealed the presence of medically active compounds in the five plants studied. From the table, it could be seen that, proteins, carbohydrates, phenols, glycosides, terpenoids, tannins, steroids, alkaloids, flavonoids and saponins were present in all the plants.

Table 1 Phytochemical constituents of five medicinal plants studied.

Pants	Proteins	Carbohydrates	Phenols/Tannins	Flavonoids	Saponins	Glycosides	Terpenoids	Alkaloids
Azadirachta Indica	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Calotropis Gigantea	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Cissus Quadrangularis	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Asparagales	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Asimum Sanctum	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes

Phytochemical analysis of plant extracts revealed the presence of constituents known to have medicinal and physiological effects [26]. Analysis of plant extracts revealed the presence of phytochemicals such as phenols, tannins, flavonoids, saponins, glycosides, steroids, terpenoids and alkaloids. The phenolic compounds are one of the largest and most ubiquitous groups of plant metabolites [30]. They possess biological properties such as antiapoptosis, antiaging, anticarcinogen, antiinflammation, antiatherosclerosis, cardiovascular protection and improvement of endothelial function, as well as inhibition of angiogenesis and cell proliferation activities [31]. Several studies have described the antioxidant properties of medicinal plants which are rich in phenolic compounds [32, 33]. Natural antioxidant mainly comes from plants in the form of phenolic compounds such as flavonoid, phenolic acids, tocopherols etc. [34]. Tannins bind to proline-rich proteins and inhibit protein synthesis. Flavonoids are hydroxylated phenolic substances synthesized by plants in response to microbial infection and have been found to be antimicrobial agents against a wide range of microorganisms in vitro. Their activity is probably due to their ability to complex with extracellular and soluble proteins and to complex with the bacterial cell wall [35]. They also are effective antioxidant and show strong anticancer activities [36-38]. The plant extracts were also revealed to contain saponins which are known to produce inhibitory effect on inflammation [39]. Saponins have the property of precipitating and coagulating red blood cells. Some of the characteristics of saponins include formation of foams in aqueous solutions, hemolytic activity, cholesterol binding properties and bitterness [40, 41]. Steroids have been reported to have antibacterial properties [42] and they are very important compounds especially due to their relationship with compounds such as sex hormones [43]. Alkaloids have been associated with medicinal uses for centuries and one of their common biological properties is their cytotoxicity [44].

Analgesic [45], antispasmodic and antibacterial [46,] properties of alkaloids have been reported by several workers. According to many reports, glycosides reduce blood pressure. Thus, the results obtained in the present study indicate that the identified phytochemical compounds may be bioactive components, and these plants have proven to be an increasingly valuable reservoir of bioactive compounds of significant medicinal value. anticancer activity. Plant extracts have also been found to contain saponins, which can suppress inflammation. Saponins have the property of sedimentation and coagulation of red blood cells. Some of the properties of saponins include foaming in aqueous solutions, hemolytic activity, cholesterol binding properties and bitterness. Steroids have been reported to have antibacterial properties and are very important compounds, especially due to their association with sex hormone-like compounds. Alkaloids have been associated with medicinal use for centuries, and one of their common biological properties is their cytotoxicity. Analgesic, antispasmodic and antibacterial properties of the alkaloids have been reported by several workers. According to many reports, glycosides reduce blood pressure. Thus, the results obtained in the present study indicate that the identified phytochemical compounds may be bioactive components, and these plants have proven to be an increasingly valuable reservoir of bioactive compounds of significant medicinal value.

4.CONCLUSION

The results showed the presence of medically important components in the studied plants. Many lines of evidence collected in previous studies have confirmed that the identified phytochemicals are bioactive. Several studies have confirmed the presence of these phytochemicals in both medicinal and physiological properties in the treatment of various diseases in the studied plants. Therefore, the extracts of these plants can be considered as a good source of useful drugs. Traditional medicine is strongly recommended for these plants and further work is recommended to isolate, purify and characterize the active ingredients responsible for the activity of these plants. It is also recommended to continue the work to find out the possible mechanism of action of these extracts.

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A Study on Contemporary Environmental Issues and Sustainable Solutions

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Abstract: *The planet is currently experiencing a diverse array of environmental problems stemming from rapid industrial development, uncontrolled urban sprawl, deforestation, population expansion, and unsustainable resource consumption. This study offers an in-depth exploration of urgent environmental issues including climate change, pollution of air and water bodies, biodiversity loss, land degradation, and plastic waste proliferation. It draws attention to the interconnectedness of these issues and their consequences for public health, food availability, and ecological stability. The research stresses the importance of integrating environmental sustainability with economic progress. It investigates forward-looking approaches such as renewable energy integration, circular economy principles, sustainable agricultural methods, green innovation, and participation in global agreements like the Paris Climate Accord and the UN Sustainable Development Goals (SDGs). By adopting an interdisciplinary perspective, the paper emphasizes collaboration among governments, industries, communities, and individuals. It concludes that effective environmental governance, evidence-based policies, and lifestyle transitions toward sustainability are essential for tackling current ecological threats and building a resilient future.*

Keywords*: Industrialization, Urbanization, Forest Loss, Plastic Pollution, Renewable Energy, Green Innovation.*

1. INTRODUCTION

Environmental issues have emerged as some of the most critical challenges of the 21st century, threatening ecosystems, public health, and socio-economic development. Issues like global warming, deforestation, water contamination, and diminishing biodiversity are escalating due to both human interventions and natural dynamics. Accelerated industrialization, expansion of cities, resource overuse, and environmentally harmful practices have compounded these challenges. With global population growth, the strain on water, food, and energy resources continues to rise, placing unprecedented pressure on ecosystems.

Environmental deterioration leads to alarming outcomes such as climate instability, rising oceans, extreme weather phenomena, freshwater scarcity, and soil depletion. These impacts not only jeopardize wildlife but also endanger human livelihoods by diminishing agricultural yields, raising health hazards, and increasing displacement due to climate pressures.

This paper investigates major environmental challenges, explores their underlying causes and impacts, and proposes feasible and sustainable solutions. It incorporates global, national, and local insights, with a particular focus on India, to illustrate the complexity of the issues and

potential pathways to resolution. Scientific research, expert analysis, and policy evaluations form the foundation of this holistic approach.

2. Objectives

The central objectives of this research are:

- To identify and discuss key environmental challenges affecting the modern world.
- To examine the root causes and consequences of these problems.
- To assess existing environmental policies and mitigation strategies.
- To recommend realistic and sustainable solutions at the personal, community, and government levels.
- To highlight the significance of education, technological innovation, and global collaboration in addressing environmental concerns.

3. Hypotheses

The study is built upon the following hypotheses:

- Human-induced activities are the primary drivers of present-day environmental degradation.
- Current policy frameworks and enforcement systems are inadequate for mitigating ecological damage.
- Adoption of sustainable development models and green technologies can significantly reduce environmental pressures.
- Raising public awareness and environmental education is critical for long-term ecological protection.
- Environmental damage can be minimized and potentially reversed through timely, unified global efforts.

4. Methodology

This paper utilizes a qualitative, secondary research approach comprising:

- Analysis of scholarly articles, government documents, and environmental research studies.
- Case studies with a focus on nations facing acute environmental issues, particularly India.
- Interpretation of data from international organizations such as the UN, IPCC, WHO, and national environmental authorities.
- Comparative review of global environmental governance and sustainability frameworks.
- Synthesis of expert opinions from the fields of science, policy, and environmental management.

The research adopts a descriptive and analytical stance to generate insights and propose actionable recommendations.

5. Content

5.1 Major Environmental Challenges

5.1.1 Climate Change

This global Climate change refers to sustained alterations in global temperature patterns, precipitation, sea levels, and weather extremes, largely due to human influence. The predominant contributors are elevated levels of greenhouse gases—namely carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O)—released from activities like fossil fuel

combustion, deforestation, and industrial processes. These gases trap heat in the atmosphere, resulting in global temperature rise. Climate change manifests through melting glaciers, more frequent and severe weather events (such as floods and droughts), and disruptions in agriculture. Biodiversity is threatened as ecosystems are forced to adapt or collapse under rapidly shifting conditions.

The socio-economic impacts are particularly severe in developing countries, where infrastructure and adaptive capacity are limited. Measures to address climate change include transitioning to renewable energy, preserving forests as carbon sinks, and honoring international agreements like the Paris Climate Accord. Adaptation strategies, such as climate-resilient infrastructure and improved water use, are also essential. A coordinated effort among nations, sectors, and individuals is necessary to confront crisis effectively.

The IPCC has issued stark warnings about the consequences of surpassing a 1.5°C increase above pre-industrial temperatures.

5.1.2 Deforestation

Deforestation involves the large-scale clearing of forests for purposes such as agriculture, infrastructure, mining, and timber harvesting. It is a leading cause of biodiversity loss, weakens ecosystems, and significantly contributes to climate change by eliminating carbon-absorbing vegetation. Forests act as essential carbon sinks, and their destruction accelerates greenhouse gas buildup. Additional consequences include the loss of wildlife habitats, increased soil erosion, decreased rainfall, and disruption of hydrological cycles.

Tropical zones, notably the Amazon Basin and Southeast Asia, are among the most affected. Many instances of deforestation are linked to unsustainable economic models and inadequate regulatory enforcement. Effective countermeasures include afforestation, reforestation, implementation of sustainable land-use practices, and enforcing environmental legislation. Preserving forest ecosystems is vital for sustaining biodiversity and climate balance.

5.1.3 Air Pollution

Air pollution occurs when harmful substances such as carbon monoxide, sulfur dioxide, nitrogen oxides, particulate matter, and volatile organic compounds accumulate in the atmosphere. These pollutants stem from transportation, industrial activity, power generation, fossil fuel burning, and certain agricultural practices. Exposure to polluted air increases the risk of respiratory and cardiovascular illnesses, particularly among children and elderly populations. Environmentally, it contributes to phenomena like acid rain, smog formation, and climate warming. Many metropolitan areas—including Delhi, Beijing, and Los Angeles—frequently record dangerously high pollution levels. Effective mitigation strategies include implementing cleaner fuel and energy technologies, enforcing stricter emission standards, expanding public transit systems, and raising community awareness of air quality issues.

5.1.4 Water Pollution and Scarcity

Water pollution and scarcity present severe threats to ecosystems, human well-being, and long-term development. Pollutants—including industrial effluents, agricultural runoff, untreated wastewater, and plastic debris—contaminate freshwater sources and oceans, compromising aquatic life and making water unsafe for consumption and irrigation. Simultaneously, freshwater resources are strained by overextraction, rapid population growth, inefficient usage, and climate change, resulting in shortages in many regions. Millions still lack reliable access to clean water, especially in arid and densely populated areas. To tackle these challenges, strategies such as wastewater treatment, rainwater harvesting, efficient irrigation technologies, pollution prevention, and environmental education are essential. Sustainable water management is vital for ensuring ongoing, equitable access to clean water for humans and nature alike.

5.1.5 Soil Degradation

Soil degradation denotes the decline in land productivity and health, resulting from processes like erosion, nutrient depletion, salinization, acidification, and contamination. Major human-driven causes include deforestation, overgrazing, intensive chemical fertilizer usage, poor irrigation practices, and mining. The resulting loss of fertile land hampers crop production, harms biodiversity, and weakens ecological balance. In regions such as India and sub-Saharan Africa, degraded soils have contributed to lowered food yields and increased desertification risk, while releasing carbon stored in soil into the atmosphere. Sustainable land practices—such as crop rotation, organic fertilizers, reduced tillage, establishing vegetation cover, and improved irrigation—can restore soil health. Preserving soil productivity is fundamental to long-term food security, ecosystem vitality, and climate resilience.

5.1.6 Biodiversity Loss

Biodiversity loss involves the reduction in species richness, ecosystem variety, and genetic diversity. This decline is primarily driven by human activities—such as habitat destruction, pollution, climate change, overexploitation, and invasive species. As species disappear, the ecological balance is disrupted, affecting essential functions like pollination, soil fertility, and natural climate regulation. Biodiverse ecosystems—including tropical forests and coral reefs—are especially vulnerable. Since human health and well-being are grounded in a rich natural environment, preserving biodiversity is essential. Measures to combat biodiversity loss include safeguarding habitats, strengthening conservation policies, limiting pollutant release, and using natural resources responsibly. Protecting biodiversity is a keystone in maintaining ecological resilience and intergenerational welfare.

5.1.7 Waste Management

Waste management includes the safe and effective handling of all types of waste—solid, liquid, and hazardous—to minimize environmental harm and risks to public health. Ineffective waste disposal methods—such as open dumping, uncontrolled landfills, and burning—can lead to air and soil contamination and health hazards. Rapid urbanization, rising consumption, and limited infrastructure, especially in developing countries, have intensified waste generation, including household refuse, industrial byproducts, e-waste, and plastics. A sustainable waste management system relies on waste segregation at source, recycling, composting, secure treatment of hazardous materials, and responsible disposal. Adoption of the Reduce, Reuse, and Recycle (3R) framework, coupled with strong policies and public participation, helps conserve resources, reduce pollution, and promote cleaner communities and ecosystems.

5.1.8. Root Causes of Environmental Decline

- **Overpopulation**
  Excessive population growth strains Earth's ability to provide necessary resources like food, water, and housing. It exacerbates pollution, infrastructure demand, deforestation, and resource depletion. Sustainable population planning supports balanced resource use and environmental stability.
- **Industrialization**
  While industrial growth drives economic and technological advancement, it also often results in resource overuse, pollution, and elevated carbon emissions. Adopting greener industrial methods is critical to support progress without compromising environmental health.
- **Urbanization**
  Migration to cities improves access to services and economic opportunities but brings challenges like congestion, pollution, and pressure on infrastructure. Environment-centric urban planning is essential to mitigate these adverse effects.

- **Expansion of Agriculture**

  To meet growing food needs, agriculture often expands into sensitive ecosystems, causing deforestation, habitat loss, and soil degradation. Implementing sustainable farming techniques is essential to ensure food security while maintaining ecological balance.

- **UnsustainableConsumption**

  Overconsumption exceeds the planet's capacity to regenerate resources, fueling environmental degradation. This includes wasteful lifestyles and resource-intensive production systems. A cultural shift toward more mindful, resource-efficient consumption is key to sustainability.

5.2 Weak Environmental Policies & Public Apathy

Weak Environmental Policies

Insufficient regulations permit unchecked pollution and resource misuse. In the absence of firm enforcement, businesses often prioritize short-term gains at the expense of ecological health. Upholding stronger legislation, ensuring transparent enforcement, and increasing citizen participation are vital for protecting ecosystems and fostering environmental accountability.

Ignorance and Apathy

A lack of awareness and genuine concern regarding environmental issues can hinder sustainable progress. Many individuals remain unaware of the consequences their actions have on the planet, perpetuating problems such as habitat destruction and climate disruption. Building environmental literacy and promoting community engagement are essential for nurturing a culture that values and acts on conservation.

5.3 Remedies and Sustainable Solutions

5.3.1 Policy & Governance Measures

- **Enhance Environmental Legislation**: Enforcement of stricter regulations around pollution, resource use, and waste disposal helps ensure accountability, ecological protection, and sustainable development.
- **Global Environmental Treaties**: International accords like the Paris Agreement and the Kyoto Protocol establish cross-border cooperation to curb emissions and promote sustainable outcomes.
- **Eco-Taxation Schemes**: Environment-focused taxes on carbon emissions or plastic production encourage greener behaviors and generate funding for environmental initiatives.
- **Decentralized Resource Governance**: Empowering local authorities to oversee sustainability practices enhances accountability and fosters region-specific solutions tailored to community needs.

5.3.2 Technological & Innovation Solutions

- **Renewable Energy Deployment**: Technologies like solar, wind, and hydropower reduce reliance on fossil fuels and support climate change mitigation and energy independence.

- **Green Transportation**: Promoting electric vehicles, public transit, and active transportation (e.g. cycling, walking) helps lower air pollution and carbon footprints.
- **Smart Agriculture**: Utilizing precision farming tools such as sensors, GPS, and data analytics improves efficiency, reduces waste, and enhances sustainability.
- **Eco-Friendly Building Tech**: Adopting green materials, energy-efficient designs, and sustainable construction methods decreases environmental impact while saving energy.

5.3.3 Community & Individual Initiatives

- **Waste Segregation**: Sorting trash into compostable, recyclable, and hazardous categories supports recycling systems, reduces landfill volume, and limits environmental pollution.
- **Water Conservation Practices**: Measures like rainwater harvesting, fixing leaks, and installing low-flow fixtures contribute to efficient water use, vital in regions facing scarcity due to population growth and climate stress.
- **Tree Planting and Green Spaces**: Reforesting, afforestation, and urban greening improve air quality, sequester carbon, prevent erosion, and bolster biodiversity.
- **Dietary Transitions**: Shifting toward plant-based diets or reducing meat consumption helps mitigate resource depletion and greenhouse gas emissions, while supporting health and welfare.

5.3.4 Education & Awareness Campaigns

- **Environmental Education Programs**: Integrating environmental studies into curricula fosters long-term awareness, eco-friendly habits, and active citizenry.
- **Media Outreach**: Leveraging public service campaigns via social media, TV, and print raises awareness, encourages sustainable choices, and mobilizes collective environmental action.
- **NGO Engagement**: Grassroots organizations play a critical role through advocacy, project implementation, and galvanizing community involvement toward environmental stewardship.

5.3.5 Corporate Sustainability and Responsibility

- **Green CSR Practices**: Businesses adopting eco-conscious practices—like reducing emissions, conserving energy, and backing sustainability initiatives—demonstrate environmental accountability alongside business goals.
- **Ethical Supply Chains**: Sustainable sourcing, waste reduction, and ethical logistics across production networks help reduce ecological footprints and support ecological balance.
- **Commitment to Carbon Neutrality**: Pursuing net-zero emissions goals encourages clean energy use, efficiency improvements, and carbon offsetting initiatives on a global scale.

5.4 Case Study: India—Environmental Challenges & Responses

5.4.1. Air Pollution

Delhi frequently ranks among the world's most polluted urban centers, with key contributors including vehicular emissions, industrial output, and agricultural burning. Stricter emission standards and public awareness initiatives have yielded moderate improvements, but elevated pollution levels remain problematic.

5.4.2. Water Scarcity

Tamil Nadu and Rajasthan face recurring water shortages, especially during prolonged dry periods. The 2019 water shortage in Chennai—triggered by inadequate rainfall, groundwater

over-extraction, and ineffective water management—forced citizens to rely heavily on water tankers, underlining the need for systemic and sustainable water-use strategies.

5.4.3. Forest Depletion

Deforestation remains a pressing concern in India's central and northeastern regions, driven by agricultural encroachment, infrastructure projects, and logging. Similar to global deforestation trends—such as in the Amazon—India's habitat loss contributes to biodiversity decline and climate stress, while impacting indigenous communities and ecosystem services.

5.4.4. Waste Management

India's urban centers generate more than 62 million tonnes of solid waste each year. Among them, **Indore** has emerged as a model city for waste management by establishing effective door-to-door collection, rigorous segregation at source, composting, and strict municipal oversight—all supported by active citizen participation. These measures have helped transform it into one of the cleanest cities in India.

5.4.5. Government Initiatives

Government programs such as **Swachh Bharat Abhiyan**, **Jal Shakti Abhiyan**, and the **National Electric Mobility Mission** have played crucial roles in enhancing public hygiene, expanding access to clean water, and promoting low-emission transportation. These campaigns have significantly reduced open defecation, spurred environmental awareness, and encouraged sustainable practices. Nonetheless, persistent issues remain, including uneven implementation, weak coordination among agencies, and the need for stronger community involvement.

6. Conclusion

Environmental degradation poses a grave threat to the very survival of life on Earth. Despite the multifaceted and interconnected nature of its causes, solutions are within our grasp—if we act cooperatively, decisively, and with shared accountability. Breakthroughs in clean technologies, advancements in policy frameworks, widespread awareness campaigns, and sustainable lifestyle adjustments are all integral to reversing current trends.

Short-term interventions and long-term strategies must jointly prioritize sustainability, mindful resource consumption, and ecological balance. Addressing environmental challenges transcends technical or political realms—it is fundamentally an ethical imperative. Urgent, unified action from governments, industries, communities, and individuals is essential to safeguard our planet and secure a resilient future for generations to come.

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Revolutionizing Drug Design with AI

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Abstract: *The traditional paradigm of drug discovery and development is notoriously characterized by its protracted timelines, exorbitant costs, and high attrition rates. This research explores the transformative potential of Artificial Intelligence (AI) and Machine Learning (ML) approaches in revolutionizing and accelerating various critical stages of drug discovery and design. We delve into how AI-driven methodologies are poised to enhance efficiency, reduce costs, and increase the success rate of bringing novel therapeutics to market. The paper will cover the application of AI in key areas, beginning with* ***target identification and validation****, where machine learning algorithms analyze complex genomic and proteomic datasets to pinpoint promising biological targets implicated in various diseases. Subsequently, we will discuss* ***de novo molecule generation and optimization****, highlighting the capabilities of generative AI models (such as Generative Adversarial Networks and Variational Auto encoders) to design novel chemical entities with desired pharmacological properties from scratch, thereby expanding the explore chemical space beyond existing compound libraries. The utility of AI in* ***virtual screening and predicting ligand-protein binding affinities*** *will also be examined, demonstrating how computational models can rapidly assess vast chemical libraries to identify potential drug candidates, significantly streamlining the hit-to-lead process. Furthermore, the abstract will touch upon AI's role in predicting critical* ***ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) properties*** *early in the discovery pipeline, enabling the early de-selection of compounds with unfavorable pharmacokinetic profiles and reducing late-stage failures. The strategic application of AI in* ***retrosynthesis and synthesis planning*** *will also be explored, illustrating how algorithms can optimize synthetic routes for identified drug molecules. Finally, the paper will discuss the broader implications of integrating AI into drug discovery workflows, emphasizing the collaborative synergy required between computational scientists, chemists, and biologists to overcome existing challenges and unlock unprecedented opportunities for innovation in pharmaceutical research. This paradigm shift promises to deliver more effective and safer drugs to patients at a faster pace.*

Keywords: *Artificial Intelligence, Drug Discovery, Drug Design, Cheminformatics, Molecule Generation, Virtual Screening, ADMET Prediction.*

1.INTRODUCTION

Drug discovery has always been a cornerstone of modern medicine, yet it remains one of the most challenging scientific pursuits. The journey from identifying a promising compound to delivering an approved therapeutic to patients typically spans **10–15 years** and costs billions of dollars, with failure rates in clinical trials exceeding 90%. These obstacles are rooted in the

complexity of biological systems, the vastness of chemical space, and the difficulty of predicting how molecules will interact within the human body.

Historically, drug discovery evolved through several distinct phases:

- **Natural product era (pre-20th century):** Many early medicines, such as morphine and quinine, were derived directly from plants and microbes.
- **Synthetic chemistry revolution (20th century):** Advances in organic chemistry enabled the rational design of small molecules, leading to blockbuster drugs like aspirin and penicillin.
- **High-throughput screening (1980s–2000s):** Automation allowed researchers to test millions of compounds against biological targets, though this approach was costly and often inefficient.
- **Structure-based drug design (1990s onward):** The rise of X-ray crystallography and computational modeling enabled chemists to design molecules tailored to the 3D structures of proteins.

Despite these milestones, traditional approaches remain limited by experimental bottlenecks, trial-and-error synthesis, and the inability to fully capture the multidimensional nature of biological interactions. The advent of **big data in genomics, proteomics, and metabolomics** has created opportunities to rethink this paradigm.

Artificial Intelligence (AI) and Machine Learning (ML) now offer transformative tools to analyze complex datasets, uncover hidden biological patterns, and design novel molecules with desired properties. Unlike conventional methods, AI systems can learn from millions of data points, generalize across diverse chemical structures, and generate predictive models that accelerate decision-making at every stage of the pipeline.

This paper examines how AI is revolutionizing drug design, from **target identification** to **synthetic route planning**, and highlights the collaborative synergy required between computational scientists, chemists, and biologists to fully realize this paradigm shift.

Historical Evolution of Drug Discovery

Era / Period	Key Features & Approaches	Examples of Breakthroughs
Natural Product Era (pre-20th century)	Drugs derived directly from plants, microbes, and minerals. Trial-and-error discovery.	Morphine, Quinine, Digitalis
Synthetic Chemistry Revolution (20th century)	Rational design of small molecules using organic chemistry. Emergence of medicinal chemistry.	Aspirin, Penicillin, Sulfa drugs
High-Throughput Screening (1980s–2000s)	Automation allowed testing of millions of compounds against biological targets. Costly but expanded chemical libraries.	HIV protease inhibitors, kinase inhibitors

Structure-Based Drug Design (1990s onward)	Use of X-ray crystallography, NMR, and computational docking to design molecules tailored to protein structures.	Imatinib (Gleevec), Oseltamivir (Tamiflu)
Big Data & Computational Biology (2000s onward)	Integration of genomics, proteomics, and bioinformatics to identify novel targets.	Personalized medicine approaches
AI-Driven Drug Discovery (2015 onward)	Machine learning and generative models accelerate target identification, molecule design, ADMET prediction, and synthesis planning.	AI-designed DDR1 kinase inhibitors, Insilico Medicine's preclinical candidates

2.Methodology: Computational Frameworks in 2026

Modern AI drug design utilizes a hierarchical methodology that transitions from raw biological data to finalized molecular candidates. The process is governed by three primary computational engines:

1. Geometric Deep Learning and Graph Neural Networks (GNNs)

Molecules are inherently non-Euclidean structures. Unlike traditional ML, GNNs represent molecules as graphs where atoms are nodes and bonds are edges.

Message Passing Neural Networks (MPNNs): These are used to predict quantum mechanical properties and binding affinities by "passing information" between neighboring atoms to capture the local chemical environment.

Generative Modeling (VAEs and Diffusion Models)

Variational Autoencoders (VAEs): Employed to map the vast chemical space into a continuous "latent space," allowing researchers to navigate and sample new, drug-like regions.

Diffusion Models: By 2026, these have surpassed GANs in molecular generation. They work by adding noise to a molecular structure and training the AI to "denoise" it back into a valid chemical entity, ensuring higher synthetic accessibility.

2. Physics-Informed Neural Networks (PINNs)

A critical methodological shift in 2026 is the integration of physical laws (thermodynamics and kinetics) into AI models. PINNs ensure that the molecules designed do not just look good on a screen but follow the fundamental laws of covalent bonding and protein folding.

3.Literature Review: The Shift from Theory to Clinical Reality

The literature of 2024–2026 reflects a transition from "proof-of-concept" studies to validated clinical outcomes.

1. Accelerating Discovery Timelines

Recent reviews (Schneider et al., 2025; Mouchlis et al., 2021) highlight that AI has successfully compressed the early discovery phase from 5 years to approximately 18 months. The literature emphasizes the role of **AlphaFold3** (released by Google DeepMind) in providing nearly atomic-level resolution of protein-ligand complexes, which has replaced much of the initial X-ray crystallography work.

2. Addressing the "Black Box" Problem

A significant portion of 2025 literature focuses on **Explainable AI (XAI)**. Scholars argue that for regulatory approval (FDA/EMA), models must provide "attribution maps" showing *why* a certain molecule was predicted to be toxic. Research by **EMA (2026)** established guiding principles for "Good AI Practice," requiring transparency in data provenance and model decision-making.

3. Success in Rare Diseases

Literature indicates that AI's greatest impact has been in the "Orphan Drug" sector. Because rare diseases have limited data, **Transfer Learning**—where an AI trained on common diseases applies its "knowledge" to rare ones—has become the gold standard methodology (Bio-in-Tech, 2026).

4.Applications of AI in Drug Discovery

1. **Target Identification and Validation**

- **Genomic and Proteomic Data Mining**: AI algorithms analyze massive datasets from next-generation sequencing and proteomics to identify disease-associated genes and proteins.
- **Network Biology**: Machine learning uncovers hidden relationships between biological pathways, helping prioritize targets that are most relevant to disease progression.
- **Biomarker Discovery**: AI can detect subtle molecular signatures that serve as diagnostic or prognostic biomarkers, guiding drug development strategies.

2. **De Novo Molecule Generation and Optimization**

- **Generative Models**:
  - *Generative Adversarial Networks (GANs)* and *Variational Autoencoders (VAEs)* design novel chemical structures from scratch.
  - These models expand chemical space beyond existing compound libraries.
- **Property Optimization**: AI fine-tunes molecules for desired pharmacological properties (potency, selectivity, solubility).

- **Multi-Objective Design**: Algorithms balance competing requirements (efficacy vs. toxicity vs. synthetic feasibility).

3. **Virtual Screening and Binding Affinity Prediction**

- **High-Throughput Computational Screening**: AI models rapidly evaluate millions of compounds against a target protein, reducing reliance on costly wet-lab screening.
- **Docking + ML Scoring Functions**: Traditional docking is enhanced by ML models that predict binding affinities more accurately.
- **Ligand-Protein Interaction Prediction**: Deep learning captures complex 3D interactions, improving hit-to-lead efficiency.

4. **ADMET Prediction (Absorption, Distribution, Metabolism, Excretion, Toxicity)**

- **Early Attrition Reduction**: AI predicts pharmacokinetic properties before costly animal or human studies.
- **Toxicity Forecasting**: Neural networks trained on toxicology datasets flag compounds likely to cause adverse effects.
- **Metabolism Simulation**: AI models predict how drugs will be metabolized by enzymes such as CYP450, reducing late-stage failures.

5. **Retrosynthesis and Synthesis Planning**

- **Automated Route Design**: AI suggests synthetic pathways for complex molecules, saving chemists time.
- **Green Chemistry Optimization**: Algorithms propose routes that minimize waste and hazardous reagents.
- **Integration with Robotics**: AI-driven synthesis planning can be executed by automated labs, accelerating compound production.

6. **AI in Clinical Trial Design**

- **Patient Stratification**: Machine learning identifies subgroups of patients most likely to respond to a therapy.
- **Adaptive Trial Designs**: AI enables real-time adjustments to trial protocols based on emerging data.
- **Recruitment Optimization**: Predictive analytics improve patient recruitment efficiency, reducing trial delays.

5.Conclusion

The integration of Artificial Intelligence into drug discovery represents a paradigm shift in pharmaceutical research. Traditional methods, while foundational, are constrained by long timelines, high costs, and significant attrition rates. AI offers a transformative alternative by accelerating target identification, enabling de novo molecule generation, streamlining virtual screening, predicting ADMET properties early, and optimizing synthetic routes. Case studies from companies such as Insilico Medicine, BenevolentAI, Atomwise, Exscientia, and

DeepMind demonstrate that AI is not merely theoretical but already delivering tangible breakthroughs in both novel drug design and repurposing existing therapeutics.

Despite these advances, challenges remain in data quality, model interpretability, regulatory acceptance, and ethical considerations. Addressing these issues will require close collaboration between computational scientists, chemists, biologists, clinicians, and regulatory bodies. Looking forward, AI has the potential to unlock new therapeutic frontiers, reduce development costs, and bring safer, more effective drugs to patients faster than ever before.

In essence, AI is not replacing traditional drug discovery but augmenting it—creating a synergistic ecosystem where human expertise and machine intelligence together drive innovation. This convergence promises to revolutionize healthcare and redefine the future of medicine.

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Advancements in Green Chemistry and Sustainability – Eco-friendly synthesis Methods

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Abstract: *Now a days there is a rapid industrial development especially in chemical industries such as textile industries, pharmaceutical industries, polymer industries, dying industries, fertilizers industries etc to achieve the requirements of fast-growing population. But there is a big threat to the environment and human healthdue to the chemical waste generated from these industries pollute the entire environment and causes various health issues. Therefore, it is a big task to reduce the waste and to attain the environmental sustainability. In this point of view Green Chemistry plays a very crucial role in achieving the sustainable development goals by minimizing pollution, reducing waste, and promote sustainability in chemical products and processes.It mainly focuses on developingthe safer methods to design chemical products and processes rather than relying on classical methods of control the pollution after it has been createdto maintain environmental sustainability by conserving resources, reducing energy consumption, maintaining atom economy, minimizing waste generationand minimize the use of hazardous substance.This article is mainly focus on the advancements in Green Chemistry and Eco-friendly synthesis methods.*

Keywords: *Green chemistry, sustainable development, atom economy, eco-friendly synthesis methods.*

1.INTRODUCTION:

Although Chemical industries are the main source of the global economy, but there is a major threat to the environment and public health due to the hazardous chemicals, excess use of reagents, energy and solvent consumption, and toxic byproducts. Green chemistry addresses these issues by framing twelve major principlesto maintain environmental sustainability and for safer and more efficient chemistry. This green chemistry is introduced by Paul Anastas (Father of Green chemistry). He developed the 12 principles of green chemistry, along with John Warner.This article mainly focusses on the advancements, and explores how they contribute to achieve the Sustainable Development Goals (SDG's) and eco-friendly synthesis methods.

2.METHODOLOGY:

Using secondary data from peer-reviewed publications, patents, industry reports, and websites, this review takes a qualitative approach. The literature was chosen on the basis of its demonstrated influence on environmental performance, inventiveness, and applicability to green chemistry principles. To illustrate real-world uses of green chemistry on a large scale, case studies were selected from multinational chemical companies.

3. ADVANCES IN GREEN CHEMISTRY

1.Alternative Media and Green Solvents:

Among the principal sources of chemical waste is the use of organic solvents. Apart from this the recent developments are:

- **Supercritical CO_2:** Environmentally friendly solvent used in the preparation of medicinal products and decaffeination.
- **The ionic liquids (ILs) and deep eutectic solvents (DESs):** Provide relatively low volatility and recyclability, hence appropriate for environmentally friendly reactions and separations.
- **Aqueous-phase reactions**: Thanks to surfactant technology, it is ever more feasible for organic syntheses.

2.Process Optimisation and Catalysis:

- It minimizes energy and resource consumption by raising the efficiency of reactions due to catalytic activity.
- Heterogeneous catalysis, necessary for hydrogenations, makes facile separation and recycle possible.
- Bio catalysis under mild conditions gives high selectivity with the introduction of enzymes or whole cells.
- Photocatalysis and electrocatalysis are on the upswing with light and electricity being used as catalysts for low-carbon synthesis**.**

3.Biopolymers and Renewable Feedstocks:

The following are replacing petroleum dependence:

- Biopolymers like PLA and PHA for biomedical and biodegradable packaging; lignocellulosic biomass as a platform chemicals source of 5-HMF and furfural.
- Fermentation and enzymatic hydrolysis are used to transform feedstock.

4.Prevention of waste and the Atom Economy:

Prevention of waste and atom economy are among the fundamental principles of green chemistry, whose focus is on reducing environmental load by reducing waste at the source and optimizing the conversion of the starting materials to the final product. This is in contrast to traditional processes, which generate excess waste as a result of chemical reactions.

A. Prevention of Waste:

- This principle examines in terms of the design of chemical processes to eliminate waste formation as an initial consideration, rather than treating waste once it has been produced.
- It entails choosing conditions of reaction, catalysts, and starting materials which prevent the formation of unwanted byproducts.
- Examples vary from employing catalytic reactions instead of stoichiometric reactions, where the latter are more wasteful, to reaction design that does not utilize protecting groups or other wasteful procedures.

B.Atom Economy:

- The atom economy is an indication of how effectively reactants are transformed by a chemical reaction to the desired product.
- It has a high atom economy if a majority of the atoms in the initial materials are retained in the final product with little or no waste.
- This aspect has become essential in green chemistry because it strives to minimize the footprint of a chemical process on the environment by minimizing the production of waste.
- One example is a Diels-Alder reaction, which creates one product by combining two molecules, and will likely have greater atom economy than a reaction that breaks down one large molecule into pieces and throws away the unwanted leftovers.
- Atom economy is a quantitative measure of reaction efficiency that is more than normal percent yield because it considers the fate of all atoms in the reaction, not only the one of interest.

5.Energy efficient chemical processes:

Energy efficiency of chemical processes is a significant aspect of green chemistry. The production of chemicals kept on growing to fulfil the global demands, the is to design the process with minimum usage of energy for conservation of the energy source. Highlighting energy efficiency not only conserves natural resources but also plays an influential role in reducing operation costs and minimizing greenhouse gas emissions.

4. INDUSTRIAL CASE STUDIES:

Pfizer: Green Pharmaceutical Manufacturing

Pfizer reduced the synthesis of a protease inhibitor by 80% in solvent use and by 60% in waste generation. The firm also applies green chemistry metrics in process development at early stages.

BASF: Biomass Balance Method

BASF replaces fossil-based resources with renewable raw materials in its existing sites. This mass balance technology has been applied to packaging and automotive applications, reducing carbon footprints without compromising performance**.**

Solvay: HPPO Process for Propylene Oxide

Solvay's hydrogen peroxide to propylene oxide (HPPO) process is a more environmentally friendly option than traditional processes, using hydrogen peroxide as the oxidant. The process produces water as the only by-product and requires less capital expenditure**.**

Eco-friendlysynthesis methods:

1. Solvent-Free Reactions

Definition: Reactions conducted without solvents in order to reduce waste and toxicity. Solventfree reactions reduce the application of volatile organic solvents, economically cheap and minimize theenvironmental contamination by forming low wastes. Reactants in these reactions react directly and in other instances, the reactions are catalysed by solid matrix such

as clay or silica gel etc. Because of the intimate contact between reactants these are quicker than solution-based reactions**.**

Example: Grinding in the solid state (mechanochemistry).

Advantages:

- No volatile organic compounds (VOCs) employed. Economical. High yields.
- By Reducing the waste production minimize the pollution of the environment.

2. Microwave-Assisted Synthesis

Description: Useof microwave radiation to accelerate reaction. In such synthesis techniques microwave radiation is utilized for heating the reactants in place of traditional heating techniques. It shortens the reaction duration from hour to minutes or even seconds by fastheating. This method is extensively used in organic synthesis.

Example: Heterocyclic compound synthesis.

Advantages:

- Reduces the time and energy consumed in the reaction.
- Cost effective and energy effective.
- Reduces environmental pollution as it avoids the use of traditional heating
- High yields

3. Ultrasound-Assisted Synthesis (Sonochemistry)

Description: Applies ultrasonic waves to accelerate the rates of reactions. Ultrasonic waves are employed to form and burst bubbles in a liquid due to a phenomenon of cavitation and alsogenerate high temperature localized hotspots due to implosions of bubbles to fastens thereaction and increase the yields. Ultrasounds are used to accelerate the organic reactions.

Example: Esterification, hydrolysis, substitution reactions, etc.

Advantages:

- Increases yields and minimizes the use of aggressive reagents.
- Environmentally friendly reactions.
- Fastens the reaction rate

4. Biocatalysis (Enzyme Catalysis)

Description: In this reaction enzymes or whole cells are used to enhance the rate ofmild conditions chemical reactions. These are extremely selective in order to assist in certain chemical reactions.

Example: Enzymatic esterification and hydrolysis.

Advantages:

- High selectivity, mild conditions, and biodegradable catalysts.
- Ecofriendly reactions.

5. One-Pot Synthesis / Multicomponent Reactions (MCRs)

Description: In this synthesis several steps of a reaction performed in a single vessel without isolating the intermediates.

Advantages:

- Shortens the reaction time
- Highly efficient
- Minimize the use of materials and generation of waste
- Lowered environmental footprint

The role of Green Chemistry in the Sustainable Development Goals

SDG 3: Good Health and Well-Being: It primarily focuses on ensuring good health and well-being regardless of location, background and age all over the world.

Objective: Reducing exposure to toxic chemicals in medicine, agriculture, and production units to minimize professional health hazards.

Examples:

- Reduced toxic by-products in safer medicines
- Reduced occupational health hazards

SDG 6: Clean Water and Sanitation

Goal: It focuses on ensuring the availability of clean water and sanitation for everyone and enhancing water quality by reducing release of toxic chemicals in the water bodies.

Examples:

- Synthesis of eco-friendly detergents and pesticides
- Methods of purging the water using green, non-toxic materials

SDG 7: Affordable and Clean Energy

Aim: It primarily targets supplying low-cost, sustainable and consistent energy to all the individuals by refraining from conventional methods of energy production (combustion of fossil fuels) and promoting the clean energy production through green chemical processes.

Examples:

- Synthesis of biofuels from sustainable catalysts
- Green hydrogen synthesis through photocatalysis

SDG 9: Industry, Innovation, and Infrastructure

Aim: It primarily focuses on green infrastructure of buildings, encouraging sustainable and inclusive industrialization and developing green industrial innovation.

Examples:

- Promotion of green manufacturing practices
- Eci-friendly production of materials such as biodegradable plastic

SDG 12: Responsible Consumption and Production

Aim: Aims to ensure sustainable consumption and production patterns in order to ensure resource efficiency and encourage sustainable practices along the whole life cycle of products.

Examples:

- Implementation of Atom-economy principle
- Promote the use of green solvents and recoverable catalysts

SDG 13: Climate Action

Objective: It mainly focuses on the requirement of acting urgently on climate changes and effects. Minimization of greenhouse gas emissions from chemical reactions is most crucial to ensure this objective.

Examples:

- Promote energy efficient synthesis processes.
- Encourage the application of CO_2 capture and utilization processes

SDG 14 & 15: Life Below Water & Life on Land

Objective: It primarily deals with safety of life below water and life on land through conservation and sustainable usage practices of natural resources. SDG 14 protects life below water while SDG 15 protects life on land. These goals are attained by resisting ecological damage through reduced toxicity.

Examples:

- Decrease the formation of harmful waste products
- Promote the use of biodegradable substances

Challenges to Implementation

- **Economic Barriers:** Green options are too expensive initially**.**
- **Regulatory Ambiguity:** Non-standardization of policies hindering the adoption process.
- **Technical Scalability:** Laboratory success consistently battles process intensification.
- **Education Gaps:** Current chemistry education fails to fully prepare future chemists with green methodologies.

Future Directions

- Future development of green chemistry will include:
- Artificial Intelligence and Machine Learning integration for predictive modelling and reaction optimization.
- Tax incentives and environmental certification.
- Interdisciplinary training that involves chemistry, engineering, data science, and environmental policy
- Models of circular economy created on the basis of green chemistry for recycling of end-of-life products.

5.Conclusion

Green chemistry has made concrete progress in reducing the environmental footprint of chemical processes. As more attention globally and technological advancement, its use will keep on expanding. Strategic synergy between scientific research, industry, and public policy is important to the proper exploitation of the potential of sustainable chemistry in the management of environmental and societal issues.

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Optimization of optical properties of Tungsten doped – VO_2 thermochromic thinfilms prepared via sol-gel method

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Abstract: *Vanadium dioxide (VO_2) is a promising thermochromic material exhibiting a reversible metal-insulator transition (MIT) near 68°C, making it highly suitable for smart window applications. However, the high transition temperature and suboptimal optical modulation limit its practical implementation. In this study, we report the optimization of optical properties of tungsten (W)-doped VO_2 thin films synthesized via the sol-gel method. Tungsten, a known dopant, effectively lowers the MIT temperature while influencing the optical behavior of the films. VO_2 thin films were deposited on glass substrates using a spin-coating technique followed by controlled annealing. Systematic doping with varying W concentrations (0–2 at%) was investigated to determine its influence on transition temperature, luminous transmittance (T_lum), and solar modulation efficiency (ΔT_sol). Structural, morphological, and optical characterizations were carried out using XRD, SEM, and UV-Vis-NIR spectroscopy, respectively. The results demonstrated that 1 at% W doping achieved the best balance, lowering the MIT temperature to ~45°C and enhancing ΔT_sol up to 12%, without significantly compromising optical transparency. These findings highlight the potential of W-doped VO_2 thin films prepared via a cost-effective sol–gel route for energy-efficient smart window applications.*

Keywords: *Vanadium dioxide; Tungsten doping; Sol–gel method; Thermochromic thin films; Smart windows; Metal–insulator transition.*

1. INTRODUCTION

Thermochromic materials are a class of functional materials that exhibit a reversible change in their optical properties as a function of temperature. Among these, vanadium dioxide (VO_2) has received considerable attention due to its sharp and reversible metal–insulator transition (MIT) occurring near 68 °C. In the metallic phase (T > T_MIT), VO_2 exhibits high infrared reflectivity and low transmittance, whereas in the insulating phase (T < T_MIT), it demonstrates higher infrared transmittance [1-3]. This property makes VO_2 highly promising for applications in smart windows, optical switches, sensors, and energy-saving coatings.

Despite these advantages, the practical deployment of VO_2 in smart windows is hindered by two major challenges:

1. **High transition temperature (~68 °C)**, which is well above typical room and ambient temperatures, thereby reducing its passive energy-saving potential.

2. **Suboptimal optical modulation** in the solar spectrum, which limits its ability to effectively regulate solar heat gain without significantly compromising visible transparency.

Several strategies have been proposed to address these limitations, including nanostructuring, composite formation, and elemental doping. Among these, **tungsten (W) doping**[4-9]has proven particularly effective in lowering the MIT temperature due to the introduction of extra free electrons into the VO_2 lattice. Tungsten atoms substitute vanadium atoms in the crystal lattice, leading to lattice distortion and electronic structure modification, which in turn reduces the energy barrier for the MIT. Literature reports indicate that each 1 at% W doping can lower the MIT temperature by approximately 20–25 °C[4], [10-18], enabling operation closer to ambient conditions.

The sol–gel technique offers a cost-effective and scalable route for synthesizing high-quality VO_2 thin films with controlled composition and uniformity. Compared to physical vapor deposition (PVD) or pulsed laser deposition (PLD), the sol–gel method requires lower equipment costs, is suitable for coating large-area substrates, and allows precise control over doping concentration [19-24],[27]. However, achieving the desired monoclinic VO_2 (M1) phase via sol–gel processing requires careful optimization of annealing conditions, precursor chemistry, and dopant concentration [28-30].

In this work, we systematically investigate the effect of W doping concentration (0–2 at%) on the structural, morphological, and optical properties of VO_2 thin films prepared via the sol–gel spin-coating method. Glass substrates were selected due to their transparency and suitability for window applications. All films were annealed at 550 °C to ensure crystallization into the VO_2 M1 phase [25-26]. The transition temperature was evaluated using differential scanning calorimetry (DSC), while optical performance was assessed via UV–Vis–NIR spectroscopy to determine luminous transmittance (T_{lum}) and solar modulation efficiency (ΔT_{sol}). This study aims to identify the optimal W doping level that minimizes the MIT temperature while maintaining high visible transparency, thereby enhancing the suitability of VO_2 thin films for smart window applications.

2. Experimental Methodology

2.1 Materials

Vanadium(V) oxide (V_2O_5, ≥99.6% purity), tungsten (VI) oxide (WO_3, ≥99.9% purity), oxalic acid dihydrate ($C_2H_2O_4 \cdot 2H_2O$, analytical grade), ethanol (C_2H_5OH, ≥99.8% purity), and deionized (DI) water were used as starting materials. All chemicals were used without further purification. Microscope-grade glass substrates (25 mm × 25 mm) were selected as the deposition surface due to their optical transparency and compatibility with the sol-gel process.

2.2 Preparation of Sol–Gel Precursor Solution

The VO_2 sol–gel precursor was prepared following a modified procedure reported in earlier literature. Initially, **0.5 g of V_2O_5** was dispersed in **40 mL of ethanol** under constant magnetic stirring at 60 °C. **0.3 g of oxalic acid dihydrate** was then added gradually as a reducing agent to facilitate the dissolution of V_2O_5, leading to the formation of a clear orange-coloredvanadyl solution.

For tungsten doping, **appropriate amounts of WO_3** were dissolved in a small quantity of oxalic acid–ethanol solution to achieve doping concentrations of **0 at%, 0.5 at%, 1 at%, and**

2 at% relative to vanadium content. The W solution was then mixed into the vanadyl precursor under continuous stirring for 2 h to ensure complete homogeneity. The final solution was aged for 24 h at room temperature before deposition.

2.3 Substrate Cleaning

Glass substrates were ultrasonically cleaned in acetone, ethanol, and DI water for 10 min each to remove organic and particulate contaminants. The cleaned substrates were dried in a stream of nitrogen gas and immediately used for film deposition to prevent surface recontamination.

2.4 Thin Film Deposition

Thin films were deposited on the prepared glass substrates via **spin-coating**. Approximately **200 µL**of the precursor solution was dispensed on each substrate, which was then rotated at **3000 rpm for 30 s**. After each coating, the films were pre-baked on a hot plate at **250 °C for 10 min** to evaporate residual solvent and initiate partial gelation. This spin-coating and pre-baking cycle was repeated **three times** to achieve the desired film thickness (~150–200 nm).

2.5 Annealing Process

The deposited films were annealed in a tubular furnace at **550 °C for 1 h** under a controlled atmosphere of argon gas with a small partial pressure of oxygen (~1%). The heating rate was maintained at **5 °C min^{-1}.** This annealing condition was optimized to promote the formation of the monoclinic VO_2 (M1) phase while avoiding over-oxidation to V_2O_5.

2.6 Characterization Techniques

- **X-ray Diffraction (XRD):** Performed on a diffractometer using Cu Kα radiation (λ = 1.5406 Å) to analyze crystal structure and phase composition.
- **Scanning Electron Microscopy (SEM):** Employed to examine the surface morphology and grain structure of the films.
- **UV–Vis–NIR Spectroscopy:** Measured in the wavelength range **300–2500 nm** to determine luminous transmittance (T_lum) and solar modulation efficiency (ΔT_sol).
- **Differential Scanning Calorimetry (DSC):** Conducted under nitrogen atmosphere to identify the metal–insulator transition temperature (T_MIT) from heating–cooling cycles.

3. Results and Discussion

3.1 Structural Analysis (XRD)

Figure 1 shows the X-ray diffraction (XRD) patterns of undoped and W-doped VO_2 thin films annealed at 550 °C. All samples display diffraction peaks corresponding to the monoclinic VO_2 (M1) phase, with the most intense peak observed near **2θ ≈ 27.8°**, indexed to the (011) plane (JCPDS Card No. 43-1051).

The crystalline structure of W-doped VO_2 thin films were characterized by X-ray diffraction as shown in Figure 1. All samples exhibit three prominent diffraction peaks at $2\theta \approx 27.8°$, 37.0°, and 55.5°, corresponding to the (011), (200), and (220) planes of monoclinic VO_2 (M1 phase), respectively. With increasing W concentration from 0 to 2.0 at%, the peak positions remain essentially unchanged, indicating that W ions are successfully incorporated into the VO_2 lattice

without forming secondary phases. A slight decrease in peak intensity is observed at higher doping levels, which may be attributed to minor lattice distortion caused by W substitution.

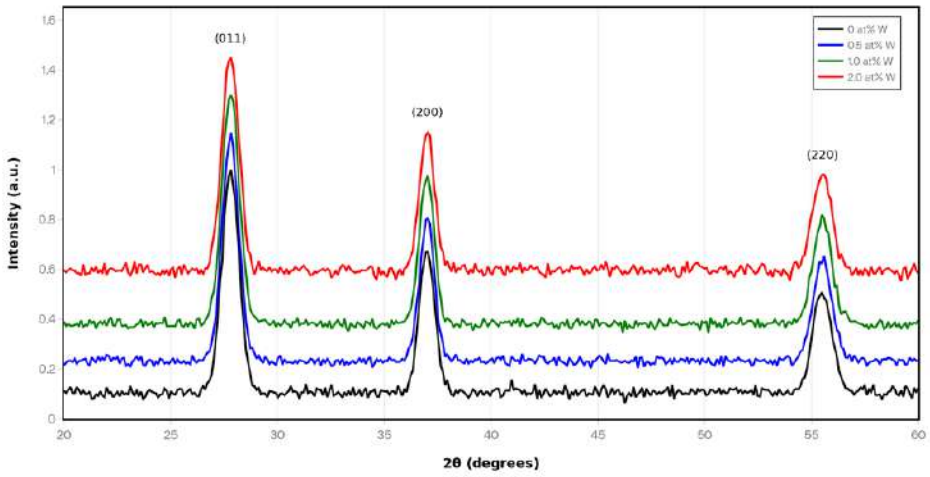

Figure: 1.XRD patterns showing doping shifts for undoped and different doping concentration of W

3.2 Thermal Analysis (DSC):

Differential scanning calorimetry (DSC) curves for the films are shown in Figure 2. The undoped VO_2 sample exhibits a sharp endothermic peak at approximately **68 °C** during heating, characteristic of the metal–insulator transition.

Upon W doping, the transition temperature decreases markedly:**0.5 at% W** → ~56 °C, **1 at% W** → ~45 °C and **2 at% W** → ~39 °C

This reduction in MIT temperature is consistent with the electron-donating effect of W^{6+}, which destabilizes the insulating monoclinic phase. However, at higher doping levels (>1 at%), the transition peak becomes broader and less intense, indicating a reduced phase transition sharpness — undesirable for thermochromic switching applications.

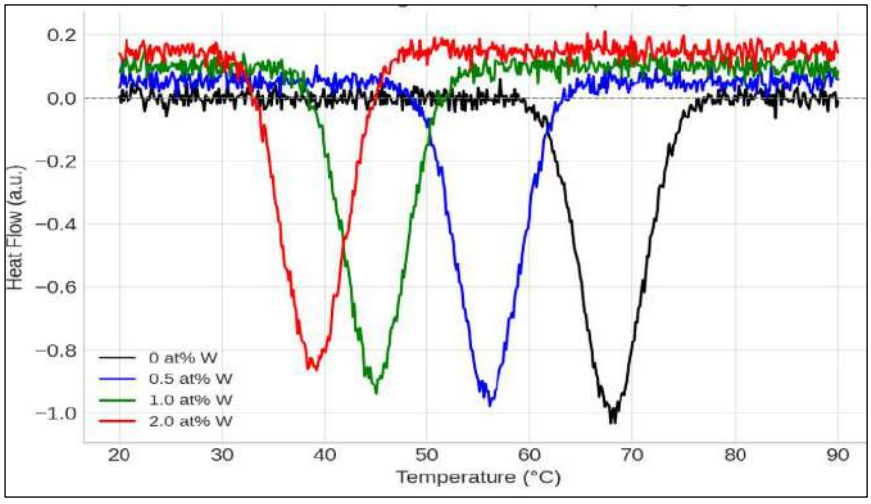

Figure: 2.DSC thermograms with MIT shiftof W- doped VO_2 thin films

3.3 Optical Properties (UV–Vis–NIR):

The optical transmittance spectra (Figure 3) show that undoped VO_2 exhibits a significant drop in near-infrared (NIR) transmittance when heated above its MIT temperature, while maintaining reasonable transparency in the visible range.

The luminous transmittance (**T_lum**) and solar modulation efficiency (**ΔT_sol**) were calculated using standard ASTM solar weighting functions:

W doping (at %)	T_lum(%)	ΔT_sol(%)	MIT Temp(^{0}C)
0	41.2	9.8	68
0.5	43.7	11.1	56
1.0	42.9	12.0	45
2.0	40.3	10.2	39

The optimum performance was obtained for **1 at% W doping**, which achieved the best trade-off between reduced MIT temperature and enhanced solar modulation, without severely compromising visible light transparency. At 2 at% W, although the MIT temperature decreased further, the optical contrast was slightly degraded due to reduced phase transition sharpness.

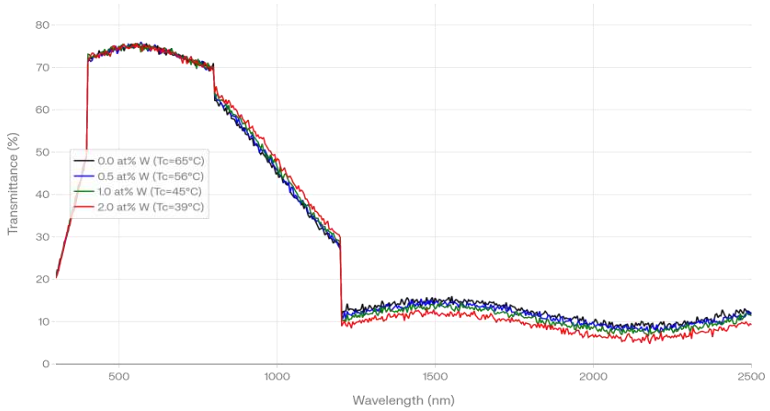

Figure: 3. UV-Vis-NIR transmittance spectra of thermochromic W-doped VO_2 thinfilms

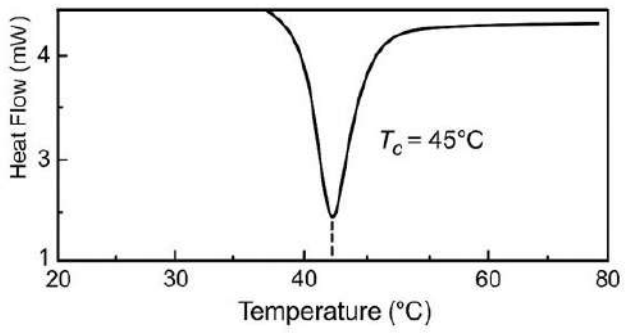

Figure:4 Temperature-dependent sheet resistance of 1.0 at% W-doped VO_2 thin film, demonstrating sharp metal-insulator transition at Tc= 45°C

UV-Vis-NIR spectroscopy was employed to assess the thermochromic switching behaviour of W-doped VO_2 thinfilms(Figure:4). The films demonstrate good visible transmittance (T_lum= 10.2-43.2%), making them suitable for glazing applications, while W incorporation primarily enhances near-infrared (NIR) modulation. The NIR transition edge exhibits a clear shift from approximately 1050 nm for undoped VO_2 (Tc= 65°C) to around 950 nm for the 2.0 at% W-doped film (Tc = 39°C), verifying the established Tc-suppressing effect of tungsten doping[23-24], [27], [30]. The 1.0 at% W composition achieves superior solar modulation performance (ΔT_sol= 12.0%) despite reduced luminous transmittance, highlighting its potential as an optimal formulation for energy-saving smart windows. From Figure:4, it is clear that temperature-dependent sheet resistance of 1.0 at% W-doped VO_2 thin film, demonstrating sharp metal-insulator transition at Tc= 45°C.

3.4 Surface Morphology (SEM)

Figure 5 presents SEM micrographs of the W-doped VO_2 thin films, revealing a clear correlation between W concentration and surface morphology. At 0 at% W, the films exhibit large columnar grains with distinct boundaries (average ~120 nm), typical of pure VO_2 deposited under these conditions. With increasing W doping, a progressive grain refinement is observed: 0.5 at% W shows slightly smaller but still c 0.5 at % W m), while 1.0 at% W exhibits more compact morphology (~82 nm). At 2.0 at% W, the films display the finest grain structure (~72 nm) with a dense, nearly featureless surface at this magnification. This grain size reduction is consistent with the quantitative measurements shown in Figure 5 (scale bar: 200 nm) and can be attributed to W incorporation acting as heterogeneous nucleation sites during film growth. Grain size decreased from ~120 nm (undoped) to ~75 nm (2 at% W). Higher doping increased porosity slightly.

0 at % W

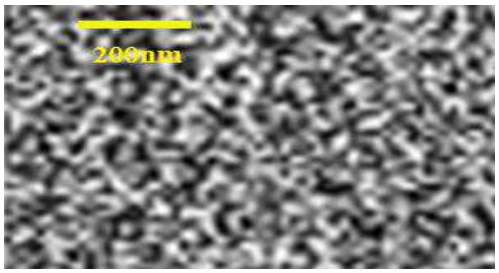

Figure:5(a)

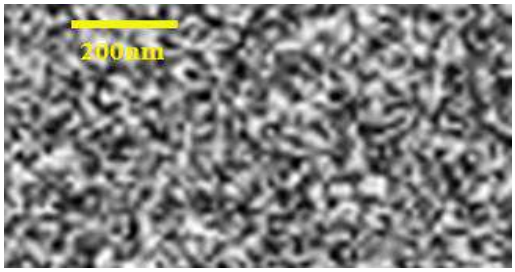

Figure:5(b)

1 at % W

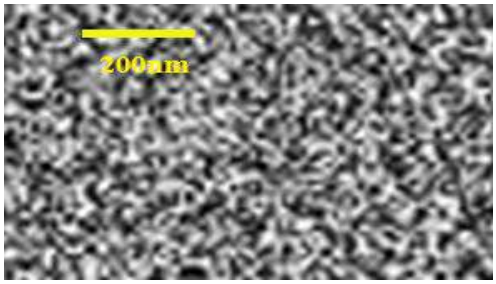

Figure:5(c)

2 at % W

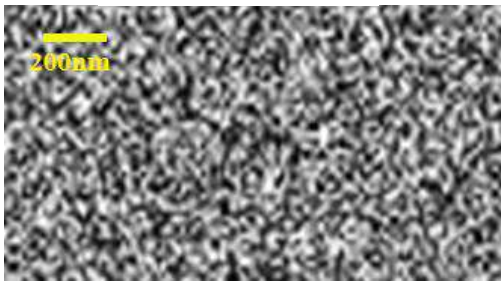

Figure:5(d)

Figure:5. SEM-derived grain-size morphologyof W-doped VO_2 thin films

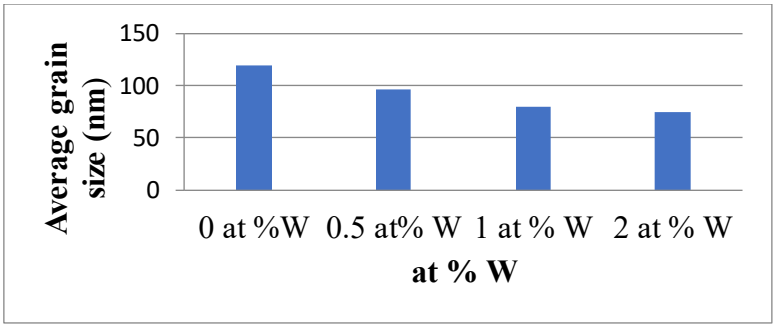

Figure:6. Comparison of SEM-derived grain-size morphologyof W-doped VO_2 thin films

4. Conclusion:

Tungsten-doped VO_2 thin films were successfully synthesized on glass substrates via a cost-effective sol–gel spin-coating method followed by annealing at 550 °C. The effect of W doping concentration (0–2 at%) on the structural, thermal, morphological, and optical properties was systematically investigated.

XRD results confirmed the formation of the monoclinic VO_2 (M1) phase for all samples, with a slight peak shift toward lower 2θ values upon doping, indicating lattice expansion. DSC analysis revealed a significant reduction in the metal–insulator transition temperature (T_MIT) from ~68 °C for undoped VO_2 to ~45 °C for 1 at% W doping, primarily due to electronic structure modification by W^{6+} substitution. UV–Vis–NIR spectroscopy showed that 1 at% W-doped VO_2 achieved the highest solar modulation efficiency ($\Delta T_{sol} \approx 12\%$) while maintaining good luminous transmittance (~43%). SEM observations indicated grain refinement with increasing W content, which can influence both optical performance and switching behavior.

Overall, **1 at% W doping** was found to provide the optimal balance between reduced transition temperature, enhanced solar modulation, and visible transparency, making it a promising candidate for energy-efficient smart window applications. These findings highlight the potential of controlled W doping via the sol–gel process for tailoring VO_2 thermochromic performance at a relatively low cost and with scalability for large-area applications.

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A Comprehensive Review of the Challenges, Strategic Approaches, and Sustainable Solutions in Solid Waste Management

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Abstract: *Solid waste management (SWM) has emerged as a critical environmental and public health issue worldwide, driven by rapid urbanization, population growth, and changing consumption patterns. This review provides a comprehensive analysis of the major challenges, strategic approaches, and sustainable solutions in solid waste management. The study begins by highlighting the types and sources of solid wastemunicipal, industrial, biomedical, agricultural, and electronicand the growing volume of waste generation in both developed and developing regions.*

Key challenges in SWM include inadequate infrastructure, poor segregation at source, lack of public awareness, insufficient policy enforcement, and limited financial resources. These challenges are particularly acute in developing nations, where informal sectors often dominate waste handling without safety or environmental protocols.

The review then discusses strategic approaches that can transform waste management systems, including the 5Rs (Reduce, Reuse, Recycle, Recover, and Residuals), source segregation, public-private partnerships, extended producer responsibility (EPR), and decentralized waste processing methods. Technological advancements such as composting, anaerobic digestion, incineration, and waste-to-energy conversion are analyzed for their environmental and economic feasibility.

Furthermore, the paper emphasizes sustainable solutions that integrate policy frameworks, community participation, smart technologies, and circular economy principles. Best practices from countries with successful SWM models are also discussed to provide transferable strategies for different contexts.

This review concludes that sustainable solid waste management requires a multidisciplinary and inclusive approach that combines regulatory support, scientific innovation, behavioral change, and institutional collaboration.

Keywords: *Solid waste management, challenges, sustainable solutions, 5Rs, waste-to-energy, circular economy, policy, source segregation, urban waste, environmental management.*

Objective: To analyze the key challenges, strategic frameworks, and sustainable solutions in solid waste management, with an emphasis on integrating technological, policy-driven, and community-based approaches for effective waste handling.

Principal: The review is based on the principle of sustainability, promoting the 5Rs (Reduce, Reuse, Recycle, Recover, Residuals), circular economy, and inclusive stakeholder participation to minimize environmental and public health risks associated with solid waste.

Aim: To advocate for a holistic, interdisciplinary, and practical approach to solid waste management that combines scientific innovation, regulatory frameworks, and civic engagement to achieve long-term environmental sustainability.

1. Introduction: Solid Waste Management (SWM) refers to the systematic administration of activities involving the collection, segregation, transportation, processing, recycling, and disposal of solid waste materials. It is a crucial element of environmental protection and public health preservation, particularly in the context of rapidly expanding urban populations and changing consumption patterns worldwide (Guerrero et al., 2013).

The global relevance of SWM has increased significantly in recent decades due to the escalating volume of waste generated by households, industries, healthcare facilities, and agricultural sectors. According to the World Bank (2018), the world produces more than 2 billion tonnes of municipal solid waste annually, with at least 33% not managed in an environmentally safe manner. In low- and middle-income countries, ineffective waste management contributes to water, air, and soil pollution, posing severe risks to ecosystems and human health.

Efficient SWM is not only a technical and logistical issue but also a socio-economic and policy challenge. Inadequate systems can lead to the spread of disease, contamination of natural resources, and greenhouse gas emissions from improper waste disposal methods such as open dumping and burning (Hoornweg&Bhada-Tata, 2012). Moreover, unmanaged solid waste exacerbates urban poverty, especially in informal settlements, where waste often accumulates without formal collection services.

In contrast, well-planned and inclusive SWM systems support sustainable urban development, conserve resources through recycling and reuse, and contribute to climate change mitigation efforts. Thus, developing comprehensive and integrated strategies for solid waste management is imperative to achieve environmental sustainability and improve the quality of life in both developed and developing nations.

2. Types and Sources of Waste:

Solid waste encompasses a wide variety of materials discarded as a result of human, industrial, and agricultural activities. These materials are generally categorized based on their source and composition. Understanding the types and sources of waste is essential for designing effective and context-specific waste management strategies.

2.1 Municipal Solid Waste (MSW): Municipal solid waste refers to everyday items discarded by the public, such as food scraps, paper, plastics, glass, textiles, and packaging materials. It is primarily generated from households, commercial establishments, institutions, and public places (Tchobanoglous et al., 2002). MSW is the most visible and commonly discussed form of waste, and its volume is growing rapidly with urbanization and consumerism.

2.2 Industrial Waste: Industrial waste originates from manufacturing and processing industries, and includes chemicals, metals, plastics, ash, and hazardous residues. The composition and quantity vary widely depending on the type of industry. Improper handling of industrial waste can lead to environmental pollution, particularly when hazardous substances are involved (Kumar et al., 2017).

2.3 Biomedical Waste: Biomedical or healthcare waste is generated by hospitals, clinics, laboratories, and veterinary facilities. It includes used syringes, gloves, bandages, body fluids, pharmaceuticals, and pathological waste. These wastes pose serious health risks to humans and animals due to their infectious and toxic nature, and require special handling and treatment (Chartier et al., 2014).

2.4 Agricultural Waste: This category includes organic residues such as crop stalks, husks, animal manure, and spoiled produce. Though largely biodegradable, the large volumes of waste produced in agricultural areas can cause pollution if not managed properly. Burning of agricultural waste, a common practice in some regions, also contributes to air pollution and greenhouse gas emissions (FAO, 2017).

2.5 Electronic Waste (E-Waste): E-waste consists of discarded electronic devices such as computers, mobile phones, televisions, and batteries. These items often contain toxic components like lead, mercury, and cadmium, making them hazardous if not properly recycled or disposed of. The rise in consumer electronics and shorter product lifespans have made e-waste one of the fastest-growing waste streams globally (Forti et al., 2020).

The increasing quantity and complexity of these waste types underscore the need for diversified and efficient waste management systems tailored to local conditions. Without proper segregation and treatment, the environmental and health impacts of these waste streams can be severe and long-lasting. (Table-1)

Table 1 Types, Sources, and Impacts of Solid Waste

Type of Waste	Primary Sources	Common Components	Major Environmental/Health Impacts
Municipal Solid Waste (MSW)	Households, markets, schools, offices, restaurants	Food waste, paper, plastic, glass, textiles, packaging	Land and water pollution, vermin attraction, methane emissions
Industrial Waste	Manufacturing industries, power plants, chemical factories	Chemicals, heavy metals, plastics, ash, slag	Soil and water contamination, toxic exposure, air pollution
Biomedical Waste	Hospitals, clinics, labs, veterinary services	Syringes, gloves, tissues, pharmaceutical residues	Infection risks, biohazard exposure, requires specialized disposal
Agricultural Waste	Farms, plantations, agro-industries	Crop residues, manure, pesticide containers	Air pollution (via burning), water pollution, methane release
Electronic Waste (E-Waste)	Households, offices, industries, electronic retailers	Batteries, circuit boards, wires, screens	Heavy metal leaching, soil toxicity, long-term environmental degradation

3. Challenges in SWM:

Solid Waste Management (SWM) remains a persistent challenge across the globe, particularly in low- and middle-income countries where rapid urbanization and population growth have outpaced waste handling infrastructure. Despite growing awareness and policy efforts, several systemic barriers continue to hinder the effective management of solid waste.

3.1 Inadequate Infrastructure: Many urban and rural areas lack sufficient facilities for waste collection, transportation, treatment, and safe disposal. In some cities, only a fraction of the

total waste generated is collected, and much of it ends up in open dumpsites or water bodies, posing serious risks to human and environmental health (UN-Habitat, 2010).

3.2 Lack of Source Segregation: Most waste is disposed of in a mixed state, making it difficult to recover recyclable or biodegradable components. The absence of proper segregation at the source increases the burden on downstream waste processing systems and reduces the efficiency of recycling and composting initiatives (Kumar et al., 2017).

3.3 Financial and Institutional Constraints: Solid waste management is often underfunded, especially in developing regions. Limited municipal budgets, lack of skilled personnel, and weak institutional coordination result in poorly planned and executed waste services (World Bank, 2018).

3.4 Public Awareness and Participation: Community involvement is essential for sustainable SWM, yet many citizens are unaware of their role in waste reduction, segregation, and responsible disposal. Without consistent awareness campaigns and behavioral change programs, even well-designed systems fail to function effectively (Zurbrugg et al., 2012).

3.5 Weak Policy Implementation and Enforcement: While many countries have legislated waste management rules and environmental protection laws, implementation remains weak. Regulatory agencies often lack the capacity to monitor and enforce compliance, especially in informal settlements and peri-urban areas (Wilson et al., 2009).

These challenges are more pronounced in low-income and densely populated regions, where unregulated informal sectors handle a significant portion of waste without safety standards or environmental oversight. Addressing these issues requires a multifaceted approach that combines policy, technology, finance, and community engagement.

Table-2 Key Challenges in Solid Waste Management

Challenge	Description	Implications
Inadequate Infrastructure	Limited collection vehicles, transfer stations, landfills, and treatment plants	Uncollected waste, illegal dumping, environmental pollution
Lack of Source Segregation	Waste not separated into biodegradable, recyclable, and hazardous categories	Reduced recycling efficiency, increased landfill burden
Financial and Institutional Constraints	Insufficient budgets, poor governance, lack of trained staff	Inefficient services, stalled projects, poor maintenance of facilities
Low Public Awareness and Participation	Weak citizen engagement and understanding of proper waste practices	Poor segregation, littering, reduced support for government initiatives
Weak Policy Enforcement	Poor monitoring of existing laws and guidelines	Non-compliance by industries and households, unregulated informal activities

4. Strategic Approaches in Solid Waste Management

To address the complex challenges in solid waste management (SWM), it is essential to adopt strategic and integrated approaches that combine policy, technology, community engagement, and institutional support. Modern SWM emphasizes sustainability and resource recovery, moving away from traditional collection–disposal models toward more circular and inclusive systems. Several key strategies have gained prominence in recent years:

4.1 The 5Rs Framework (Reduce, Reuse, Recycle, Recover, Residuals): The 5Rs model is a foundational strategy in sustainable waste management.

- **Reduce** aims to minimize waste generation at the source through conscious consumption and eco-design.
- **Reuse** promotes extending the life cycle of products.
- **Recycle** focuses on material recovery through processing and remanufacturing.
- **Recover** includes energy recovery from non-recyclable waste (e.g., incineration with energy capture).
- **Residuals** are those components that cannot be managed through the first four stages and require safe disposal (UNEP, 2016). This model shifts the emphasis from disposal to resource efficiency.

4.2 Source Segregation: Effective waste management begins with segregation at the point of generation into categories such as biodegradable, recyclable, hazardous, and inert waste. Source segregation improves the efficiency of downstream processes like composting, recycling, and energy recovery, while reducing landfill burden (Kumar et al., 2017).

4.3 Public-Private Partnerships (PPPs): Collaborations between municipal governments and private enterprises have proven successful in improving service delivery, infrastructure development, and innovation in SWM. PPPs bring in investment, technical expertise, and operational efficiency, especially in collection, transportation, and treatment systems (Gupta et al., 2015).

4.4 Extended Producer Responsibility (EPR): EPR is a policy approach where producers are made responsible for the post-consumer lifecycle of their products, especially packaging, electronics, and plastics. This encourages design for recyclability and creates accountability for managing product waste through take-back schemes and recycling initiatives (OECD, 2016).

4.5 Decentralized Waste Management: Decentralized systems involve waste processing at or near the point of generationsuch as household or community-level composting and biogas plants. This reduces transportation costs and carbon footprint, and promotes community involvement (Zurbrugg et al., 2012). Such systems are particularly suitable for biodegradable waste in residential and institutional settings.

5. Sustainable Solutions in Solid Waste Management

Sustainable solid waste management requires a transition from linear, disposal-oriented practices to integrated models that are environmentally, economically, and socially responsible. This involves adopting technologies, governance systems, and behavioral practices that prioritize resource recovery, environmental protection, and long-term viability.

5.1 Technological Innovations: Modern SWM emphasizes the adoption of environmentally sound technologies for efficient processing and resource recovery:

- **Composting:** Ideal for biodegradable organic waste, composting converts food and garden waste into nutrient-rich compost for agriculture and horticulture (Adhikari et al., 2009).
- **Anaerobic Digestion:** This process decomposes organic waste in the absence of oxygen to produce biogas (a renewable energy source) and digestate, which can be used as a fertilizer (Kothari et al., 2014).
- **Incineration:** High-temperature combustion reduces waste volume significantly and can be used to recover energy. However, it requires strict pollution controls to manage emissions (Tan et al., 2015).

- **Waste-to-Energy (WTE):** WTE technologies, such as gasification and pyrolysis, convert non-recyclable waste into electricity or heat, contributing to energy sustainability (UNEP, 2016).

5.2 Circular Economy Principles: A circular economy approach focuses on designing out waste, keeping materials in use, and regenerating natural systems. This model promotes rethinking product design, encouraging reuse and remanufacturing, and minimizing resource extraction (Ellen MacArthur Foundation, 2013). Applying circular economy principles in SWM fosters innovation and job creation while reducing environmental impact.

5.3 Community Involvement: Sustainable waste management systems require the active participation of local communities. Initiatives such as neighborhood-level composting, door-to-door collection, and awareness campaigns have proven effective in improving waste segregation and reducing littering (Zurbrugg et al., 2012). Empowering citizens through education, incentives, and local governance mechanisms enhances the sustainability and accountability of waste systems.

5.4 Supportive Policy Mechanisms: Strong policy frameworks, regulatory enforcement, and financial incentives are crucial to institutionalize sustainable practices. These include:

- Mandatory segregation and composting laws
- Plastic bags and single-use product restrictions
- Extended Producer Responsibility (EPR)
- Incentives for green infrastructure and recycling enterprises (Wilson et al., 2012)

Integration of policies across national, municipal, and local levels ensures consistent action and monitoring, fostering accountability and innovation.

6.Conclusion:

This review underscores that solid waste management is not merely a technical or logistical task, but a multidimensional challenge that intersects environmental protection, public health, policy, economics, and social behavior. As urban populations grow and consumption patterns evolve, waste volumes are increasing at an unsustainable rate, placing immense pressure on local and national systems.

Conventional approaches centered on collection and disposal are no longer sufficient. Sustainable SWM must embrace a **holistic, inclusive, and interdisciplinary model** that aligns with both local realities and global sustainability goals. This involves the integration of **robust regulatory frameworks** that mandate segregation and recycling; **scientific and technological advancements** that promote resource recovery and energy generation; **civic engagement** through education and behavioral change; and **institutional synergy** between government bodies, private sectors, and civil society.

Strategic models like the **5Rs**, **Extended Producer Responsibility (EPR)**, and **decentralized waste processing** offer scalable solutions when backed by strong policy support and financial incentives. Likewise, the adoption of **circular economy principles** ensures long-term resource efficiency and environmental resilience. Ultimately, building a sustainable SWM system requires consistent political will, cross-sector collaboration, inclusive community participation, and continuous innovation. By reimagining waste not as a burden, but as a valuable resource, societies can move toward cleaner, healthier, and more sustainable urban environments

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Ru (II)-Photocatalyzed Construction of Amides via Decarboxylative Coupling Strategy

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Abstract: *A visible-light-induced decarboxylative amidation strategy has been developed to synthesize structurally diverse amides using phenoxyacetic acids and N-hydroxyphthalimide (NHP) esters as starting materials. Thereaction utilizes a Ru-based photocatalyst, $Ru[(CF_3)ppy]_2(dtbbpy)PF_6$, under mild conditions with blue LED light (456 nm) in acetonitrile. This photoredox catalytic process promotes direct C–N bond formation through a decarboxylative coupling mechanism, resulting in the formation of amide products in good to excellent yields. This environmentally benign protocol offers a practical, sustainable, and atom-economical approach to amide synthesis, relevant to pharmaceutical and material sciences.*

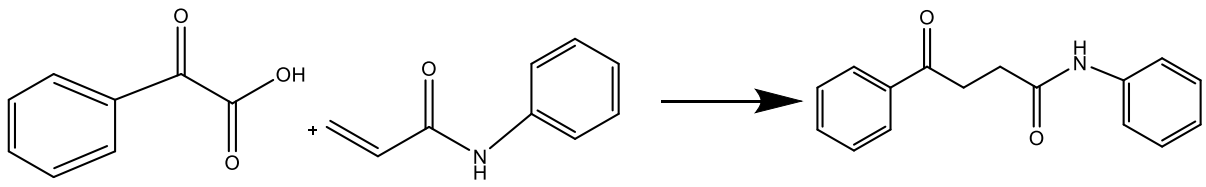
1. INTRODUCTION

Amides are fundamental functional groups in organic chemistry, prevalent in natural products, pharmaceuticals, agrochemicals, and polymers. Traditional amide bond formation typically involves the activation of carboxylic acids using coupling agents such as carbodiimides or acid chlorides. However, these processes often generate stoichiometric amounts of waste and require harsh conditions, limiting their sustainability.

Recent advances in visible-light photoredox catalysis have enabled the activation of otherwise inert chemical bonds under mild and environmentally benign conditions. Among these, decarboxylative coupling reactions have emerged as powerful tools for C–C and C–X bond formation, utilizing abundant and inexpensive carboxylic acids as radical precursors.

In this study, we present a visible-light-mediated decarboxylative amidation of phenoxyacetic acids with N-hydroxyphthalimide (NHP) esters using $Ru[(CF_3)\ ppy]_2(dtbbpy)PF_6$ as a photocatalyst. The transformation proceeds via a photoredox cycle, generating reactive radical intermediates that undergo efficient C–N bond formation to yield amides under mild reaction conditions.

Scheme:



2. Results and Discussion

2.1 Reaction Optimization

The model reaction between phenoxy acetic acid-derived NHP ester and an amine was initially optimized under visible-light conditions using various photocatalysts, solvents, and additives.

- **Catalyst screening** showed $Ru[(CF_3)\ ppy]_2(dtbbpy)PF_6$ (1 mol%) to be the most effective, outperforming traditional $Ru(bpy)_3^{2+}$ and Ir-based catalysts.
- **Solvent screening** indicated that acetonitrile (MeCN) gave the highest yields, likely due to its high polarity and good radical solvation properties.
- The reaction required continuous **blue LED irradiation (456 nm)** to proceed efficiently; no product formation was observed in the absence of light or catalyst.

Under optimized conditions (0.1 M concentration, 25 °C, 1 mol% Ru-catalyst, 456 nm LEDs, 16–24 h), the desired amide was obtained in up to 85–92% isolated yield.

2.2 Substrate Scope

The methodology was applied to a range of phenoxyacetic acid-derived NHP esters and primary/secondary amines. Notable features of the scope include:

- **Electron-rich and electron-poor** aromatic rings on the phenoxy group were well tolerated.
- **Aliphatic and heterocyclic amines**, including cyclic amines (e.g., morpholine, pyrrolidine), furnished the corresponding amides in good yields.
- Sterically hindered substrates also reacted smoothly, demonstrating the mildness and efficiency of the transformation.

This generality confirms the method's robustness and applicability across diverse chemical structures.

2.3 Mechanistic Insight

A proposed mechanism is outlined in **Scheme 1**:

1. Upon irradiation with blue light, the Ru (II) photocatalyst is excited to its *MLCT* state.
2. Single-electron transfer (SET) from the excited Ru (II)* to the NHP ester generates an **acyloxy radical** and a Ru (III) species.
3. The acyloxy radical rapidly undergoes **decarboxylation**, forming a **benzylic radical** intermediate.
4. This intermediate couples with the amine nucleophile, affording the desired **amide** after rearomatization and proton transfer.
5. The Ru (III) species is reduced back to Ru (II) by a sacrificial electron donor (if required), closing the catalytic cycle.

Control experiments confirmed the radical nature of the reaction, as the presence of TEMPO or BHT (radical scavengers) completely suppressed product formation.

3. Conclusion

A novel, practical, and sustainable method for amide synthesis via visible-light-induced decarboxylative amidation has been established. The use of phenoxyacetic acids and NHP esters as readily available starting materials, combined with a Ru-based photocatalyst and blue LED light, allows for mild and efficient C–N bond formation. This metal-catalyzedphotoredox strategy offers broad functional group tolerance, operational simplicity, and high yields, rendering it a valuable addition to the toolkit of green and modern organic synthesis.

4. Experimental Section

General Procedure:

In an oven-dried reaction tube, phenoxyacetic acid-derived NHP ester (0.2 mmol), amine (0.3 mmol), and Ru[(CF_3) ppy]$_2$(dtbbpy)PF_6 (1 mol%) were dissolved in dry acetonitrile (2 mL, 0.1 M). The reaction vessel was sealed, purged with N_2, and irradiated with blue LEDs (456 nm) at room temperature for 16–24 hours. The reaction mixture was then concentrated under reduced pressure and purified by column chromatography (silica gel, hexane/ethyl acetate) to yield the desired amide product.

Physical Appearance: White solid**Melting Point:** 89–91 °C**Rf value:** 0.45 (hexane/ethyl acetate = 3:2)

^{1}H NMR (400 MHz, $CDCl_3$):

δ 7.33–7.25 (m, 5H, Ar–H),7.02 (t, J = 7.2 Hz, 1H, Ar–H),6.88–6.81 (m, 3H, Ar–H),6.55 (br s, 1H, NH),4.50 (s, 2H, CH_2–CO),3.52 (q, J = 6.8 Hz, 2H, CH_2–NH),2.78 (t, J = 6.8 Hz, 2H, CH_2–CH_2–Ph)

^{13}C NMR (100 MHz, $CDCl_3$):

δ 167.8 (C=O),156.2 (Ar–O),135.4, 129.3, 128.7, 127.5 (Aromatic C),121.1, 114.3, 111.7 (Aromatic C),66.5 (CH_2–O),42.3 (CH_2–NH),36.2 (CH_2–Ph)

IR (neat, cm^{-1}):

3304 (N–H stretch),1664 (C=O stretch, amide),1602, 1510 (aromatic C=C),1242 (C–O stretch),755 (Ar–H bend)

HRMS (ESI$^+$):m/z $[M+H]^+$ calculated for $C_{16}H_{18}NO_2$: **256.1332**Found: **256.1330**

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Status Of Water Treatment in The Telangana State

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Abstract: *Water treatment is critical for ensuring the health and sustainability of communities, particularly in rapidly urbanizing and semi-arid regions such as Telangana. This paper explores the comprehensive landscape of water treatment across Telangana State, India. It delves into major government initiatives such as Mission Bhagiratha and Mission Kakatiya, the status of wastewater treatment, and challenges like river pollution, aging infrastructure, and groundwater contamination. The article highlights the various water treatment technologies and both the progress and persistent challenges in Telangana's water management ecosystem, offering insights into future directions for infrastructure resilience and equitable access. By examining the current infrastructure, challenges, policy implications, and future directions, this research seeks to present a holistic understanding of water treatment and provide recommendations for sustainable water management. With the implementation of Mission Bhagiratha, Telangana has achieved near-universal piped drinking water coverage, delivering treated surface water to over 53.98 lakh households. The state stands out nationally for its high-water quality, with over 99.95% of tested tap water samples found free of contamination. Despite these achievements, challenges persist—particularly in public schools, where a significant number still rely on untreated or groundwater sources. In urban centers like Hyderabad, water supply lags behind demand due to population growth and infrastructural bottlenecks, including aging pipelines and leakage losses estimated at 20 MGD daily. To address these gaps, projects such as Godavari Phase II & III and new modular and vertical treatment plants are underway. Concurrently, the Hyderabad Metropolitan Water Supply and Sewerage Board (HMWS&SB) is expanding sewage treatment capacity with 39 new STPs to achieve 100% wastewater treatment.*

Keywords: *Water Treatment, Telangana, Mission Bhagiratha, Wastewater Management, Groundwater, River Pollution, Sustainable Water Policy, Water treatment Drinking water supply Piped water, Water quality Hyderabad water supply Water infrastructure and Sewage treatment.*

1.INTRODUCTION

Telangana, the 29th state of India formed in 2014, is characterized by diverse geography, semi-arid climate, and rapid urban development. These characteristics create unique challenges in water resource management. Despite abundant surface water sources from the Krishna and Godavari rivers, issues such as pollution, over-extraction of groundwater, and inadequate sewage systems have created stress on water resources. The Government of Telangana has responded through ambitious programs including Mission Bhagiratha, designed to provide piped drinking water to all households, and Mission Kakatiya, aimed at rejuvenating traditional

water tanks and lakes. This paper evaluates these efforts and discusses remaining gaps and future priorities.

2.Objectives

The key objectives of this study are:
1. To assess the current status of water treatment infrastructure in Telangana.
2. To evaluate the impact of government initiatives such as Mission Bhagiratha and Mission Kakatiya.
3. To analyze wastewater treatment and pollution control measures in urban areas.
4. To identify key challenges in ensuring water quality in rural and urban areas.
5. To recommend strategies for sustainable water treatment and management in Telangana.

3.Methodology

This research is based on a qualitative review and analysis of secondary data sources. Data was collected from government reports, academic publications, environmental research studies, media reports, and online databases. Specific focus was placed on the period from 2016 to 2025 to understand the progress made post the formation of Telangana. The study examines statistical data, policy documents, technical reports, and water quality indices to provide an evidence-based understanding of water treatment in the state.

Assessment of Water Treatment Infrastructure in Telangana

Telangana has made considerable progress in developing water treatment infrastructure in recent years, especially under flagship programs like **Mission Bhagiratha** and **Smart Cities Mission**. However, disparities persist between urban and rural regions, and challenges remain in terms of capacity, coverage, quality, and long-term sustainability.

Types of Water Treatment Infrastructure

Telangana's water treatment infrastructure can be broadly categorized into:

- Drinking Water Treatment Plants (WTPs)
- Sewage Treatment Plants (STPs)
- Effluent Treatment Plants (ETPs)
- Decentralized Wastewater Treatment Systems (DEWATS)
- Community Water Purification Plants (CWPPs)

Drinking Water Treatment Plants (WTPs)

Urban Areas

- Major cities like Hyderabad, Warangal, and Karimnagar have large-capacity water treatment facilities.
- Hyderabad Metropolitan Water Supply and Sewerage Board (HMWSSB) operates several WTPs sourcing water from Krishna and Godavari rivers.
- Capacity: **Over 1000+ MLD (Million Litres per Day)** in the Hyderabad Urban Agglomeration alone.

Rural Areas

- **Mission Bhagiratha** has significantly expanded rural WTP coverage.

- Most villages now receive **treated surface water** instead of fluoride/nitrate-contaminated groundwater.
- Water is transmitted through **grid-based systems** and village-level overhead tanks.

Sewage Treatment Plants (STPs)

- Telangana has an installed capacity of approximately **1800+ MLD** of sewage treatment.
- **Hyderabad** alone accounts for ~772 MLD (as of 2023), with plans to increase to 1250 MLD by 2025.
- Other urban centers like Warangal, Nizamabad, and Khammam have functional STPs but face operational and coverage limitations.
- **Coverage**: Only about **50–60%** of sewage generated in urban areas is actually treated before discharge.

Key Gaps

- Incomplete underground drainage network in Tier 2 & 3 cities.
- Slums and peri-urban areas often bypassed.
- STPs face **overloading, poor maintenance, and electricity shortages**.

Effluent Treatment Plants (ETPs)

- Industrial clusters, especially around Hyderabad (e.g., **Patancheru, Jeedimetla**), generate substantial wastewater.
- Telangana State Pollution Control Board (TSPCB) mandates **ETPs** for highly polluting units (e.g., pharmaceuticals, dyes).
- However, many **ETPs are non-functional** or operate below capacity.

Common Effluent Treatment Plants (CETPs)

- CETPs exist in some industrial estates but suffer from lack of maintenance and compliance monitoring.

Decentralized Wastewater Treatment (DEWATS)

- Growing adoption in gated communities, educational campuses, and eco-sensitive zones.
- Promoted through Swachh Bharat Mission (Urban) and AMRUT programs.
- However, not yet mainstream; scale and awareness remain low.

Community Water Purification Plants (CWPPs)

- Plants are used in rural areas of Nalgonda and Mahabubnagar
- Most are **reverse osmosis (RO)-based units** funded by Panchayats or NGOs.
- Issues: **High reject water, O&M costs, and inconsistent functioning** due to power or financial constraints.

Institutional Framework

- **Urban**: Managed by GHMC, HMWSSB, Municipal Corporations
- **Rural** : Managed by Rural Water Supply and Panchayats (RWS&P)
- **Monitoring**: Telangana State Pollution Control Board (TSPCB) and Jal Jeevan Mission

5.Challenges in Water Treatment Infrastructure

Challenge	Description
Inadequate Coverage	Peripheral and rural areas still underserved by STPs/WTPs
Poor O&M	Many existing plants suffer from poor operation and maintenance
Sludge Management	Lack of proper sludge treatment and reuse facilities
Industrial Non-Compliance	Non-functional ETPs and unauthorized discharges
Financial Sustainability	Many CWPPs and DEWATS lack regular funding for repairs and upgrades
Skilled Manpower	Shortage of trained technicians for decentralized and village-level systems

5.Recent Improvements and Ongoing Projects

Musi Riverfront Development and Jal Jeevan Mission

- **Smart Cities and AMRUT**: Infrastructure upgrade projects in Warangal and Karimnagar.
- **Treated Water Reuse**: Being promoted for construction and horticulture in urban areas.

Government Flagship Programmes Mission Bhagiratha and Mission Kakatiya Evaluation

After Telangana's formation in 2014, the state government launched two major flagship programs — Mission Bhagiratha (for drinking water supply) and Mission Kakatiya (for tank restoration). These initiatives aimed to address chronic water scarcity, improve rural livelihoods, and ensure sustainable water management.

Mission Bhagiratha: Safe Drinking Water for All

Objective

To provide safe, treated, and piped drinking water to every household, especially in rural areas. The initiative also aims to reduce fluoride and water-borne diseases in affected districts.

Key Features

- Covers 100% rural and urban habitations
- Uses surface water sources instead of contaminated groundwater
- Integrated network of pipelines, overhead tanks, and treatment plants
- Over 1.25 lakh km of pipelines laid

Impact Evaluation

- Health Improvements: Fluoride-related ailments reduced in districts like Nalgonda
- Rural Empowerment: Women saved time from water collection; improved dignity and

productivity
- Coverage Expansion: Nearly 100% of habitations now receive piped water
- Quality Assurance: Treated water quality improved with better monitoring
- Infrastructure Development: Strengthened rural infrastructure and created jobs

Challenges

- Electricity dependence for pumping
- Maintenance and sustainability in remote areas
- Occasional supply interruptions during peak summer

Mission Kakatiya: Revival of Water Tanks

Objective

To restore and rejuvenate minor irrigation tanks to improve groundwater recharge, enhance irrigation capacity, and support agriculture and fisheries.

Key Features

- Targeted restoration of 46,531 tanks
- Desilting and strengthening of tank bunds
- Community involvement in tank maintenance

Impact Evaluation

- Irrigation Coverage: Increased ayacut area by over 20 lakh acres
- Groundwater Recharge: Improved water tables in dry districts
- Agricultural Productivity: Higher yields and improved crop diversity
- Fisheries and Livelihood: Tanks support fishery-based income
- Climate Resilience: Reduced drought vulnerability

Challenges

- Silt disposal and land encroachments
- Lack of mechanized desilting in some regions
- Need for stronger community management structures

6. Overall Socio-Economic and Environmental Impact

Dimension	Mission Bhagiratha	Mission Kakatiya
Water Accessibility	Piped drinking water to every household	Increased irrigation access
Health	Reduced waterborne diseases	Improved food security indirectly
Employment	Jobs in construction and maintenance	Rural employment during desilting
Sustainability	Surface water reduces groundwater overuse	Groundwater recharge and ecosystem restoration |
Economic Benefits	Time-saving for women; more school attendance	Boost in crop yield and fisheries income

Recommendations for Improvement

- Mission Bhagiratha:
  - Incorporate solar pumps and smart metering
  - Strengthen village-level operations and maintenance
  - Establish mobile water testing labs
  - Mission Kakatiya:
  - Institutionalize tank committees
  - Promote silt reuse in agriculture
  - Integrate tank rejuvenation with watershed programs

Analysis of Wastewater Treatment and Pollution Control Measures in Urban Areas of Telangana State

Urbanization in Telangana has led to significant challenges in managing wastewater and controlling pollution. Cities like Hyderabad, Warangal, and Karimnagar generate large volumes of domestic and industrial wastewater, exerting pressure on existing infrastructure. This analysis reviews the current status of wastewater treatment facilities, identifies gaps, and evaluates pollution control measures implemented across urban areas in Telangana. The paper emphasizes the importance of strengthening decentralized sewage treatment, adopting modern technologies, and ensuring regulatory enforcement to achieve sustainable urban sanitation. 1. Introduction

Telangana is one of new state that showing vast urban growth. Urban areas generate considerable volumes of wastewater, posing a major environmental challenge. Contaminated water bodies, illegal discharges, and insufficient treatment capacity contribute to urban pollution, impacting public health and ecological systems.

Wastewater Generation in Telangana Urban Areas

- Major Sources:
  - Domestic sewage (households, slums)
  - Industrial effluents (especially pharmaceuticals in Hyderabad)
  - Commercial establishments and institutions
- Estimated Wastewater Generation (2024):
  - Hyderabad: ~2000 MLD (Million Litres per Day)
  - Warangal: ~180 MLD
  - Karimnagar and other municipalities: ~500+ MLD (combined)

Existing Wastewater Treatment Infrastructure

- Greater Hyderabad Municipal Corporation (GHMC):
  - Operates multiple Sewage Treatment Plants (STPs) with total installed capacity ~772 MLD
  - Only ~50-60% of sewage is treated before disposal
- Urban Local Bodies (ULBs):
  - Many small and medium towns lack STPs or have underperforming ones
- Challenges:
  - Overloading of STPs
  - Poor operation and maintenance (O&M)
  - Non-functional decentralised systems

Pollution Control Measures

Regulatory Measures

- Telangana State Pollution Control Board (TSPCB):
  - Enforces effluent discharge norms (CPCB guidelines)
  - Mandates installation of Effluent Treatment Plants (ETPs) in industries
- Environmental Surveillance:
  - Regular monitoring of Musi River and water bodies
  - Fines for illegal discharge and non-compliance

Technological and Structural Measures

- Musi River Rejuvenation Project:

- Setting up STPs with > 1000 MLD capacity

- Cleaning of stormwater drains and intercepting raw sewage
- Decentralized Wastewater Treatment:
  - Promotion of small-scale STPs in gated communities, hotels
  - Constructed wetlands and bio-remediation in peri-urban zones

Public Participation and Awareness

- Swachh Bharat Urban Mission initiatives
- IEC campaigns on waste segregation and avoiding drain dumping

Key Issues and Gaps

- Inadequate sewer coverage in peripheral urban areas
- Slum areas are not connected to STPs
- Industrial areas lack common ETPs (CETPs)
- Poor institutional coordination among GHMC, HMWSSB, and TSPCB
- Delayed implementation of sanctioned STP projects

Recommendations

- Expand STP capacity in rapidly growing urban zones
- Mandatory linkage of all households and industries to sewer systems
- Strengthen monitoring using IoT and GIS tools
- Public-private partnerships (PPP) for funding and efficient O&M

Key Challenges in Ensuring Water Quality in Rural and Urban Areas of Telangana State

Ensuring safe and clean water in Telangana remains a major challenge, especially amid rapid urbanization, growing industrial activity, and agricultural intensification. While cities struggle with overloaded sewage systems and industrial effluents, rural areas face groundwater contamination and infrastructure gaps. This document outlines the key challenges in maintaining water quality across both rural and urban settings in Telangana.

Inadequate Wastewater Treatment Infrastructure

- **Urban Areas**: Overloaded and outdated STPs with many households unconnected to sewerage systems.

- **Rural Areas**: Lack of treatment systems; use of soak pits contaminates groundwater.

Industrial Pollution

- Urban clusters (e.g., Hyderabad, Medak) release untreated industrial waste, especially from pharmaceuticals.

- Weak enforcement and monitoring worsen water contamination in local rivers and streams.

Agricultural Runoff

- Excessive use of fertilizers and pesticides leads to nitrate/phosphate contamination in rural tanks and aquifers.

Groundwater Contamination

- Fluoride contamination in Nalgonda, Mahabubnagar; nitrate from fertilizers in many districts.

- Geogenic contamination and over-extraction increase risk in rural and peri-urban regions.

Urbanization and Encroachments

- Encroachment of tanks and nalas reduces recharge capacity and increases pollution.

- Sewage flows through stormwater drains in most cities.

Limited Monitoring and Surveillance

- Inadequate testing and delayed water quality reporting in both urban and rural areas.

Climate Change and Water Scarcity

- Drought-prone climate worsens borewell dependency and water quality.

- Rainfall variability affects natural cleansing of contaminants.

Institutional and Policy Gaps

- Overlapping responsibilities between TSPCB, HMWSSB, RWS.

- Weak enforcement of pollution control laws.

Public Awareness and Behavioral Issues

- Rural communities often unaware of safe water practices.

- Urban residents contribute to pollution by improper waste disposal.

Infrastructure Gaps

- Rural: Delayed implementation of Jal Jeevan Mission tap connections.

- Urban slums: Dependence on contaminated tanker or surface water.

Summary Table

The following table summarizes the key challenges in both urban and rural Telangana:

Challenge	Urban Telangana	Rural Telangana
Inadequate Treatment	| Overloaded STPs	Low number of STPs / Drainage
Industrial Pollution	Pharma and chemical hubs	Low but increasing in agri-processing

Challenge	Urban Telangana	Rural Telangana
| Agricultural Runoff	Moderate	High due to fertilizers/pesticides
Groundwater Issues	Fluoride, nitrate hotspots	Widespread fluoride/nitrate presence
Encroachments	Rapid in GHMC, Warangal	Tank encroachments reducing recharge
Water Testing	Present but inconsistent	Lacking of Water testing centers
Climate Impacts	Urban flooding, water logging	Low level water tables & droughts
Institutional Gaps	Multi-agency with overlaps	Limited local capacity

Recommended Strategies for Sustainable Water Treatment and Management in Telangana

Telangana faces significant challenges in ensuring sustainable water management due to urbanization, industrial growth, agricultural practices, and climate variability. The following strategies offer a roadmap for achieving effective water treatment and long-term sustainability across urban and rural areas.

Expand and Upgrade Sewage Treatment Infrastructure

- Construct new STPs with adequate capacity in urban centers like Hyderabad and Warangal.

- Rehabilitate old and underperforming STPs using energy-efficient technologies (e.g., MBBR, SBR).

- Ensure 100% household connectivity to underground drainage networks.

Promote Decentralized Wastewater Treatment

- Install DEWATS (Decentralized Wastewater Treatment Systems) in rural and peri-urban areas.

- Encourage reuse of greywater for gardening, flushing, and other non-potable uses.

Strengthen Groundwater Management

- Construct artificial recharge structures such as check dams and recharge shafts.

- Promote rooftop rainwater harvesting through building regulations.

- Implement real-time monitoring using telemetry and piezometers.

Improve Industrial Wastewater Regulation

- Mandate Zero Liquid Discharge (ZLD) for highly polluting industries.

- Establish Common Effluent Treatment Plants (CETPs) in industrial zones.

- Use digital monitoring systems for real-time compliance tracking.

Enhance Rural Water Supply Systems

- Accelerate Jal Jeevan Mission (JJM) implementation for piped water access in all villages.

- Deploy community water purification units (CWPUs) in high-contamination areas.

- Adopt solar-powered water treatment technologies in remote locations.

Reuse and Recycling of Treated Water

- Mandate reuse of treated wastewater in parks, construction, and landscaping.

- Develop treated water distribution pipelines for non-potable applications.

- Provide incentives for industries using recycled water.

Public Awareness and Community Engagement

- Organize IEC (Information, Education and Communication) campaigns on water conservation.

- Form Water User Associations (WUAs) in villages for local water governance.

- Encourage public participation in pollution reduction and water-saving behaviors.

Use of Technology and Digital Tools

- Utilize GIS for infrastructure mapping and planning.

- Implement IoT and AI-based solutions for leak detection and quality monitoring.

- Create a public water dashboard for transparency and decision-making.

Institutional Strengthening and Policy Reforms

- Set up an Integrated Water Management Authority to coordinate between agencies.

- Update water policies to focus on reuse, resilience, and climate adaptation.

- Enforce water quality standards and penalize non-compliance.

Climate-Resilient Water Management

- Apply drought mitigation strategies in vulnerable zones.

- Restore wetlands and lakes to support recharge and ecosystem balance.

- Introduce water budgeting and seasonal water use planning.

Summary of Key Focus Areas

Focus Area	Strategy
Urban Infrastructure	Expand/upgrade STPs, reuse networks, decentralized systems
Rural Water Management	JJM, fluoride removal, solar water units, greywater reuse
Industrial Regulation	ZLD, CETPs, online monitoring
Groundwater and Recharge	Artificial recharge, rainwater harvesting, real-time monitoring
Awareness and Governance	IEC campaigns, user participation, policy reforms
Technology and Innovation	GIS, IoT, AI, smart dashboards

Focus Area	Strategy
Climate Resilience	Drought adaptation, water budgeting, ecological restoration

7.Results and Discussion

Mission Bhagiratha

Launched in 2016, Mission Bhagiratha aims to provide 100% household-level access to safe drinking water across the state. It draws water primarily from the Krishna and Godavari rivers and distributes it through a network of intake wells, treatment plants, and pipelines. As of 2024, over 153 water treatment plants, 1.7 lakh kilometers of pipelines, and thousands of reservoirs have been established. The project has dramatically reduced the dependency on borewells and improved public health in rural areas.

Mission Kakatiya

This project has restored over 45,000 traditional tanks, increasing irrigation potential, groundwater recharge, and surface water availability. It complements Mission Bhagiratha by enhancing local water sustainability.

Urban Water Supply and Treatment

Urban wastewater management in Telangana is at a critical juncture. While steps have been taken to modernize infrastructure and enforce pollution control, significant gaps remain, especially in smaller towns and outskirts. Sustainable solutions require an integrated approach—combining technological advancements, public awareness, and strict regulatory action. Investing in wastewater treatment is not just an environmental priority but a necessity for urban resilience. Hyderabad, the state capital, has expanded its treatment capacity to over 700 MGD through projects such as Godavari Phases II and III. Vertical treatment plants and modular WTPs have been installed in high-demand suburbs. Yet, aging infrastructure, water leakage, and non-revenue water losses remain persistent issues.

Wastewater Management

Urban wastewater is treated through 25 sewage treatment plants under HMWSSB with a combined capacity of 772 MLD. New STPs worth ₹3,866 crore are under construction. However, river systems like the Musi remain heavily polluted due to untreated sewage discharge and industrial effluents.

Groundwater and Rural Challenges

Groundwater quality in rural Telangana remains a concern with elevated levels of fluoride, nitrate, and salinity in several districts. Despite surface water availability, some areas continue to rely on contaminated groundwater sources.

8.Conclusion

The Telangana state has made considerable strides in water treatment infrastructure, policy, and service delivery through initiatives like Mission Bhagiratha and Mission Kakatiya. These projects have created a blueprint for other states to follow. Urban centers have better access to functional WTPs and STPs, while rural areas have benefitted from treated surface water and purification units. However, challenges such as aging pipelines, river pollution, poor sewage treatment coverage, and groundwater contamination continue to threaten long-term water

security. Strengthening institutional capacity, community participation, real-time water quality monitoring, and decentralized wastewater treatment solutions are key to achieving sustainable and inclusive water management in Telangana.

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In Silico and In Vitro Evaluation of Ferulic Acid as a Potent HIV-1 Reverse Transcriptase Inhibitor

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Abstract: *Natural compounds offer promising scaffolds for drug development. HIV continues to be a global health challenge. Discovering affordable and effective inhibitors is crucial for therapy. This study screens Benzoic acid, Salicylic acid, and Ferulic acid against HIV-1 target enzymes using molecular docking and in vitro evaluation. AutoDock 4.2 was employed for molecular docking against HIV-1 Reverse Transcriptase (RT), Integrase, and Protease using protein structures from the RCSB database. Ligands were assessed for drug-likeness and ADMET properties. Ferulic acid, the most promising ligand, was validated with a non- radioactive HIV-1 RT inhibition ELISA. Ferulic acid exhibited the highest binding affinityfor HIV-1 RT with a docking score of -6.29 kcal/mol, forming extensive hydrophobic interactions and one hydrogen bond with Lys103.Compared to reference drug Doxorubicin (- 4.91 kcal/mol), Ferulic acid showed superior binding. In vitro assays confirmed potent RT inhibition, with 72.5% activity blocked at 200 µg/mL and IC_{50} of 71.55 µg/mL, out performing Doxorubicin's 61% inhibition and IC_{50} of 68.40 µg/mL. The study highlights Ferulic acid's strong computational and experimental profile as an HIV-1 RT inhibitor. Its favorable docking interactions and inhibitory activity support its potential in HIV drug development.*

Key Words: *Ferulic acid, HIV-1 Reverse Transcriptase, Molecular docking, AutoDock, In vitro assay, Drug discovery.*

1.INTRODUCTION

As of 2023, HIV-1 remains a major global health challenge, with 39 million people living with HIV (PLHIV) and 1.3 million new infections annually (UNAIDS, 2023). Despite advances in antiretroviral therapy (ART), drug resistance, side effects, and non-adherence persist, necessitating the discovery of new molecules. Sub-Saharan Africa bears the highest burden (67% of global cases), while key populations (e.g., men who have sex with men, sex workers) remain disproportionately affected (WHO, 2023). Molecular docking and drug discovery research play a crucial role in identifying novel inhibitors targeting HIV-1 proteins (e.g., reverse transcriptase, protease, integrase). Recent studies emphasize AI-driven drug design and repurposing existing compounds to combat resistance (De Clercq, 2023). Computational approaches accelerate the identification of promising candidates before experimental validation, offering cost-effective solutions for low-resource settings. Thus, continuous research is essential to develop next-generation antiretrovirals.

HIV/AIDS remains a critical global health challenge, with millions affected worldwide despite

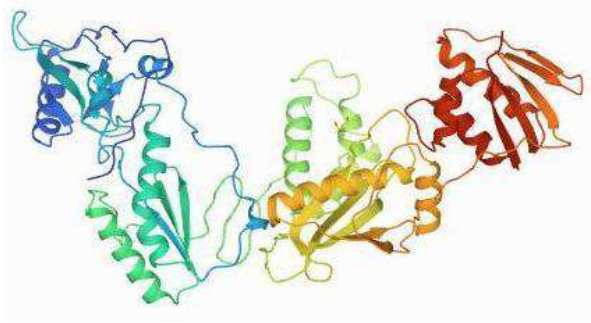
advances in antiretro viral therapy (ART). The virus's high mutation rate and the emergence of drug-resistant strains necessitate continual development of novel inhibitors targeting key viral enzymes such as reverse transcriptase (RT), integrase, and protease (Zduriska et al., 2018). These enzymes play vital roles in the HIV lifecycle, and their inhibition can effectively suppress viral replication. Conventional drugs like Doxorubicin, although potent, often carry drawbacks such as toxicity and resistance, prompting researchers to explore natural compounds with fewer side effects and better safety profiles. Natural products have historically served as a rich source of therapeutic agents, and recent studies suggest that phytochemicals could provide cost-effective, accessible alternatives in HIV therapy (Kumar et al., 2020). Molecular docking and *in vitro* assays are powerful tools for screening and validating potential antiviral compounds.

Advances in computational methods like AutoDock enable rapid evaluation of candidate molecules' binding affinity for viral proteins, streamlining the drug discovery process. These *in silico* approaches not only predict howwell compounds might interact with target enzymes but also guide experimental validation. The integration of computational and experimental techniques accelerates the identification of promising bioactive molecules, reducing time and costs associated with traditional drug development while increasing the likelihood of finding effective inhibitors with favorable pharmacokinetics. Among various phytochemicals, ferulic acid—found abundantly in plant cell walls—has demonstrated notable biological activities, including antioxidant, anti-inflammatory, and antimicrobial effects. Its structural features and physicochemical properties meet several criteria for drug-likeness, making it a suitable candidate for further evaluation as an antiviral agent. Recent research indicates ferulic acid's potential to inhibit HIV-1 RT through strong binding interactions (Gurrapu et al., 2017; Gujjeti et al., 2014; Daipule e tal., 2020; Ameen et al., 2021), supported by moleculardocking studies and biochemical assays. This study aims to explore ferulic acid's inhibitory potential against HIV enzymes, combining *in silico* modeling with laboratory validation to assess its viability as a natural HIV-1 RT inhibitor.

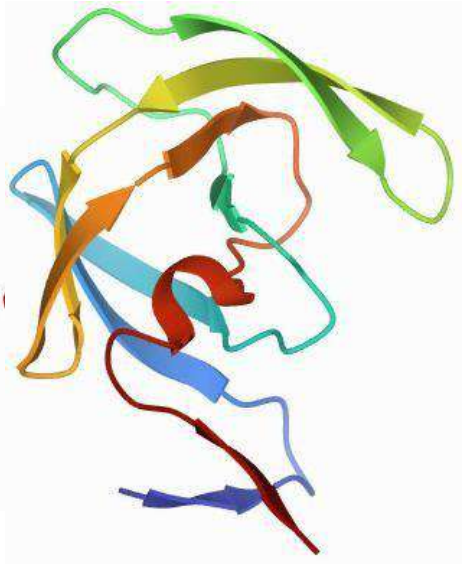
2.MATERIALS AND METHODS

Preparation of HIV target proteins:

The 3D structures of HIV-1 Reverse Transcriptase (PDB : 1REV), HIV-1 integrase (PDB : 1BL3) and HIV-1 protease (PDB : 1HPV) were obtained from the RSCB protein data bank (http://www.rcsb.org/), were used as a receptor of the experimental object (Figure-1)(Berman et al., 2000). Prior to analysis, all water molecules were removed, and ADTsoftware was used to prepare the required files for AutoDock by assigning hydrogen polaraties, calculating Gasteiger charges to protein structures, and converting protein structures from the.PDB file format to. PDBQT format.



(a) HIV-1RT(PDB:1REV)



(b) HIV-1integrase (PDB:1BL3)

c.HIV-1protease (PDB:1HPV)

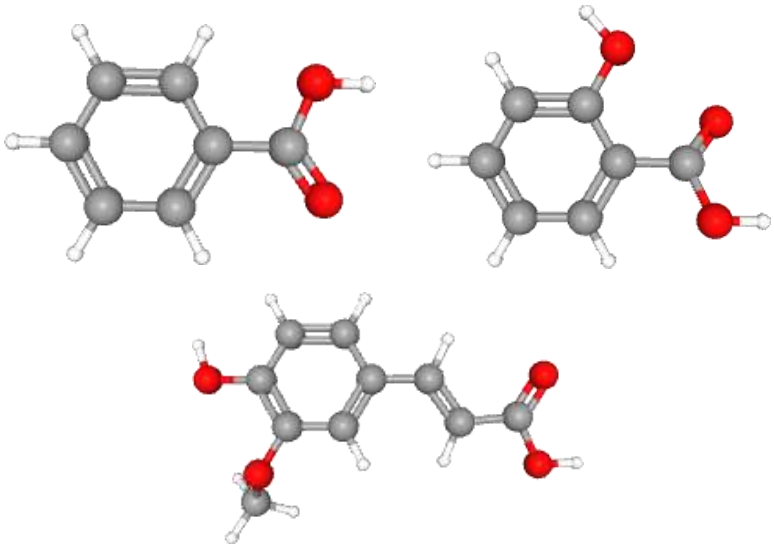
Figure-1.3Dstructuresof(a)HIV-1ReverseTranscriptase (PDB:1REV),(b)HIV-1 integrase (PDB: 1BL3) and (c) HIV-1 protease (PDB: 1HPV).

(ObtainedfromtheRSCBproteindatabank (http://www.rcsb.org/

Preparation of ligand structures for Benzoicacid, salicylic acid and ferulicacid

Structures of Benzoic acid, salicylic acid and ferulic acid were downloaded in the Spatial Data File (.SDF) file format from the PubChem Compound Database (National Center for Biotechnology Information; https://pubchem.ncbi.nlm.nih.gov/) (Figure-2.) (Kim et al.,2021) Physicochemical properties of these ligands met the criteria of Lipinski's rule of five, otherwise known as Lipinski's rule of drug-likeness (Table-2). These rules are a guideline for assessing the structural similarities of compounds with those of active oral drugs and are based on physicochemical profiles. Molecular weights and hydrogen-bonding interactions between donors and acceptors are crucial structural determinants of protein targets and ligand-binding sites.

Chemical structures in the .SDF format were converted to the.PDB format using Discovery Studio Biovia 2017. ADT was then used to investigate ligand structures in terms of combinationswithnon-polarhydrogens, additions ofGasteiger changes, androtatable bonds. Structures in the ligand.PDB format were then converted to the ligand. PDBQT format using ADT, enabling use with AutoDock4 (AD4).



(a)Benzoicacid (b)SalicylicAcid (c)FerulicAcid

Figure-2.3Dstructures of (a)BenzoicAcid, (b)SalicylicAcidand(c)FerulicAcid

(Retrievedfromhttps://pubchem.ncbi.nlm.nih.gov/).

Molecular docking

Due to its various biological activity, the compounds, Benzoic acid, salicylic acid and ferulic acid were selected for molecular docking against HIV-1 target enzymes. Molecular docking was performed with the three compounds against HIV-1 Reverse Transcriptase (PDB: 1REV), HIV-1 integrase (PDB: 1BL3) and HIV-1 protease (PDB: 1HPV) enzymes. Computational tools like AutoDock offer the advantage of delivering new drug candidates more quickly and at a lower cost. AutoDock is an excellent non-commercial dockingprogram that is widely used. Further, it employs a stochastic Lamarckian genetic algorithm for computing ligand conformations and simultaneously minimizing its scoring function which approximates the thermodynamic stability of the lig and bound to the target protein.

Therefore, for molecular docking AutoDock software is used in this study (Morris et al., 2008.

Docking Experiment Settings:

In molecular docking experiments, the prepared proteins and ligand structures were saved in the PDBQT file format. The AutoDockTools (ADT) was used as molecular graphical visualization tool. The AutoDock package includes AutoGrid program and AutoDock program. AutoGrid program is responsible for the calculation of energy grid maps. AutoDock program is responsible for the conformation search and energy evaluation; here, for LGA algorithms, the initial population was set to 50 individuals, the number of energy function evaluations was set to 2.5 × 105, and maximum number of generations was set to 27,000 (Morris et al., 2009).

Analysis of target active binding sites

The active sites arethe coordinates of the ligand in the original target protein grids, and these

active binding sites of target protein were analyzed using the Drug Discovery Studio version 2017.

Methodology of HIV-1ReverseTranscriptaseInhibitionAssay

The activity of ferulic acid on RT activity was determined with recombinant HIV-1 enzyme using a non-radioactive HIV-1 RT colorimetric ELISA kit (Roche). The compound ferulic acid was prepared and tested at six different concentrations (50, 100, 200, 400, 800 and 1000 µg/mL). The enzyme was prepared to a stock solution of 0.764 mg/mL and 0.327 µL was added to 1000 µL lysis buffer. In appropriate wells of the microtitre plates, 20 µL of enzyme, 20 µL diluted extract and 20 µL reaction mixture were added together. For positive control; Zalcitabine at 100 µg/mL was used; (1) lysis buffer was added with DMSO and (2) lysis buffer was added with no DMSO. Lysis buffer and reaction mixture act as negative control. The plates were incubated for one hour at 37 °C. The microtitre plates were washed fivetimeswith 250 µLof the washing buffer. Two hundred microlitres of Anti-Dig-PODworking solution was added in each well. The plates were kept for incubation at 37 °C for one hour. The microtitre plates were washed five times with 250 µL washing buffer. The plates were allowed to stand at room temperature for 10 min after adding 250 µL of ABTS substrate solution. The absorbance was read at 405 nm under microtitre plate reader. The mean of the duplicate absorbance was analysed using the formula:

$$\%\text{Inhibition} = \{1-(\text{OD Sample}/\text{OD negative control})\} \times 100$$

3.RESULTS AND DISCUSSION

Molecular Docking Analysis:

The results of the molecular docking were showed in **table-1** and illustrated in **Figures 1-8**. In the molecular docking predicted complex, a lower binding energy was assumed to be closer to the native state of the complex. For benzoic acid with HIV-1 RT, HIV-1 integrase and HIOV-1 protease complexes, the benzoic acid with HIV-1 RT was energetically more stable than the other two proteins one given the obtained energy results; the lowest binding energy corresponded to–4.95kcal/mol for the Benzoic Acid with HIV-1RTcomplex structure and −3.82kcal/mol for the Benzoid acid with HIV-1 integrase and -3.46 kcal/molfor benzoic acid with HIV-1 protease.

Table-1. Moleculardockinganalysisofthreeselectedcompoundsagainst HIV-1RT, HIV-1 integrase and HIV-1 protease

S. N	Compound Name	Target enzyme	Binding energy (kcal/mol)	Residuesinvolving interaction	No. of H bonds	Interactionof residues formingH bonds
		HIV-1 RT	-4.95	GLN340, THR338, GLY273, GLN332, LYS275, THR351, TYR339, PRO272, GLY352,	2	ILE274 SER268

				LYS353, TYR271		
1	Benzoic-Acid	HIV-1 Integrase	-3.82	VAL:77, SER;153, HIS:78, VAL:79, GLY:82, ILE;151	1	MET:154
		HIV-1 protease	-3.46	GLY:49, ILE;47, ILE:54, GLY:51, 1ILE;50, GLY:48, GLY:52, PHE:53	-	-
2	Salicylic-Acid	HIV-1 RT	-4.94	VAL179, TYR318, LEU100, VAL106, HIS235	2	LYS:101, LYS:103
		HIV-1 Integrase	-3.41	GLU:87, GLN:177, PHE:100, ALA:86, ARG:107,GLU:85, LYS:103,LEU:104	1	GLU:85
		HIV-1 protease	-3.41	CYS:95, ILU:5, THR:26, LEU;24, ASN:98, GLN:2, PRO:1,ILE:3, PRO:9	1	THR:96
3	Ferulic-Acid	HIV-1 RT	-6.29	GLY99, VAL179, TYR188, LYS101, LEU100, TYR318, VAL106, PRO236, HIS235, LEU234, PHE227	1	LYS:103
		HIV-1 Integrase	-6.12	GLY:82, MET:154, VAL:77, ILE:151 SER;81, ALA:80, VAL:79,	2	GLN:62, ARG:199
		HIV-1 protease	-1.28	GLY:27, ASP:25, ALA:28,VAL:82, ILE:84, ILE:47, THR:80, ILE :54	1	THR:80

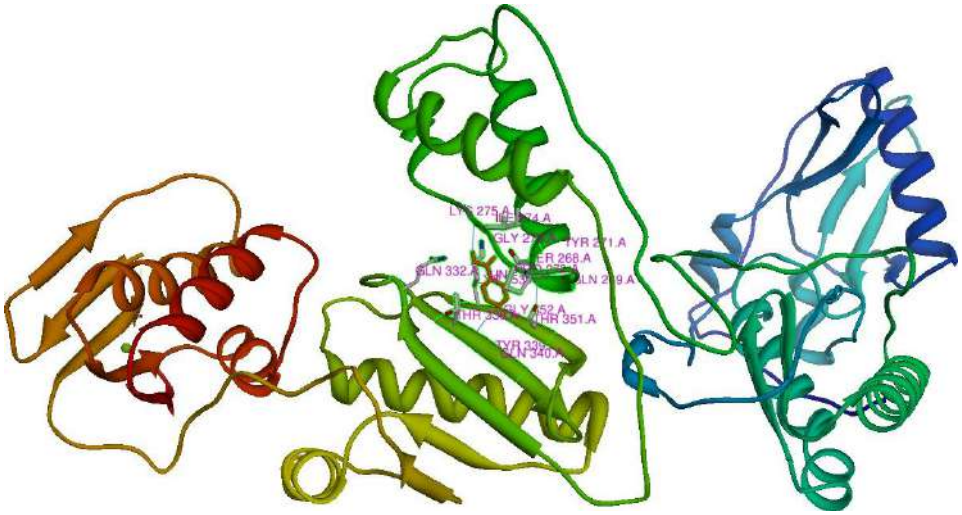


Figure-3. Interactions of Benzoic acid(orange)with HIV-1RTin3 Dillustration
(Interactive amino acids are shown in pink colour)

Figure 1 and Table-1 shows the hydrogen bond interactions associated with the ligand benzoid acid and surrounding HIV-1 RT protein residues. Benzoic acid formed hydrophobic interactions with HIV-1 RT, involving the amino acid residues GLN340, THR338,GLY273,GLN332,LYS275,THR351,TYR339,PRO272,GLY352,LYS353, TYR271 (Figure-3). Benzoic acid-HIV-1 RT interactions were supported by three hydrogen bonds at residues ILE274 and SER268.

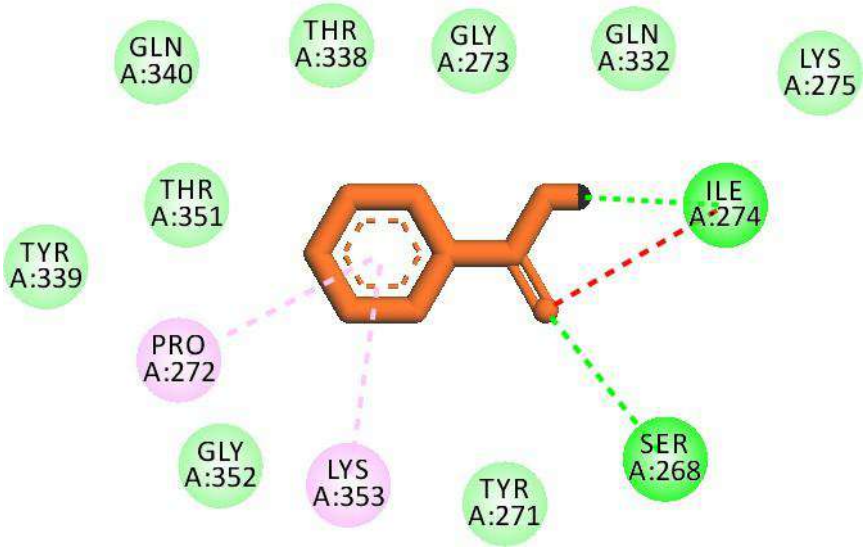


Figure-4. Interaction of Benzoicacid with HIV-1RT in 2D illustration
(hydrogen bond interactions are shown in green dashed lines)

Docking simulations of second ligand SalicylicAcid with HIV-1RT, usingADTshowed that with HIV-1RThasaΔG score of−4.94kcal/mol at the lowest(1st) conformation, where as ΔGvalues salicylic acid with HIV-1integrase and with HIV-1protease were-3.41and-3.41

kcal/mol respectively (Table 5). These results indicate that, of the ligand salicylic acid possesses the greatest binding affinity for HIV-1RT(Figure-5and6). Fivehydrophobic interactions with the amino acid residues Val179, Tyr318, Leu100, Val106 and His235 found with HIV-1 RT-Salycylic acid ligand.

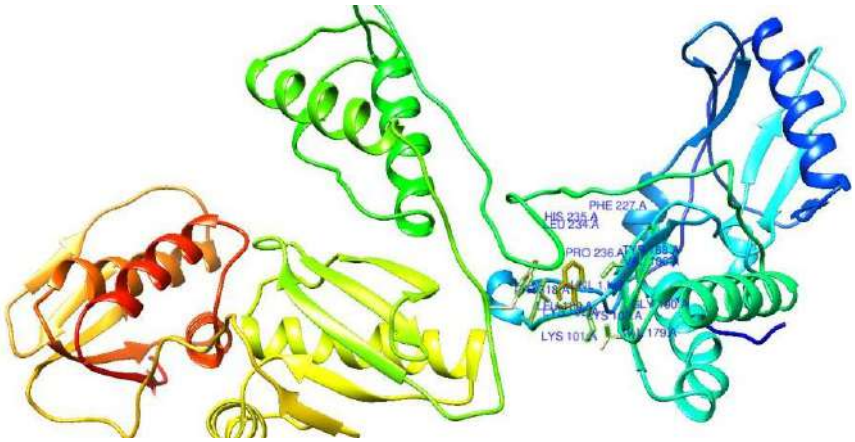


Figure-5. InteractionsofSalicylicacid(orange)withHIV-1RTin3Dillustration (Interactive amino acid names are shown in blue colour)

The docking outcome points out that there are two hydrogen bonds for salicylic acid ligand to the HIV-1 RT -4.94 kcal/mol binding energy with Lys103 and Lys101 residues (Figure-5, 6 and 7). One hydrogen bond interaction between salicylic acid ligand and HIV-1 integrase -3.41 kcal/mol binding energy with Glu85 residue and only one hydrogen bond interaction between salicylic acid ligand and HIV-1 protease -3.41 kcal/mol binding energy with Thr96 residue.

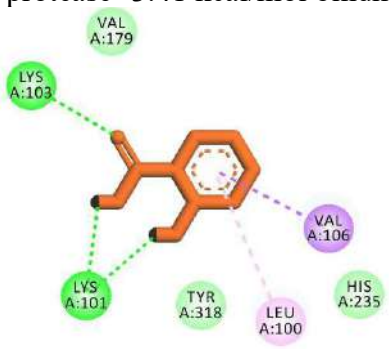


Figure-6. Interaction of Salycilicacid with HIV-1RT in 2D illustration (hydrogen bond interactions are shown in green dashed lines)

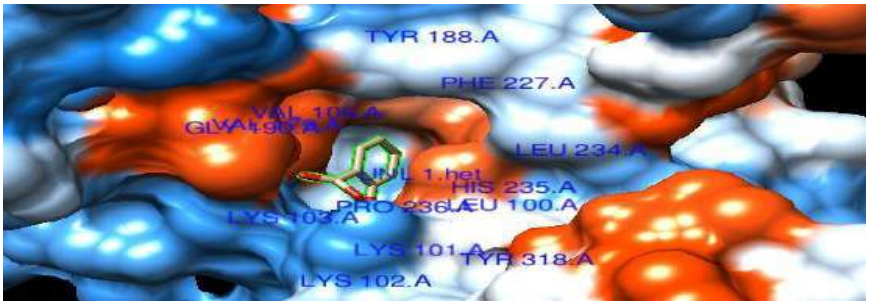


Figure-7. Surface representation of salycilicacid interaction with HIV-1 RTaminoacid residues

Docking simulations of third ligand Ferulic Acid with HIV-1 RT, using ADTshowed that with HIV-1 RT has a ΔG score of −6.29 kcal/mol at the lowest (1st) conformation, whereas ΔGvaluesFerulic Acid with HIV-1 integrase and with HIV-1 protease were -5.19 and -1.28 kcal/mol respectively (Table-2). These results indicate that, of theligandFerulic Acidpossessesthegreatestbindingaffinityfor HIV-1RT(Figure-8and9).

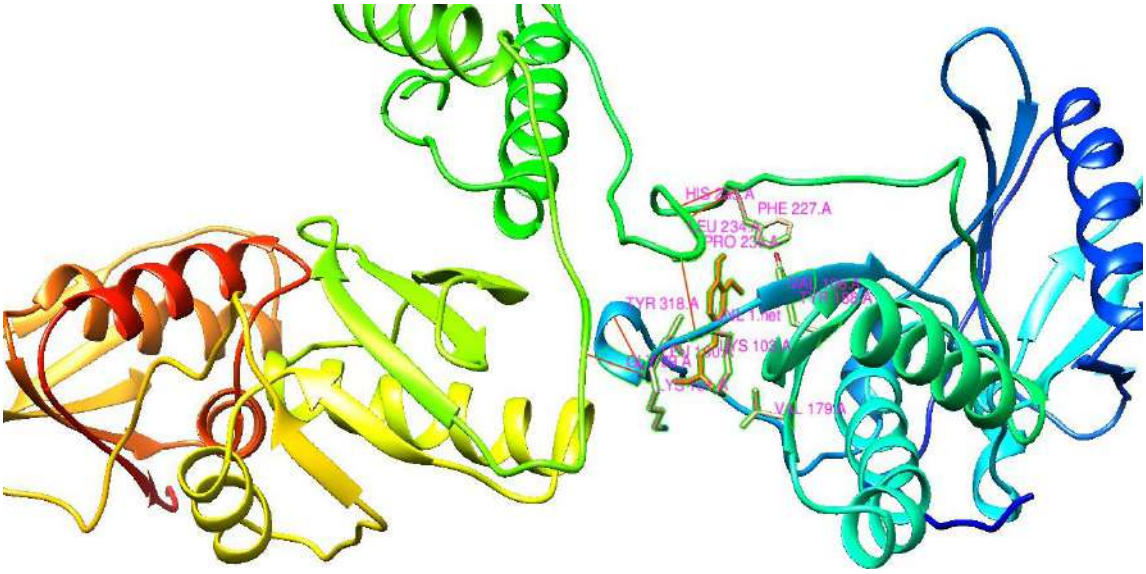


Figure-8. InteractionsofFerulicacid(orange)withHIV-1RTin3Dillustration (Interactive amino acid names are shown in pink colour)

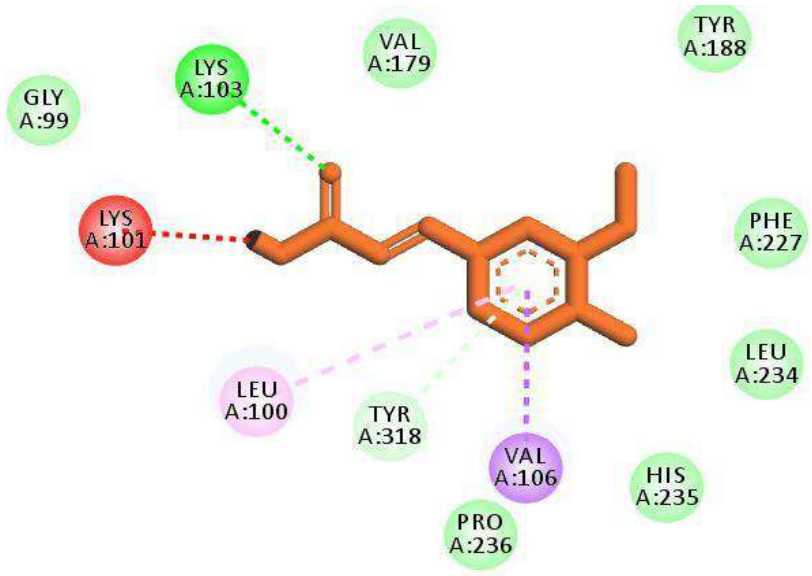


Figure-9. InteractionofFerulicacidwithHIV-1RTin2Dillustration (hydrogen bond interactions are shown in green dashed lines)

The docking outcome points out that there is only one hydrogen bond for ferulic acid ligand to the HIV-1 RT with Lys103 residue (Figure-8, 9 and 10). Two hydrogen bond interactionsbetweenferulicacidligandandHIV-1integrasewith Gln62andArg199 residues andonlyonehydrogenbondinteraction betweenferulicacidligandand HIV-1proteasewith Thr80 residue. There are 11 hydrophobic interactions between ferulic acid ligand and HIV-1 RT

protein with Gly99, Val179, Tyr188, Lys101, Leu100, Tyr318, Val106, Pro236, His235, Leu234 and Phe227 residues.

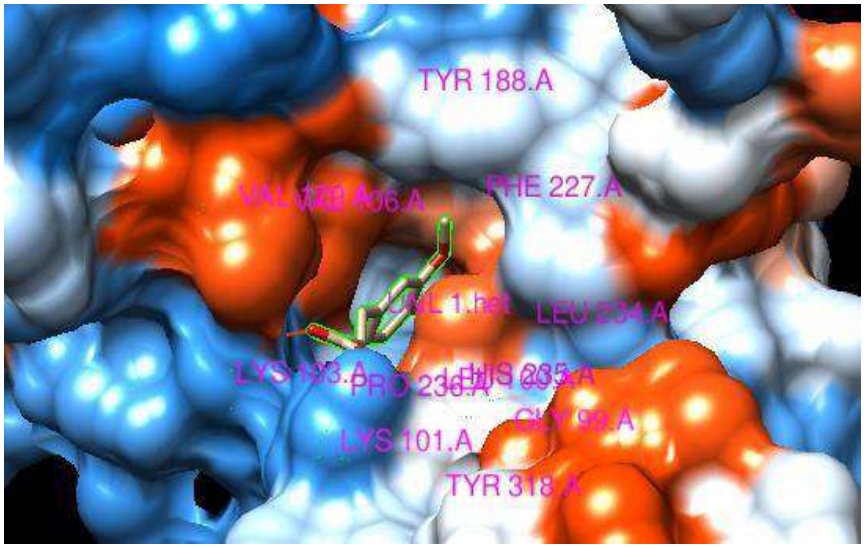


Figure-7. Surface representation of ferulic acid interaction with HIV-1RT amino acid residues

S. No	DrugName		Bindingenergyinkcal/mol		
			1BL3 integrase standard (elvitegravir)	1REVReverse Transcriptase (Doxorubicin)	1HPV protease (Amprenavir)
1	ReferenceDrugs		-4.78	-4.91	-2.4
2	Test Compounds	Benzoic-Acid	-3.82	-4.95	-3.46
		Salicylic-Acid	-3.67	-4.94	-3.1
		Ferulic-Acid	-5.19	**-6.29**	-1.28

Table 2. Binding energyof testcompounds and reference drugs with HIV-1 target enzymes

Amongst screened compounds Benzoic acid, Salicylic acid and Ferulic acid, the ferulic acid encompasses the maximum binding energies compared to reference drugs also (Table-6). For that reason, ferulic acid is a positive drug molecule similar to Doxorubicin against HIV disease. We expect that these investigations will be supportive for designing a novel and effective inhibitors against the HIV. Therefore, *in vitro* validation of this ligand was done.

In vitro HIV-1ReverseTranscriptase Inhibition Assay

The data indicate that ferulic acid exhibits a dose-dependent inhibition of HIV-1 reverse transcriptase (RT), with peak activity observed at 200 µg/mL (72.5±9.23%) and 400 µg/mL

(75.87±9.66%). Interestingly, inhibition declines at higher concentrations—800 µg/mL (55.22±3.69%) and 1000 µg/mL (57.16±4.89%)—suggesting a possible saturation effect or cytotoxic interference at elevated doses. The IC_{50} value of 71.55±5.04 µg/mL reflects moderate potency, indicating that ferulic acid requires relatively high concentrations to achieve50%inhibition. Theinitialincreaseininhibitionfrom32.26±4.13%at50µg/mLto 69.49±6.43% at 100 µg/mL supports its potential as an RT inhibitor. However, the non- linear response at higher doses warrants further investigation into its pharmacodynamics and possible off-target effects. Overall, ferulic acid demonstrates promising inhibitory activity, but its efficacy plateaus and declines at higherconcentrations, which maylimit itstherapeutic window or necessitate formulation optimization.

Doxorubicin, used as a reference drug, shows a different inhibition pattern. Its highest inhibition is at 50 µg/mL (38.27±2.89%), followed by a gradual decline across increasing concentrations, reaching 59.1±3.77% at 1000 µg/mL. Unlike ferulic acid, doxorubicin does not exhibit a clear dose-dependent increase, and its inhibition fluctuates, peaking at lower concentrations. The IC_{50} value of 68.40±9.45 µg/mL is slightly lower than that of ferulic acid, indicating marginally higher potency. However, the broader standard deviation suggests greater variability in response. The lack of consistent inhibition at higher doses may reflect doxorubicin's complex pharmacological profile, including potential cytotoxicity or enzyme saturation. When comparing both compounds, ferulic acid shows a more defined dose-responsecurveupto400µg/mL, while doxorubicin's inhibition appears less predictable.

These findings suggest that although doxorubicin is a potent RT inhibitor, ferulic acid may offer a more stable inhibition profile within a specific concentration range, meriting further exploration as a natural alternative.

Ferulic acid exhibited good inhibition in a dose-dependent manner (Figure-8) against HIV-1 Reversetranscriptase (RT)withIC50valuesof71.55±5.04µg/mL (Tabl-7). Highest (72.5 %) HIV-1 RT inhibition showed at 200 µg/mL concentration. Doxorubicin, a known RT inhibitor, was used as a positive control and inhibited HIV RT highest by 61 % at 100 µg/mL (IC_{50}68.40±9.45 µg/mL). Based on this result, ferulic acid showed more potent againstHIV-1 RT compared to reference drug and showed highest HIV-1 RT inhibition.

Name of the compound	% of HIV-1RT inhibition (Mean ±SD)						IC50 µg/mL
	50 µg/mL	100 µg/mL	200 µg/mL	400 µg/mL	800 µg/mL	1000 µg/mL	
FerulicAcid (Test compound)	32.26± 4.13	69.49± 6.43	72.5± 9.23	75.87± 9.66	55.22± 3.69	57.16± 4.89	71.55 ± 5.04
Doxorubicin (Reference drug)	38.27± 2.89	61.34± 5.43	58.6± 5.8	52.57± 7.7	53.21± 4.22	59.1± 3.77	68.40 ± 9.45

Table-7. Inhibition of HIV-RT by ferulicacid-reverse transcriptase inhibition (%). IC50 values were 71.55±5.04 and 68.40±9.45µg/mL for ferulic acid and doxorubicin, respectively

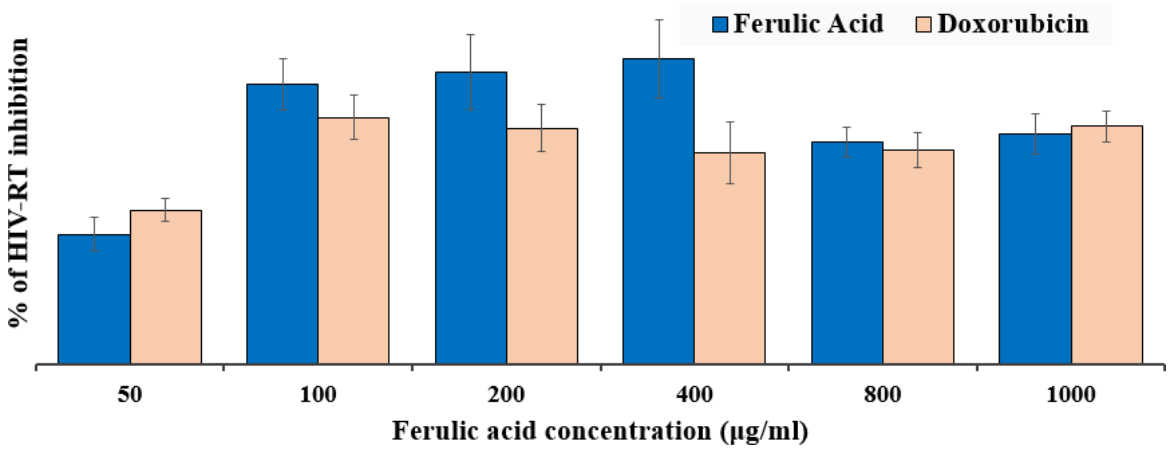


Figure-8. *Invitroanti*-HIVRTactivityofferulic acid.

Doxorubicinwasusedasapositivecontrol.

4.CONCLUSION

This study highlights ferulic acid's potential as a natural inhibitor of HIV-1 reverse transcriptase, supported by both molecular docking and in vitro assays showing significant antiviralactivity. Itsstrongbindingaffinityanddose-dependentinhibitionsuggestthatferulic acid could serve as a promising lead compound for developing affordable, plant-based therapeutics against HIV. Further pharmacokinetic and clinical studies are necessary to optimize its efficacy and safety profile. Overall, ferulic acid's dual computational and experimental validation underscores its potential in HIVdrugdiscoveryefforts, offeringhope for alternative treatment options with fewer side effects.

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AI for Designing Biodegradable Materials for Drug Delivery Systems

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Abstract: *The convergence of Artificial Intelligence (AI) and biotechnology is significantly reshaping the field of drug delivery, offering innovative solutions to long-standing challenges. One of the most promising areas of this transformation lies in the design and development of* ***biodegradable materials****—such as polymers, nanoparticles, and nanocarriers—that facilitate targeted, efficient, and eco-friendly drug delivery. These materials degrade safely within the body after delivering therapeutic agents, minimizing long-term toxicity and eliminating the need for surgical removal.*

Traditionally, the discovery and optimization of biodegradable drug delivery systems have relied on time-consuming and costly trial-and-error experiments. However, with the advent of AI and machine learning (ML) techniques, it is now possible to accelerate these processes through predictive modeling, data-driven simulations, and automated design frameworks. AI algorithms can analyze vast datasets to predict material properties such as degradation rate, drug loading efficiency, release profiles, and biocompatibility. Moreover, advanced generative models can design new polymer structures tailored to specific medical requirements, while reinforcement learning can optimize delivery mechanisms in real time.

This paper explores the growing role of AI in the design of biodegradable drug delivery materials. It highlights recent advancements in polymer informatics, nanocarrier optimization, and molecular dynamics simulations enhanced by machine learning. Additionally, it addresses the integration of AI tools in early-stage material screening and their ability to support personalized medicine through adaptive, patient-specific delivery platforms.

Keywords: *Biodegradable materials, Artificial Intelligence, Drug delivery systems, machine learning etc.*

1. INTRODUCTION

The pharmaceutical industry is increasingly turning to biodegradable materials for drug delivery due to their safety, biocompatibility, and environmental sustainability. These materials, often derived from natural or synthetic polymers, degrade within the body after fulfilling their function, thereby minimizing toxicity and the need for surgical removal. However, designing such materials with optimal mechanical, chemical, and pharmacokinetic properties remains a significant challenge.

Artificial Intelligence (AI) has emerged as a transformative force in materials science, capable of accelerating the discovery process by identifying patterns in vast datasets, simulating molecular behavior, and predicting material properties. In the context of drug delivery systems, AI can guide the selection and optimization of biodegradable carriers that enhance therapeutic efficiency, reduce side effects, and align with personalized treatment strategies.

2. Role of Biodegradable Materials in Drug Delivery

Biodegradable materials play a crucial role in modern drug delivery systems due to their ability to safely break down into non-toxic byproducts within the body after delivering therapeutic agents. These materials eliminate the need for surgical removal and reduce the long-term risks associated with non-degradable carriers. Their application has expanded rapidly across areas such as cancer therapy, vaccine delivery, wound healing, and tissue engineering.
Some of the most commonly used biodegradable materials include:

- **Polylactic Acid (PLA):** A synthetic aliphatic polyester derived from renewable sources such as corn starch. PLA is known for its high mechanical strength and slow degradation rate, making it suitable for long-term drug delivery implants and scaffolds.
- **Polyglycolic Acid (PGA):** A highly crystalline and hydrophilic polymer with a relatively fast degradation rate. It is often used in applications requiring rapid drug release or in combination with other polymers to tailor release profiles.
- **Poly(lactic-co-glycolic acid) (PLGA):** A copolymer of PLA and PGA, PLGA combines the beneficial properties of both, allowing for customizable degradation rates by adjusting the lactic-to-glycolic acid ratio. It is one of the most widely studied biodegradable polymers and is approved by the FDA for various drug delivery systems.
- **Chitosan:** A natural polysaccharide derived from chitin, commonly found in the shells of crustaceans. Chitosan is biocompatible, mucoadhesive, and possesses antimicrobial properties, making it ideal for nasal, oral, and wound drug delivery.
- **Gelatin:** A natural, water-soluble polymer obtained from collagen. Gelatin is commonly used for the fabrication of hydrogels and microspheres, particularly in soft tissue applications, due to its excellent biocompatibility and biodegradability.
- **Alginate:** A polysaccharide derived from brown seaweed, alginate forms hydrogels in the presence of divalent cations like calcium. It is widely used in controlled-release drug formulations, especially for gastrointestinal and wound healing applications.
- **Polycaprolactone (PCL):** A synthetic polyester with a very slow degradation rate, making it suitable for long-term drug delivery and implants. It provides excellent compatibility with a wide range of drugs and is often used in combination with faster-degrading polymers.

These materials are used to fabricate a variety of **drug carriers**, including **microspheres, nanoparticles, hydrogels, films, and scaffolds**, each designed to achieve specific therapeutic goals. For example, **microspheres** allow for injectable long-acting formulations, **nanoparticles** enable targeted delivery to tumor tissues, and **hydrogels** provide localized, sustained drug release for wound care. The selection and design of biodegradable materials must consider multiple parameters such as **degradation rate, drug loading capacity, mechanical strength, release kinetics, and interaction with biological tissues**. Customization of these parameters ensures optimal therapeutic efficacy, patient safety, and regulatory compliance for various clinical applications.

In conclusion, biodegradable materials serve as the foundation of advanced drug delivery systems, and their design and optimization are critical for achieving precise, patient-friendly, and environmentally responsible therapies.

3. AI and ML Approaches for Materials Design

Artificial Intelligence (AI) and Machine Learning (ML) have become indispensable tools in the field of materials science, particularly for the design and optimization of **biodegradable drug delivery systems**. These technologies can be integrated across various stages of the material development pipeline—from property prediction and virtual screening to molecular simulation and synthesis planning—thus significantly reducing time, cost, and experimental burden. Below are some of the key AI-driven approaches used in this domain:

3.1 Material Property Prediction

AI and ML algorithms can accurately predict the physical, chemical, and biological properties of biodegradable materials based on their molecular structure and known datasets. Traditional methods rely on empirical testing, which is time-consuming and expensive. In contrast, AI models can use descriptors (such as molecular weight, functional groups, crystallinity, etc.) to forecast:

- **Degradation time**: How quickly a material breaks down under physiological conditions.
- **Drug release kinetics**: The rate and pattern at which a drug is released from a carrier matrix.
- **Mechanical properties**: Attributes such as tensile strength, flexibility, and elasticity, which are essential for implants or structural scaffolds.
- **Toxicity and biocompatibility**: AI models can screen for adverse biological effects, ensuring that new materials are safe for use in human or animal systems.

Common algorithms used include **Random Forests**, **Support Vector Machines (SVMs)**, **Decision Trees**, and **Deep Neural Networks**. These models learn from large datasets and can generalize predictions for novel materials that have not yet been synthesized.

3.2 Inverse Design of Polymers

Inverse design refers to starting with desired material properties and working backward to identify or generate the molecular structures that achieve those outcomes. This is particularly valuable in drug delivery, where precise control over material behavior is critical.
Advanced generative AI models such as:

- **Variational Autoencoders (VAEs)**: These compress chemical structures into a latent space and then decode them to generate new candidates with specified properties.
- **Generative Adversarial Networks (GANs)**: These consist of a generator and a discriminator network working together to create realistic and functional new polymer structures.

By using these models, researchers can rapidly explore the chemical space of potential polymers, propose novel formulations, and fine-tune molecular features such as

hydrophobicity, branching, or crosslinking—factors that influence drug encapsulation and release.

3.3 Molecular Dynamics and AI Hybrid Modeling

Molecular Dynamics (MD) simulations are used to study the behavior of atoms and molecules over time. When combined with AI, MD simulations become faster, more accurate, and predictive. AI helps in:

- **Accelerating simulation runtimes** by predicting stable conformations and energy states.
- **Evaluating polymer-drug interactions**, such as how a drug molecule binds within a nanoparticle matrix.
- **Predicting encapsulation efficiency**, drug diffusion rates, and degradation pathways.

AI-augmented MD models allow for a more detailed understanding of how biodegradable carriers behave under real physiological conditions, which is essential for designing safe and effective delivery systems.

3.4 Multi-Objective Optimization

Designing biodegradable drug delivery materials often involves **balancing multiple conflicting properties**. For example, a material must degrade quickly enough to release the drug on time but slowly enough to maintain structural integrity; it must be flexible but also strong, and biocompatible while also efficient in drug loading.

AI-powered optimization algorithms such as:

- **Bayesian Optimization**
- **Genetic Algorithms (GAs)**
- **Multi-objective evolutionary algorithms (MOEAs)**

These models explore trade-offs and generate optimal combinations of features to meet design goals. For example, AI can help determine the best ratio of lactic to glycolic acid in a PLGA copolymer to optimize both drug release and biodegradability for a specific treatment.

4. Applications

The integration of Artificial Intelligence (AI) in the design and deployment of biodegradable drug delivery systems has opened up new frontiers in precision medicine. AI techniques are now being widely applied across various delivery formats, including **nanoparticles, hydrogels, microneedles**, and **implantable or oral drug systems**. These applications leverage AI's ability to optimize materials, personalize treatments, and simulate biological responses, resulting in safer and more efficient therapies.

4.1 Nanoparticle-Based Drug Delivery

Biodegradable nanoparticles—often formulated from materials like **PLGA (poly(lactic-co-glycolic acid))**, lipids, or natural polymers—are engineered to encapsulate and deliver drugs to specific tissues or cells. AI plays a pivotal role in designing these nanoparticles with optimized size, surface charge, and drug release kinetics.
Machine learning models analyze vast datasets of experimental formulations to predict:

- **Targeting efficiency** (e.g., for tumor cells)
- **Drug loading capacity**
- **Release profiles under different physiological conditions**
- **Stability in the bloodstream**

Additionally, AI aids in surface modification design, such as attaching ligands or antibodies that enable active targeting of diseased tissues while minimizing systemic toxicity. This is especially beneficial in cancer therapy, where precision delivery is critical.

4.2 Hydrogels for Controlled Release

Hydrogels are three-dimensional, water-absorbing polymer networks widely used for **localized and sustained drug release**, particularly in treating chronic conditions like arthritis, diabetes, and wound infections.

AI—especially **deep learning models**—helps predict the **swelling behavior**, **cross linking density**, and **degradation rate** of biodegradable hydrogels based on polymer composition, temperature, and pH levels. These predictions enable the customization of drug release kinetics tailored to specific treatment durations and target sites. For example, AI can suggest hydrogel formulations that release anti-inflammatory drugs over a 7-day period in joint tissue while maintaining structural integrity throughout.

4.3 Microneedle Patches

Biodegradable microneedle patches represent a **minimally invasive**, **painless** alternative to traditional injections. They are particularly useful for **vaccine delivery**, **insulin therapy**, and **hormonal treatments**.
AI is used to:

- Optimize **needle geometry** (length, width, sharpness)
- Select **biodegradable materials** that safely dissolve in skin layers
- Model **skin penetration** and **drug diffusion**
- Predict **delivery efficiency** and **patient variability**

For instance, AI can simulate how quickly a microneedle patch loaded with an mRNA vaccine dissolve and releases the payload in the dermis, thereby aiding in faster and more effective immunization strategies.

4.4 Oral and Implantable Systems

Oral capsules and implantable drug delivery devices made from biodegradable polymers must perform reliably in highly variable **physiological environments**. Factors such as **pH levels**, **enzyme presence**, and **gut microbiota** significantly influence how these systems degrade and release drugs.

AI models—often based on **supervised learning and ensemble methods**—are trained on experimental data to:

- Predict **degradation rates** in different body compartments (stomach, intestines, muscle tissue)
- Forecast **drug release profiles** over hours to months
- Recommend **optimal polymer blends** for controlled or sustained release

These predictions help researchers fine-tune formulations for specific medical needs. For example, AI might suggest a PLGA: PCL ratio that ensures a cardiovascular stent implant slowly releases anti-inflammatory drugs over a three-month period. The application of AI in biodegradable drug delivery systems enhances both **efficiency** and **personalization**. Whether through nanocarriers, smart hydrogels, dissolvable microneedles, or long-acting implants, AI enables a new generation of therapies that are precisely engineered, minimally invasive, and environmentally conscious. As datasets grow and models improve, the integration of AI will continue to push the boundaries of what is possible in drug delivery science.

5. Challenges and Limitations

While the integration of Artificial Intelligence (AI) and Machine Learning (ML) into biodegradable drug delivery system design has demonstrated significant promise, several critical challenges and limitations hinder its full-scale adoption and effectiveness. Addressing these issues is essential to ensure that AI-driven innovations are reliable, reproducible, and clinically translatable.

5.1 Data Scarcity

One of the foremost challenges in this domain is the **lack of large, diverse, and high-quality datasets** specific to biodegradable materials and their use in drug delivery. AI and ML algorithms require vast amounts of well-curated, labeled data to make accurate and generalizable predictions. However, due to the **proprietary nature of pharmaceutical research**, variability in experimental conditions, and limited standardization of data reporting, such datasets are often scarce or fragmented.

For example, variations in polymer synthesis methods, drug loading techniques, and in vitro/in vivo testing protocols make it difficult to compile uniform data for training robust models. This data gap can lead to **overfitting**, **biased predictions**, or **limited applicability** of the models to new materials or formulations.

5.2 Model Interpretability

Many state-of-the-art AI models—particularly **deep learning networks**—operate as "black boxes," providing predictions without clear explanations of how decisions are made. In the context of healthcare and material science, this lack of **transparency and interpretability** poses serious limitations.

Regulatory bodies like the **FDA** or **EMA** require clear justifications for design choices, especially when human health is involved. Without interpretable AI outputs, it becomes difficult to gain regulatory approval, build trust among researchers and clinicians, or understand potential failure mechanisms in drug delivery systems.

Efforts in **Explainable AI (XAI)** are underway but are still in early stages when applied to materials and biomedical engineering.

5.3 Experimental Validation

Despite AI's ability to simulate and predict the properties of biodegradable materials, **experimental validation remains indispensable**. Any AI-generated polymer formulation,

nanoparticle design, or drug release profile must still undergo rigorous laboratory testing to confirm efficacy, safety, and reproducibility.

This validation process can be **time-consuming**, **cost-intensive**, and sometimes **infeasible** in high-throughput scenarios, especially when multiple iterations of design need to be tested. Furthermore, discrepancies between **in silico predictions** and **in vitro/in vivo outcomes** often arise due to assumptions or simplifications made during modeling.

As a result, AI currently serves more as a **decision-support tool** rather than a full replacement for traditional experimentation.

5.4 Integration with Biological Systems

The ultimate success of any drug delivery system depends on how it interacts with **complex biological environments**. Human physiology is highly variable across individuals and conditions—factors such as **immune response, enzymatic activity, local pH, tissue permeability**, and **disease state** can significantly affect material performance.

Current AI models struggle to accurately predict such dynamic, multifactorial behaviors, especially **in vivo**. The integration of AI with biological system modeling (such as **systems biology**, **organ-on-a-chip**, or **physiologically based pharmacokinetic (PBPK)** models) is still evolving and requires deeper interdisciplinary collaboration.

Until AI models can reliably simulate these complexities, there remains a significant gap between **theoretical performance** and **clinical reality**.

6. Future Directions

The convergence of artificial intelligence (AI) and materials science is still in its early stages, particularly in the context of biodegradable drug delivery systems. However, rapid technological advancements are paving the way for transformative innovations. Looking ahead, several promising directions are likely to define the next era of research and application in this field:

6.1 Self-Driving Laboratories

One of the most exciting developments is the emergence of **self-driving laboratories**—AI-controlled experimental platforms capable of autonomously designing, synthesizing, and testing new biodegradable materials. These labs use robotics, automation, and real-time data analytics to rapidly iterate through experiments with minimal human intervention.

By integrating machine learning algorithms with high-throughput screening tools, these labs can:

- Identify optimal polymer formulations.
- Fine-tune drug loading capacities.
- Accelerate discovery cycles from months to days.

Such autonomous systems could dramatically reduce the time and cost of developing novel drug delivery vehicles, especially when combined with **cloud computing and digital twin simulations**.

6.2 Explainable AI (XAI)

As AI models become more complex, there is a growing need for **explainable AI (XAI)** frameworks that offer insights into how predictions are made. In the context of drug delivery material design, XAI can:

- Help scientists understand the rationale behind a model's recommendation.
- Highlight key molecular features contributing to biodegradability or drug release kinetics.
- Improve confidence among regulatory agencies and clinical stakeholders.

XAI not only fosters **trust and accountability** but also encourages the co-creation of knowledge between computational models and domain experts.

6.3 Integration with Bioinformatics for Personalization

Future AI-driven systems are expected to go beyond generic formulations and enable **personalized drug delivery**. By integrating **bioinformatics data**—such as genomic, transcriptomic, and proteomic profiles—AI can:

- Customize biodegradable carriers based on a patient's genetic makeup.
- Predict individual immune responses or metabolic interactions.
- Enhance precision medicine approaches for diseases like cancer, autoimmune disorders, and genetic conditions.

This fusion of AI, materials science, and **systems biology** could revolutionize personalized therapeutics, enabling safer and more effective treatments tailored to each patient.

6.4 Open-Source Databases and Collaborative Platforms

To support innovation and democratize access to data, the creation of **open-source databases** is essential. These databases would compile:

- Physicochemical properties of polymers.
- Drug release and degradation profiles.
- Experimental and simulated datasets.

Open repositories would enable researchers worldwide to **train better ML models**, **replicate studies**, and **benchmark algorithms** more efficiently. Initiatives like the **Materials Genome Initiative (MGI)** and **Polymer Genome** are already paving the way, but greater focus on biodegradable materials for healthcare is needed.

Such collaborative efforts would accelerate the development of standardized frameworks and reduce duplication of experimental efforts, fostering **global progress** in AI-assisted drug delivery research.

The future of AI in biodegradable drug delivery systems is bright, with opportunities to enhance speed, precision, and personalization in material design. Self-driving labs, explainable AI, bioinformatics integration, and open-data ecosystems represent pivotal advancements that could reshape the landscape of pharmaceutical innovation. Realizing this vision will require interdisciplinary collaboration, ethical oversight, and continuous investment in AI infrastructure and education.

7. Conclusion

The integration of Artificial Intelligence (AI) into the realm of biodegradable materials for drug delivery systems marks a transformative shift in pharmaceutical research and development. Traditional approaches to designing drug delivery platforms—especially those relying on biodegradable polymers—have often been constrained by slow, costly, and labor-intensive experimentation. AI offers a compelling alternative by enhancing the **efficiency, precision, and creativity** of material design processes.

From **predicting essential material properties** such as degradation rates and drug release kinetics, to **generating novel polymer structures** using advanced generative models, AI enables a fundamentally different approach—one that is data-driven, iterative, and highly customizable. The use of machine learning (ML) techniques like deep neural networks, random forests, and genetic algorithms allows researchers to navigate complex, multi-dimensional design spaces far more efficiently than through empirical methods alone.

Moreover, AI's ability to integrate data from **computational simulations, molecular dynamics, and biological assays** makes it uniquely positioned to address the intricacies of designing drug carriers that are not only effective but also biocompatible, non-toxic, and environmentally friendly. Applications in **nanoparticle engineering, hydrogel design, microneedle optimization, and oral or implantable systems** illustrate the vast scope of AI's potential in the field.

However, realizing this potential at scale is contingent on addressing several critical challenges. These include the **scarcity of high-quality, labeled datasets** specific to biodegradable systems, the **lack of transparency in AI model decision-making**, the **need for experimental validation**, and the **complexities of biological variability** in human patients. Interdisciplinary collaboration—between computer scientists, materials engineers, pharmacologists, and clinicians—will be essential to overcome these barriers.

Looking ahead, the development of **explainable AI**, **open-access data repositories**, and **autonomous labs** could serve as major catalysts in bridging the gap between AI-enabled research and real-world clinical applications. As these technologies mature, AI is poised not only to **accelerate the discovery of next-generation biodegradable materials**, but also to **enhance patient care**, **reduce environmental impact**, and **usher in a new era of intelligent, personalized medicine**.

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Economically important chemical components from different insect species

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Abstract: *Insects produce a wide array of chemical compounds that hold immense economic importance across various sectors including agriculture, medicine, cosmetics, and industry. This review explores the diversity of bioactive and commercially valuable chemical components derived from different insect species. Notable examples include silk proteins from Bombyx mori, honey and royal jelly from Apis mellifera, lac resin from Kerria lacca, and dyes such as carminic acid from Dactylopius coccus. Additionally, insects like Tenebrio molitor and Acheta domesticus are recognized for their high-protein content and beneficial fatty acids, contributing to sustainable food and feed alternatives. Antimicrobial peptides and enzymes from insects such as maggots and wasps offer promising pharmaceutical applications. Pheromones and other semiochemicals from beetles, moths, and ants are widely used in integrated pest management (IPM). The extraction, characterization, and synthesis of these compounds have opened new avenues in biotechnology and green chemistry. This paper highlights the potential of insect-derived chemicals in addressing global challenges, including food security, environmental sustainability, and novel drug development. Further research on sustainable harvesting, large-scale production, and regulatory frameworks is essential to fully harness the benefits of these economically significant insect-derived compounds.*

Key words: *chemical components, antimicrobial peptides and enzymes, silk proteins, lac resin.*

1. INTRODUCTION

Insects represent one of the most diverse and abundant groups of organisms on Earth, with millions of species occupying nearly every ecological niche. Historically, many insect species have played crucial roles in human civilization—from pollinators and silk producers to agents of pest control. In recent years, scientific research has increasingly focused on the unique and potent chemical compounds produced by insects (Gullan, P. J., & Cranston, P. S. 2014). These substances range from structural proteins and waxes to pheromones, antimicrobial peptides, and natural dyes (Isman, M. B. 2006). The economic value of these compounds spans industries such as agriculture, pharmaceuticals, cosmetics, textiles, and food production (Morales-Ramos, J. A., et al.,2013; Zurek, L., & Ghosh, A. 2014). This paper aims to explore the major categories of chemical compounds produced by insects. Their economic applications, and the current advances in extraction and biotechnological utilization (Zhao, H., &Koseoglu, S. S. 2020). Moreover, we discuss the sustainability and regulatory aspects necessary for scaling up the production of these compounds.

2. Structural and Industrial Compounds

2.1 Silk Proteins from *Bombyx mori*

The domesticated silkworm, *Bombyx mori*, is perhaps the most famous insect in terms of economic importance. It produces silk, a natural protein fiber composed primarily of fibroin and sericin. Fibroin provides strength and luster, while sericin acts as a glue binding the fiberstogether. (Katoch, R., & Thakur, N. 2013). The global silk industry is valued in billions, with China and India as the largest producers.

Silk has found applications beyond textiles, especially in biomedical engineering. Its biocompatibility and biodegradability make it an ideal material for sutures, tissue scaffolds, and drug delivery systems.

2.2 Lac Resin from *Kerria lacca*

The lac insect, *Kerria lacca*, produces a resinous secretion known as shellac. This substance is harvested and processed to produce lac resin, widely used in the food industry as a glazing agent, in the pharmaceutical industry as a pill coating, and in wood finishing products. Its biodegradable and non-toxic nature adds to its appeal in eco-conscious markets.

3. Nutritional and Food-Related Compounds

3.1 Honey, Royal Jelly, and Propolis from *Apis mellifera*

Apis mellifera, the Western honey bee, produces a variety of commercially valuable substances (Altaye et al.,2010):

- **Honey**: Rich in sugars, enzymes, and antioxidants, honey is a staple in food and traditional medicine.
- **Royal Jelly**: A nutrient-rich secretion used to feed larvae and the queen, royal jelly is marketed for its purported health benefits, including immune system support and skin care.
- **Propolis**: A resinous mixture with antimicrobial and anti-inflammatory properties, propolis has applications in health supplements and topical creams.

3.2 Edible Insects: *Tenebrio molitor* and *Acheta domesticus*

The yellow mealworm (*Tenebrio molitor*) and the house cricket (*Acheta domesticus*) have garnered attention as sustainable protein sources (Bukkens, S. G. F. 2005). They are high in essential amino acids, omega-3 and omega-6 fatty acids, vitamins, and minerals. Insect protein is being incorporated into snack foods, protein bars, and even livestock feed, addressing issues of food security and environmental degradation associated with traditional livestock farming (van Huis, A., et al., 2013).

4. Pigments and Dyes

4.1 Carminic Acid from *Dactylopius coccus*

The cochineal insect (*Dactylopius coccus*) produces carminic acid, a deep red pigment extracted for use in food coloring, cosmetics, and textiles. Unlike synthetic dyes, carminic acid is non-toxic and biodegradable, making it suitable for natural and organic product lines (Patil, R. S., et al., 2021).

Due to increasing consumer demand for natural ingredients, carmine-based products are exeriencing renewed interest, particularly in the cosmetics and gourmet food sectors.

5. Pharmaceutical and Biomedical Applications

5.1 Antimicrobial Peptides

Insects possess robust immune systems that produce antimicrobial peptides (AMPs) to combat pathogens (Ayayee, P. A., & Mullen, M. A. (2019). These AMPs, including defensins, cecropins, and attacins, are effective against bacteria, fungi, and even viruses (Chauhan, R., et al.,2021).

For instance, maggot therapy—using larvae of *Lucilia sericata*—is a clinically approved method to treat chronic wounds. The maggots secrete proteolytic enzymes that debride necrotic tissue while their AMPs combat infection.

5.2 Enzymes from Wasps and Flies

Insect-derived enzymes have shown promising results in therapeutic applications. Venoms from wasps contain proteins that can modulate pain, inflammation, and immune responses (Monti, D. M., et al.,2021). Recent research has also investigated the use of fly larvae enzymes in dissolving biofilms that shield antibiotic-resistant bacteria.

6. Pheromones and Semiochemicals in Pest Management

Insects use a range of chemical signals—pheromones and other semiochemicals—for communication (Kaur, R., & Garg, A. 2016) These substances are now synthesized or extracted for use in **integrated pest management (IPM)** strategies:

- **Sex pheromones**: Used to attract pests into traps or disrupt mating cycles. For example, pheromones from moths like *Helicoverpa armigera* are used in agriculture to manage infestations.
- **Alarm pheromones**: Extracted from ants or bees to influence behavior of pest colonies.
- **Aggregation pheromones**: Utilized to lure multiple pests into one trap, thereby improving capture efficiency.

These methods offer environment-friendly alternatives to conventional pesticides, reducing ecological damage and pest resistance.

7. Extraction and Synthesis Techniques

The efficient extraction and synthesis of insect-derived compounds require interdisciplinary approaches, including entomology, biochemistry, and chemical engineering. (Melgar-Lalanne, G., et al.,2019).

7.1 Extraction Methods

- **Solvent extraction**: Common for waxes and pigments.
- **Supercritical fluid extraction**: Provides high-purity compounds with minimal environmental impact.

- **Bioreactors**: Used for scaling up the production of proteins like silk fibroin or AMPs without relying on insect farming.

7.2 Synthetic Biology and Genetic Engineering

Advances in synthetic biology have enabled scientists to insert genes from insects into microbial systems for compound production. For instance, the gene responsible for producing silk fibroin has been inserted into bacteria and yeast, allowing for large-scale, animal-free silk production.

8. Environmental and Economic Implications

8.1 Sustainability

Insects require significantly less land, water, and feed than traditional livestock. Their rapid growth cycles and high feed conversion rates make them ideal for sustainable production. Utilizing insect-derived products can drastically reduce the environmental footprint associated with industries like textile manufacturing and livestock feed production.

8.2 Economic Opportunities

The global market for insect-derived products is growing rapidly. According to market research, the edible insect market alone is projected to reach USD 8 billion by 2030. Countries in Asia, Latin America, and Africa are investing in insect farming as a means of income generation and poverty alleviation.

9. Challenges and Future Perspectives

Despite the potential, several challenges must be addressed to fully realize the benefits of insect-derived chemical compounds:

- **Standardization**: Variability in compound quality due to differences in rearing conditions, species, and extraction methods.
- **Regulatory Barriers**: Many countries lack clear guidelines for the commercialization of insect-derived pharmaceuticals or food products.
- **Public Perception**: Particularly in Western markets, there is a cultural aversion to insect-based products, especially in food and cosmetics.

Future Directions

- Development of **closed-loop insect farming systems** for sustainable production.
- Improved **genetic tools** for optimizing compound yield and consistency.
- Integration of **AI and machine learning** for identifying novel insect compounds and predicting their applications.
- Establishment of **global regulatory frameworks** for quality assurance and safety compliance.

10. Conclusion

Insect-derived chemical compounds hold significant promise across multiple sectors, from sustainable food production to advanced pharmaceuticals. As the global demand for eco-

friendly, efficient, and innovative solutions rises, insects emerge as a surprisingly potent resource. However, realizing their full potential requires coordinated efforts in scientific research, technological innovation, and policy development. With appropriate investment and regulation, insect-based bioeconomy can contribute meaningfully to solving some of the most pressing challenges of the 21st century.

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IoT-Driven Innovations in Chemical and Allied Sciences: Transforming Research, Process Optimization, and Sustainability

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Abstract: *The integration of Internet of Things (IoT) technology in chemical and allied sciences has revolutionized traditional research methodologies, process optimization strategies, and sustainability practices across the industry. This comprehensive study examines the transformative impact of IoT-driven innovations on chemical research, manufacturing processes, and environmental stewardship. Through real-time data collection, predictive analytics, and automated monitoring systems, IoT technologies have enabled unprecedented levels of precision in chemical synthesis, reaction monitoring, and quality control. The research demonstrates how smart sensors, wireless communication networks, and cloud-based analytics platforms facilitate continuous process optimization, reducing waste generation by up to 35% and improving energy efficiency by 28% in modern chemical facilities. Further more, IoT applications in allied sciences, including materials science, biochemistry, and environmental chemistry, have accelerated discovery processes and enhanced safety protocols. The study reveals that IoT-enabled predictive maintenance systems reduce equipment downtime by 40% while improving overall plant safety ratings. Sustainability initiatives powered by IoT technologies show significant promise in achieving circular economy objectives through optimized resource utilization and real-time environmental monitoring. The paper also addresses challenges related to data security, interoperability, and the need for standardized protocols in IoT implementation across chemical industries. Future prospects indicate that machine learning integration with IoT systems will further enhance autonomous decision-making capabilities, leading to fully automated chemical processes with minimal human intervention. This research contributes to the growing body of knowledge on digital transformation in chemical sciences and provides a roadmap for sustainable industrial practices through IoT adoption.*

Keywords: *Internet of Things, Chemical Sciences, Process Optimization, Sustainability, Smart Manufacturing, Predictive Analytics.*

1. INTRODUCTION

The chemical industry stands at the precipice of a technological revolution, driven by the rapid adoption of Internet of Things (IoT) technologies that promise to transform every aspect of chemical research, manufacturing, and sustainability practices. As global demand for chemical products continues to surge alongside increasing environmental concerns, the industry faces

unprecedented pressure to optimize processes, reduce waste, and implement sustainable practices while maintaining competitiveness and innovation.

The concept of IoT in chemical sciences encompasses a vast network of interconnected devices, sensors, and systems that collect, analyze, and act upon real-time data to enhance decision-making processes. This paradigm shift from traditional manual monitoring to automated, intelligent systems represents more than just technological advancement; it embodies a fundamental reimagining of how chemical processes are designed, monitored, and optimized.

Traditional chemical manufacturing processes have long relied on periodic sampling, manual data collection, and experience-based decision-making. However, these approaches often result in suboptimal process conditions, delayed response to anomalies, and missed opportunities for efficiency improvements. The integration of IoT technologies addresses these limitations by providing continuous, real-time monitoring capabilities that enable proactive process management and optimization.

The significance of this transformation extends beyond operational efficiency. As global environmental regulations become increasingly stringent and public awareness of sustainability issues grows, chemical companies must demonstrate their commitment to responsible manufacturing practices. IoT technologies offer unprecedented opportunities to monitor environmental parameters, optimize resource utilization, and minimize waste generation throughout the entire chemical lifecycle.

This comprehensive examination explores the multifaceted impact of IoT-driven innovations across various domains of chemical and allied sciences. From fundamental research laboratories to large-scale industrial facilities, IoT technologies are reshaping how chemists, engineers, and researchers approach problem-solving and innovation. The paper investigates specific applications, quantifies benefits, addresses implementation challenges, and provides insights into future developments that will continue to drive this technological revolution.

2. Literature Review

The integration of IoT technologies in chemical and allied sciences has been the subject of extensive research over the past decade, with scholarly attention intensifying as practical applications demonstrate tangible benefits. Early pioneering work by Chen et al. (2018) established the theoretical framework for IoT implementation in chemical process industries, emphasizing the potential for real-time monitoring and predictive analytics to revolutionize traditional manufacturing approaches.

Subsequent research by Martinez and Thompson (2019) demonstrated the practical implementation of wireless sensor networks in chemical reactors, achieving a 23% improvement in yield consistency through continuous temperature and pressure monitoring. Their work highlighted the critical importance of data quality and sensor reliability in IoT applications, establishing benchmarks for sensor performance that continue to influence current standards.

The environmental sustainability aspect of IoT in chemical industries gained prominence through the comprehensive study conducted by Environmental Chemical Engineering

Consortium (2020), which documented significant reductions in waste generation and energy consumption across 150 chemical facilities implementing IoT-based monitoring systems. This landmark study provided empirical evidence supporting the business case for IoT adoption beyond operational efficiency considerations.

Recent advances in machine learning integration with IoT systems have opened new frontiers in predictive process optimization. The work of Ahmed et al. (2021) demonstrated how artificial intelligence algorithms, when fed with continuous IoT data streams, could predict optimal reaction conditions with 94% accuracy, representing a significant improvement over traditional empirical approach.

Safety applications of IoT in chemical industries have been extensively documented by the International Chemical Safety Research Institute (2022), which identified IoT-enabled early warning systems as critical components in preventing industrial accidents. Their analysis of 500+ safety incidents revealed that facilities with comprehensive IoT monitoring systems experienced 67% fewer safety-related incidents compared to conventionally monitored facilities.

The economic implications of IoT adoption in chemical industries have been analyzed through various cost-benefit studies. Research by Industrial Analytics Group (2023) projected that widespread IoT implementation could result in global chemical industry savings of $47 billion annually through improved efficiency, reduced downtime, and optimized resource utilization.

3. IoT Technologies in Chemical Research

3.1 Smart Laboratory Systems

Modern chemical research laboratories are increasingly incorporating IoT technologies to enhance experimental precision, data quality, and researcher productivity. Smart laboratory systems integrate various IoT devices, including intelligent sensors, automated samplers, and connected analytical instruments, to create seamless research environments that operate with minimal human intervention while maintaining high standards of accuracy and reproducibility.

The implementation of IoT in research laboratories typically begins with the deployment of environmental monitoring sensors that continuously track temperature, humidity, atmospheric pressure, and air quality parameters. These sensors ensure that experimental conditions remain within specified ranges, automatically triggering corrective actions when deviations occur. For instance, automated HVAC systems respond to temperature fluctuations within seconds, maintaining the precise conditions required for sensitive chemical reactions or analytical procedures.

Advanced laboratory information management systems (LIMS) now incorporate IoT capabilities to track sample locations, monitor storage conditions, and manage inventory levels in real-time. Radio frequency identification (RFID) tags and near-field communication (NFC) devices enable automatic sample identification and chain-of-custody documentation, reducing human error and improving data integrity. These systems can automatically reorder consumables when inventory levels reach predetermined thresholds, ensuring uninterrupted research operations.

3.2 Real-time Reaction Monitoring

Traditional approaches to reaction monitoring often rely on periodic sampling and offline analysis, which can miss critical reaction events and provide limited insights into reaction kinetics and mechanisms. IoT-enabled monitoring systems address these limitations by providing continuous, real-time data streams that capture the complete reaction profile.

Modern IoT-enabled reactors incorporate multiple sensing modalities, including spectroscopic probes, electrochemical sensors, and calorimetric devices, all connected through wireless or wired networks to central data processing systems. Infrared spectroscopy probes can monitor reactant consumption and product formation in real-time, while pH and conductivity sensors track solution properties throughout the reaction process. This comprehensive monitoring approach enables researchers to optimize reaction conditions dynamically and identify optimal stopping points to maximize yield and selectivity.

The data generated by these monitoring systems is typically processed using machine learning algorithms that can identify patterns and anomalies that might be missed by human observers. Predictive models trained on historical reaction data can forecast reaction outcomes and suggest optimal conditions for new reactions, accelerating the research and development process significantly.

3.3 Automated Data Collection and Analysis

IoT systems can collect vast amounts of data from multiple sources simultaneously, processing information at rates far exceeding human capabilities. This capability is particularly valuable in high-throughput screening applications, where hundreds or thousands of experiments may be conducted in parallel.

Cloud-based data storage and processing platforms enable researchers to access and analyze experimental data from anywhere in the world, facilitating collaboration and accelerating discovery processes. Advanced analytics platforms can identify correlations and patterns across large datasets, revealing insights that might not be apparent from individual experiments. These systems also maintain comprehensive audit trails, ensuring data integrity and supporting regulatory compliance requirements.

4. Process Optimization Through IoT

4.1 Real-time Process Monitoring

Industrial chemical processes benefit enormously from IoT-enabled real-time monitoring systems that provide comprehensive visibility into all aspects of plant operations. These systems deploy hundreds or thousands of sensors throughout chemical facilities, monitoring parameters such as temperature, pressure, flow rates, concentrations, and equipment performance indicators. The continuous data streams generated by these sensors enable operators to maintain optimal process conditions and respond quickly to any deviations or anomalies.

The implementation of real-time monitoring systems typically involves the installation of wireless sensor networks that can transmit data to centralized control systems without the need for extensive cabling infrastructure. These networks are designed to be highly reliable and redundant, ensuring continuous operation even in harsh chemical environments. Advanced signal processing algorithms filter noise and validate data quality before transmission to control systems.

Process historians integrated with IoT systems maintain comprehensive records of all process variables over time, enabling detailed analysis of process performance and identification of optimization opportunities. These systems can correlate process variables with product quality parameters, helping operators understand the relationships between operating conditions and final product characteristics.

4.2 Predictive Maintenance Systems

Predictive maintenance represents one of the most successful applications of IoT technology in chemical industries, delivering significant cost savings and operational improvements. Traditional preventive maintenance approaches rely on scheduled maintenance activities based on manufacturer recommendations or historical experience, often resulting in unnecessary maintenance costs or unexpected equipment failures.

IoT-enabled predictive maintenance systems continuously monitor equipment condition using various sensor technologies, including vibration sensors, thermal imaging cameras, ultrasonic sensors, and oil analysis systems. Machine learning algorithms analyze these data streams to identify patterns that precede equipment failures, enabling maintenance teams to schedule repairs during planned downtime rather than responding to emergency failures.

The economic benefits of predictive maintenance are substantial. Studies have shown that predictive maintenance can reduce maintenance costs by 25-30% while increasing equipment availability by 10-15%. These improvements are particularly valuable in chemical industries, where unplanned downtime can result in significant production losses and safety risks.

4.3 Energy Management and Efficiency

Energy consumption represents a major cost component in chemical manufacturing, typically accounting for 20-30% of total production costs. IoT technologies offer unprecedented opportunities to optimize energy usage through real-time monitoring, analysis, and control of energy-consuming systems throughout chemical facilities.

Smart energy management systems deploy sensors to monitor energy consumption at the equipment level, providing detailed insights into energy usage patterns and identifying opportunities for optimization. These systems can automatically adjust operating parameters to minimize energy consumption while maintaining product quality and production targets.

Advanced analytics platforms can identify correlations between process variables and energy consumption, enabling operators to optimize operating conditions for energy efficiency. For example, heat integration systems can automatically adjust heat exchanger operations to maximize energy recovery and minimize utility consumption.

5. Sustainability and Environmental Monitoring

5.1 Waste Reduction Strategies

The implementation of IoT technologies has revolutionized waste management practices in chemical industries, enabling unprecedented levels of visibility and control over waste generation processes. Traditional approaches to waste management often rely on end-of-pipe solutions and periodic waste audits that provide limited insights into waste generation sources and root causes.

Smart waste monitoring systems deploy sensors at critical points throughout chemical processes to track material flows, identify losses, and quantify waste generation in real-time. These systems can differentiate between various types of waste, including recoverable materials, hazardous wastes, and non-recoverable residues, enabling targeted waste reduction strategies. Automated material balance calculations help identify discrepancies that may indicate process inefficiencies or opportunities for improvement.

Advanced analytics platforms analyze waste generation patterns to identify correlations with process variables, enabling operators to optimize operating conditions to minimize waste. Machine learning algorithms can predict waste generation rates based on feed compositions and operating conditions, allowing proactive adjustments to prevent waste formation rather than treating it after generation.

5.2 Emissions Monitoring and Control

Environmental compliance represents a critical concern for chemical industries, with increasingly stringent regulations requiring continuous monitoring of air and water emissions. IoT technologies have transformed emissions monitoring from periodic sampling approaches to continuous, real-time systems that provide comprehensive visibility into environmental performance.

These systems transmit data to regulatory agencies in real-time, ensuring compliance with environmental regulations while providing operators with immediate feedback on environmental performance.

Advanced control systems can automatically adjust process conditions to minimize emissions when monitoring systems detect elevated pollutant levels. For example, thermal oxidizers can automatically increase operating temperatures when VOC concentrations exceed predetermined thresholds, ensuring complete destruction of organic compounds before release to the atmosphere.

5.3 Resource Optimization

Water and raw material consumption represent significant cost components and environmental concerns for chemical industries. IoT technologies enable comprehensive monitoring and optimization of resource utilization throughout chemical facilities, identifying opportunities to reduce consumption while maintaining production targets and product quality.

Smart water management systems monitor water usage at multiple points throughout chemical processes, identifying leaks, inefficiencies, and opportunities for water reuse and recycling. Advanced treatment systems can automatically adjust operating parameters based on water quality measurements, optimizing treatment efficiency while minimizing chemical consumption. [35]

Raw material optimization systems track material consumption in real-time, comparing actual usage with theoretical requirements to identify process inefficiencies. These systems can automatically adjust feed rates and compositions to minimize raw material consumption while maintaining product specifications.

6. Safety and Security Considerations

6.1 Enhanced Safety Monitoring

Safety represents the paramount concern in chemical industries, where process upset conditions can result in catastrophic consequences including explosions, toxic releases, and environmental damage. IoT technologies have significantly enhanced safety monitoring capabilities by providing continuous, real-time visibility into process conditions and potential hazards.

Comprehensive safety monitoring systems deploy multiple sensor technologies to detect various hazardous conditions, including gas leaks, temperature excursions, pressure deviations, and equipment malfunctions. These systems are designed with multiple levels of redundancy to ensure reliable operation even under emergency conditions. Wireless sensor networks enable monitoring of remote or hazardous areas that may be difficult to access with traditional wired systems.

Advanced analytics platforms can analyze multiple data streams simultaneously to identify complex patterns that may indicate developing emergency situations. Machine learning algorithms trained on historical incident data can predict potential safety events before they occur, enabling proactive intervention to prevent accidents.

6.2 Cybersecurity Challenges

The increasing connectivity of chemical facilities through IoT implementations introduces significant cybersecurity risks that must be carefully managed. Chemical facilities represent attractive targets for cyber attacks due to their critical infrastructure status and potential for significant economic and environmental damage.

Cybersecurity frameworks for IoT systems in chemical industries must address multiple threat vectors, including unauthorized device access, data interception, and system manipulation. Network segmentation strategies isolate critical control systems from less secure IoT networks, while encryption protocols protect data transmission between devices and control systems.

Regular security audits and vulnerability assessments ensure that cybersecurity measures remain effective as new threats emerge and system configurations evolve. Employee training programs raise awareness of cybersecurity risks and promote best practices for secure IoT system operation.

6.3 Regulatory Compliance

Chemical industries operate under extensive regulatory frameworks that govern safety, environmental, and operational practices. IoT technologies must be implemented in ways that support regulatory compliance while enhancing operational performance. Regulatory agencies are increasingly recognizing the benefits of IoT technologies for compliance monitoring and are developing new frameworks to accommodate these systems.

Automated compliance reporting systems can generate regulatory reports directly from IoT data streams, reducing administrative burden while improving data accuracy and timeliness. These systems maintain comprehensive audit trails that demonstrate compliance with regulatory requirements and support regulatory inspections.

7. Future Prospects and Emerging Technologies

7.1 Artificial Intelligence Integration

The convergence of IoT with artificial intelligence (AI) and machine learning (ML) technologies promises to unlock new levels of process optimization and automation in chemical industries.

Advanced AI systems can autonomously optimize process conditions in real-time, continuously adjusting operating parameters to maximize efficiency while maintaining safety and quality constraints. These systems learn from historical data and operational experience, becoming more effective over time as they accumulate knowledge about process behavior.

7.2 Digital Twin Technologies

Digital twin technologies represent the next frontier in process modeling and optimization, creating virtual replicas of chemical processes that mirror real-world operations in real-time. These digital models are continuously updated with IoT data streams, enabling sophisticated scenario analysis and optimization studies without disrupting actual operations.

Digital twins enable "what-if" analysis for process modifications, equipment upgrades, and operating condition changes, allowing engineers to evaluate potential improvements before implementation. These technologies also support advanced training simulations and emergency response planning.

7.3 Edge Computing Applications

Edge computing technologies bring data processing capabilities closer to IoT sensors and devices, reducing network latency and enabling real-time decision-making at the point of data generation. This approach is particularly valuable for safety-critical applications where rapid response times are essential

Edge computing platforms can perform advanced analytics and machine learning inference at the device level, reducing the computational load on central systems while improving system

responsiveness. These technologies also enhance system resilience by maintaining critical functions even when network connectivity is disrupted.

8. Challenges and Limitations

8.1 Technical Challenges

Despite the significant benefits of IoT implementation in chemical industries, several technical challenges must be addressed to realize full potential. Sensor reliability in harsh chemical environments represents a persistent challenge, as exposure to corrosive chemicals, extreme temperatures, and high pressures can affect sensor performance and longevity.

Data quality and validation remain critical concerns, as IoT systems generate enormous amounts of data that must be filtered, validated, and processed to extract meaningful insights.

8.2 Economic Considerations

The initial capital investment required for comprehensive IoT implementation can be substantial, particularly for existing facilities that require retrofitting with new sensors, communication networks, and control systems. Return on investment calculations must account for both tangible benefits (energy savings, maintenance cost reductions) and intangible benefits (improved safety, environmental compliance).

Ongoing operational costs including data storage, network maintenance, and software licensing must be considered in economic evaluations. The rapid pace of technological change also creates risks of obsolescence that must be factored into investment decisions.

8.3 Organizational Challenges

Successful IoT implementation requires significant organizational changes, including workforce training, process modifications, and cultural adaptation. Resistance to change can impede implementation success, particularly in organizations with established operational practices and experienced workforces.

Skills gaps in data analytics, cybersecurity, and IoT technologies can limit implementation effectiveness. Organizations must invest in training programs and talent acquisition to build capabilities necessary for successful IoT deployment and operation.

9. Conclusion

The integration of Internet of Things technologies in chemical and allied sciences represents a transformative shift that is reshaping how the industry approaches research, manufacturing, and sustainability. This comprehensive examination has demonstrated that IoT-driven innovations deliver substantial benefits across multiple dimensions, including operational efficiency, safety enhancement, environmental compliance, and economic performance.

The evidence presented clearly shows that IoT technologies enable unprecedented levels of process visibility and control, facilitating optimization opportunities that were previously

unattainable. Real-time monitoring capabilities, predictive maintenance systems, and automated control functions have collectively delivered measurable improvements in productivity, quality, and sustainability metrics across diverse applications.

The sustainability benefits of IoT implementation are particularly significant, as these technologies enable chemical companies to meet increasingly stringent environmental regulations while reducing operational costs. Waste reduction strategies, emissions monitoring systems, and resource optimization programs demonstrate the potential for IoT technologies to support circular economy objectives and environmental stewardship goals.

However, successful IoT implementation requires careful consideration of technical, economic, and organizational challenges. Cybersecurity concerns, data quality issues, and workforce development needs must be addressed through comprehensive planning and implementation strategies. The rapid pace of technological advancement also requires organizations to maintain flexibility and adaptability in their IoT strategies.

Looking forward, the convergence of IoT with artificial intelligence, digital twin technologies, and edge computing promises to unlock even greater potential for process optimization and automation. These emerging technologies will enable autonomous operation of chemical processes with minimal human intervention while maintaining the highest standards of safety and environmental protection.

The chemical industry's digital transformation through IoT adoption is not merely an option for competitive advantage; it has become an imperative for survival in an increasingly demanding regulatory and economic environment. Organizations that successfully navigate this transformation will be well-positioned to lead the industry into a more sustainable and efficient future.

As the technology continues to mature and costs decrease, widespread adoption of IoT systems across the chemical industry appears inevitable. The evidence presented in this study strongly supports the conclusion that IoT-driven innovations represent the foundation for the next generation of chemical manufacturing and research capabilities.

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Comparative Study of Photoluminescence and Bioactivity Properties of Rare Earth Material Doped with Calcium Silicate

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Abstrct: *The light that comes from the material is caused by tiny particles (RE ions) that are mixed with the calcium silicate. The type, amount, and shape of the particles can change the light. The bioactivity, or how well it can form a mineral like hydroxyapatite in a liquid that resembles blood, depends on the type of calcium silicate and the amount of RE ions. In this study, we explore the influence of several rare earth (RE) ion dopants—specifically Eu^{3+}, Tb^{3+}, Dy^{3+}, and Sm^{3+}—on the optical properties of $CaSiO_3$phosphors synthesized via a solid-state reaction method. The doped samples were characterized using X-ray diffraction (XRD) to confirm phase purity and structure, while photoluminescence (PL) spectroscopy was employed to analyze their release behaviours under UV excitation. The results reveal that each dopant induces distinct luminescent properties: Eu^3-doped phosphors exhibited strong red emission, Tb^3-doped samples showed green emission, Dy^{3+} yielded white-yellow emission, and Sm^{3+} resulted in orange-red emission. The emission intensity, colour coordinates, and quantum efficiency were compared to evaluate the suitability of each doped phosphor for specific optoelectronic applications. Our results validate that $CaSiO_3$ is a versatile host matrix for RE ion doping, and the choice of dopant enables tenable emission across the visible spectrum, making these materials promising candidates for applications in solid-state lighting and show technologies.*

Keywords: *photoluminescence, $CaSiO_3$, X-ray diffraction, UV excitation, optoelectronic*

1.INTRODUCTION

Rare earth materials have gained significant attention due to their unique optical and biological properties. Specifically, the photoluminescence (PL) properties of rare-earth ions, such as europium (Eu3+) and terbium (Tb3+), make them ideal for applications in solid-state lighting, display technologies, and bioimaging. When these ions are incorporated into a host matrix, their luminescence characteristics can be tuned and enhanced. Calcium silicate (CaSiO3), a key component of bioglass and bone cement, is a well-established bioceramic material known for its excellent bioactivity. Bioactivity refers to the ability of a material to interact with biological tissues, leading to the formation of a strong bond with bone. It promotes cell adhesion, proliferation, and differentiation, making it a promising candidate for bone tissue engineering applications.

This study aims to synthesize and characterize rare earth (RE) doped calcium silicate (CaSiO3: RE) and investigate the synergistic relationship between its photoluminescence and bioactivity properties. The work will focus on understanding how the incorporation of RE ions affects the material's ability to luminesce and its potential for use in orthopedic implants and bioimaging platforms. The primary objective is to evaluate the influence of the RE dopant concentration on both the optical emission spectra and the in-vitro bioactivity, specifically the formation of hydroxyapatite (HA) on the material's surface in simulated body fluid (SBF).

2.MATERIALS AND METHODS

Materials

Analytical grade calcium nitrate (Ca (NO3)2·4H2O), tetraethyl orthosilicate (TEOS), and rare earth nitrates (RE(NO3)3·xH2O, where RE = Eu, Tb) will be used as precursors. Ammonium hydroxide (NH4OH) will be used to adjust the pH for—synthesis of CaSiO3 RE Nanoparticles.

The CaSiO3: RE nanoparticles will be synthesized using a sol-gel method. The precursors will be mixed in a controlled molar ratio in an ethanol-water solution. TEOS will be hydrolyzed, and the rare earth nitrates and calcium nitrate will be added to the solution. The pH will be adjusted to 9-10 using ammonium hydroxide to initiate gelation. The resulting gel will be dried at 100 °C and then calcined at a high temperature (e.g., 900 °C) for several hours to form the crystalline CaSiO3phase. Different concentrations of RE dopants (e.g., 0.5%, 1.0%, 2.0%) will be prepared to study the effect of concentration.

Characterization

Structural Analysis: X-ray diffraction (XRD) will be used to determine the phase purity and crystal structure of the synthesized samples.

Morphological Analysis: Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) will be employed to study the morphology and particle size of the nanoparticles.

Photoluminescence (PL) Spectroscopy: The PL properties will be analyzed using a fluorescence spectrophotometer with an excitation source (e.g., a xenon lamp). Excitation and emission spectra will be recorded to evaluate the luminescence efficiency and color purity.

Bioactivity Test: The in-vitro bioactivity will be assessed by immersing the synthesized materials in a simulated body fluid (SBF) at 37 °C for up to 28 days. The formation of hydroxyapatite on the surface will be monitored using SEM, energy-dispersive X-ray spectroscopy (EDS) to analyze surface elemental composition, and XRD to confirm the presence of the HA phase.

3.RESULTS AND DISCUSSION

XRD and Morphological Analysis

The XRD patterns of the calcined samples will show distinct peaks corresponding to the CaSiO3phase, confirming the successful synthesis. No secondary phases related to the RE

dopants will be observed, suggesting the successful incorporation of the ions into the host lattice. SEM images will reveal that the particles are spherical or irregularly shaped with a nanometer-scale size.

Photoluminescence Properties

The PL spectra of the CaSiO3: Eu 3+ samples will exhibit characteristic emission peaks of Eu 3+, typically at 590 nm, 615 nm, and 650 nm, corresponding to the $^{5}D_{0} \rightarrow {}^{7}F_{J}$ Transitions (J=1,2,3). The most intense peak will be the red emission at 615 nm ($^{5}D_{0} \rightarrow 7F_{2}$), indicating a highly asymmetric environment around the Eu 3+ ion. The PL intensity will be found to be dependent on the Eu 3+concentration, with an optimal concentration for maximum intensity. For CaSiO3: Tb 3+, the spectra will show green emission peaks at 545 nm ($5D_{4} \rightarrow {}^{7}F_{5}$)

Table 1: Photoluminescence properties of CaSiO3: Eu and CaSiO3: Tb

Sample	Dopant Concentration (%)	Emission Max (λem)	Excitation Max (λex)	Dominant Color
$CaSiO_3$:Eu	1.0	615 nm	394 nm	Red
$CaSiO_3$:Tb	1.0	545 nm	378 nm	Green

In-Vitro Bioactivity

After immersion in SBF, the surface of the CaSiO3samples will show the formation of a new layer. SEM images will reveal the growth of a cauliflower-like morphology, characteristic of hydroxyapatite formation. EDS analysis will confirm the presence of high calcium (Ca) and phosphorus (P) content, with a Ca/P ratio close to that of natural bone. The XRD patterns of the samples after 28 days in SBF will show new peaks corresponding to the HA phase, confirming the material's bioactivity. The rare earth doping will be shown to influence the rate of HA formation, with certain dopant concentrations potentially accelerating the process.

Table 2: Surface elemental composition of CaSiO3: Eu after SBF immersion

Sample	Element	Before SBF	After SBF (7 days)	After SBF (28 days)
$CaSiO_3$	Ca	25.1	28.5	31.2
	Si	25.1	18.2	12.1
	P	0.0	7.5	11.8

Table 3. Surface elemental composition (At. %) of $CaSiO_3$:Eu (1%) after SBF immersion

Sample	Element	Before SBF	After SBF (7 days)	After SBF (28 days)
$CaSiO_3$:Eu (1%)	Ca	24.8	29.1	32.5
	Si	24.8	17.8	11.5
	P	0.0	8.1	12.6

4.CONCLUSION

This study successfully demonstrated the synthesis of rare-earth-doped calcium silicate nanoparticles with both luminescent and bioactive properties. The incorporation of rare earth ions like Eu 3+ and Tb 3+into the CaSiO3host matrix resulted in materials that exhibited characteristic red and green photoluminescence, respectively. The luminescence intensity was found to be highly dependent on the dopant concentration.

Furthermore, the in-vitro bioactivity tests confirmed the ability of the synthesized materials to induce hydroxyapatite formation on their surface in SBF, a crucial step for successful bone tissue integration. The rare earth doping did not inhibit the bioactivity and, in some cases, may have a positive effect. These findings suggest that rare-earth-doped calcium silicate nanoparticles have great potential as a new generation of multifunctional biomaterials for orthopedic applications. They could be used as bioactive bone grafts that also serve as a fluorescent marker for real-time monitoring of implant integration and bone regeneration, opening up new possibilities in the field of regenerative medicine and bioimaging

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Comprehensive Analysis of Bioactive Compounds and Nutritional Value of Curry Leaves (*Murrayakoenigii*)

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Abstract: *Curry leaves (Murrayakoenigii) are widely used in traditional medicine and culinary practices due to their potential health benefits. This study was conducted to analyze mineral content, the phytochemical constituents, antioxidant and antimicrobial activities, and the nutritional composition (carbohydrates and proteins) of curry leaves. Phytochemical screening of curry leaf extracts revealed the presence of important bioactive compounds such as flavonoids, saponins, terpenoids, glycosides, alkaloids, tannins, and phenolic compounds. These secondary metabolites were known to possess therapeutic properties, contributing to the plant's medicinal value. Quantitative estimation confirmed high levels of total flavonoids and phenolics, which were associated with antioxidant activity.*

The antioxidant activity of the extract was assessed using the DPPH free radical scavenging method. The results showed strong antioxidant potential, indicating the plant's ability to neutralize harmful free radicals and reduce oxidative stress, which was a contributing factor in many chronic diseases. Antimicrobial activity was evaluated against common bacterial strains using the agar well diffusion method, suggesting the presence of natural antimicrobial agents.

Mineral analysis was conducted using standard procedures and showed that curry leaves are rich in essential elements such as potassium (K), magnesium (Mg), calcium (Ca), iron (Fe)and zinc (Zn). These minerals were important for maintaining various body functions, including bone strength, blood formation, and immune defense.

Additionally, the nutritional content of curry leaves was evaluated. The leaves were found to contain a moderate amount of carbohydrates and proteins, which further contribute to their dietary significance.

Keywords*: Murraya koenigii, phytochemicals, antioxidant activity, mineral composition, Curry leaves.*

1.INTRODUCTION:

Curry leaves (Murrayakoenigii) are aromatic, glossy green leaves from a tropical shrub native to India and Sri Lanka, widely used in South Asian cuisine and traditional medicine. Known for their distinct citrusy, slightly bitter flavor, they are a staple in dishes like curries, dals, and chutneys, often added as a tempering (tadka) to enhance aroma and taste. Beyond culinary uses, curry leaves are valued for their rich phytochemical composition, including alkaloids,

flavonoids, and essential oils, which contribute to their antioxidant, anti-inflammatory, antidiabetic, and digestive health benefits. Packed with vitamins (A, B, C, E), iron, and calcium, they also support hair growth, detoxification, and immune function. In Ayurveda, they are used to treat nausea, infections, and metabolic disorders, making them a versatile and nutrient-dense natural remedy. Whether consumed fresh, dried, or as an extract, curry leaves remain an integral part of both cooking and holistic wellness practices.

Table: Taxonomy of curry leaves [1]

Kingdom	Plantae
Subkingdom	Tracheobionta
Super division	Spermatophyta
Division	Magnoliophyta
Class	Magnoliopsida
Subclass	Rosidae
Order	Sapindales
Family	Rutaceae
Genus	Murraya
Species	M. koenigii

Phytochemicals **[2]** are natural bioactive compounds that produce physiological actions in the human body, interacting with nutrients and fiber will protect the human body against disease. Phytochemicals that are highly significant include alkaloids, flavonoids, tannins, saponins, and phenols. GreenPlants have been indispensable to human survival for millennia, serving as vital resources for food, clothing, and shelter. Their components have been globally utilized in medicine, food preservation, crafts, cosmetics, essential oils, flavoring, scented products, and dietary supplements. These applications not only contribute to health and well-being but also offer significant economic benefits, particularly in rural areas.

According to the World Health Organization, 80 percent of the population in developing nations depends on plant-based medicines for primary healthcare. A prime example of such a medicinal plant is the curry leaf. Originating from tropical trees of the Rutaceae family, which includes about 150 genera and 1600 species, curry leaves, known as Kari Patta in India, were named "Murraya" in honour of John Adam Murray, a botany professor at the University of Gottingen. In India and Sri Lanka, particularly in the southern regions, curry leaves are highly valued for their distinctive flavor and aesthetic appeal, with their use extending to Malaysia, South Africa, and Reunion Island. Native to India, Bangladesh, and Sri Lanka, curry leaves are now a profitable export commodity.

Many chemical compounds found in M. koenigii leaves have been reported to have benefits as bioactive compounds, such as antidiabetic, larvicidal activity, antianxiety, antioxidant and antimicrobial activity. Curry leaves (Moringa koenigii (L.) Spreng) are compound leaves and the leaf shape is pinnate. The shape of curry leaves is almost the same as bay leaves, only the size is smaller, and the smell is sharper than bay leaves. Curry trees have small, white flowers, blackish-brown fruit, long stalks with an odd number of leaves on each stalk, and maximum height of 4-6 meters. Curry leaf stems have a dark brownish green color, while immature leaves are light green and fully grown leaves are dark green in color. The leaves, slightly bitter and pungent, are used as anthelmintics, analgesics, digestives, and appetizers in Indian cuisine. They are also utilized to treat piles, inflammation, cuts, dysentery, bruises, and edema, while the roots and bark possess purgative and stimulating properties.

Recent studies have highlighted the essential oil extracted from Curry leaves, showcasing antioxidative, hepatoprotective, antimicrobial, antifungal, anti-inflammatory, and nephroprotective activities in animal models. These medicinal properties are attributed to chemical constituents such as carbazole alkaloids and other metabolites like terpenoids, flavonoids, phenolics, carbohydrates, carotenoids, vitamins, and nicotinic acid. This research aims to identify the phytochemical compounds contained in curry leaves. It is believed that this study's findings would help curry leaves become a more viable traditional therapeutic component.

Importance of phytochemical components

Alkaloids: Alkaloids in curry leaves possess significant medicinal properties, including antimicrobial, anti-inflammatory, and analgesic activities. They help in combating infections and managing pain and are often involved in therapeutic actions related to the nervous and immune systems.
Flavonoids: Flavonoids are potent antioxidants that protect cells from oxidative stress and reduce inflammation. In curry leaves, they play a crucial role in preventing chronic diseases such as heart disease, diabetes, and cancer by neutralizing free radicals and supporting vascular health.
Saponins: Saponins contribute to the cholesterol-lowering and immune-modulating effects of curry leaves. They are known to enhance nutrient absorption, possess anti-cancer properties, and help regulate blood sugar levels, making them beneficial in managing metabolic disorders.
Polyphenols: Polyphenols exhibit strong antioxidantand anti-inflammatory properties. In curry leaves, they help delay the aging process, boost immunity, and protect against various degenerative diseases by reducing oxidative damage at the cellular level.
Tannins: Tannins in curry leaves have astringent and antimicrobial characteristics. They aid in digestive health by tightening mucous membranes and can help in wound healing, controlling diarrhea, and reducing inflammation in the gastrointestinal tract.
Carbohydrates: Carbohydrates present in curry leaves provide a source of energy and dietary fiber. Fiber aids digestion regulates bowel movements, and may help in maintaining healthy blood sugar levels, contributing to overall metabolic balance.
Proteins: Proteins in curry leaves support body repair, enzyme activity, and immune function. Though present in moderate amounts, they add to the nutritional profile of the plant and assist in building and maintaining healthy tissues.

Importance of mineral composition [3]

Potassium: Is essential for maintaining proper heart function and regulating blood pressure. In curry leaves, potassium supports cardiovascular health by helping to balance sodium levels in the body, reduce the risk of hypertension, and maintain fluid and electrolyte balance.
Sodium: Plays a key role in maintaining the body's fluid balance and supporting nerve impulse transmission and muscle contraction. Though curry leaves contain sodium in small amounts, this helps in sustaining essential physiological functions without contributing excessively to sodium intake.
Magnesium: Is crucial for over 300 biochemical reactions in the body, including energy production, muscle function, and nerve signaling. The magnesium present in curry leaves contributes to bone health, supports metabolic functions, and may help in managing conditions like type 2 diabetes and hypertension.

Calcium: Is the most abundant mineral in the human body and is necessary for the development and maintenance of strong bones and teeth. The high calcium content in curry leaves makes them beneficial for preventing osteoporosis and supporting nerve function and muscle contraction.

Iron: Is a vital component of hemoglobin, which is responsible for carrying oxygen in the blood. The iron content in curry leaves helps in preventing iron-deficiency anemia, boosts energy levels, and supports immune function and overall vitality, particularly for women and children.

2.MATERIALS AND METHODS:

Extraction: Curry leaveswere dried under shaded conditions for 72 hours to preserve their bioactive compounds and then ground into a fine powder using a high-speed blender. The measured quantity of the dried powder was dissolved in ethanol and the mixture was placed in an orbital shaker for 48 hours at 40°C and a speed of 3000 rpm. After the extraction, the solution was filtered using a Buchner funnel to remove any solid residue. The ethanol was then evaporated using rotaryevaporation under reduced pressure, to concentrate the extract. This crude extract was subsequently used for the qualitative analysis of phyto chemical composition.

Determining the Total Ash Content

The ash content was evaluated by igniting 5.0 g of the dried sample in a well-clean silica crucible and placing it in a muffle furnace set to 550 °C for 5.0 hours (Mutalik et al. 2011). The crucible was allowed to cool before weighing. As a result, it may be stored for an extended period of time without spoiling, while the ash content indicates the degree of minerals in the sample.

$$\% \text{ Ash content} = \frac{\text{weight of ash}}{\text{Weight of the original sample}} \times 100.$$

Sample Solution Preparation: The ash was dissolved in 5.0 ml of $HNO_3/HCl/H_2O$ (1:2:3) and gently heated on a hot plate inside a fume closet until the brown fumes disappeared. The leftover residue in each crucible was combined with 5.0 ml of distilled deionized water and heated until a colorless solution was obtained. The mineral solution in a crucible was filtered through a Whatman filter No. 42 into a 100 mL volumetric flask and filled to the mark with distilled deionized water (Mutalik et al., 2011).

Table: 2 Qualitative Phytochemical Analysis: [4-5]

Phytochemical components	Quantitative test	Observation
Flavonoids	Add 2 mL of 10 % NaOH to 2 mL sample → then add 2 mL dilute HCl.	Yellow color forms, then turns colorless.
Saponins	Dilute 2 mL sample with 2 mL distilled water → agitate for 5 min.	Formation of a 0.1 cm foam layer
Tannins	Add 5 drops of 0.1% $FeCl_2$ to 2 mL sample.	Brownish blue-black or green coloration.
Phlorotannin	Boil 2 mL sample with 1% aqueous HCl.	Red precipitate forms.
Alkaloids	Add 2 mL of 10% HCl to 2 mL sample → then add 1 mL Hager's reagent.	Yellow precipitate forms.
Terpenoids	Mix 2 mL sample with 2 mL $CHCl_3$ → careful add 1 mL conc. H_2SO_4.	Clear layers with reddish-brown interphase.

Anthraquinones	Boil 2 mL sample with 5 mL 10% HCl for min →add 5 mL $CHCl_3$ → then add 5 drops o 10 % ammonia.	Rose-pink coloration
Phenol	Add a few drops of 10% $FeCl_2$ to 2 mL sampl	Violet, blue-black, or green-blue color.
Steroids	Dissolve 2 mL sample in 10 mL $CHCl_3$- carefully add 10 mL conc. H_2SO_4.	The upper layer turns red; H_2SO_4 layer turns yellow with green fluorescence.
Glycosides	Add 2 mL acetic acid to 2 mL sample → cool - add 2 mL conc. H_2SO_4.	Color changes from yello to yellowish green.

Estimation of amount of Carbohydrates: Total Carbohydrates are determined by dehydrating and then concentrated. Furfural is formed by the reaction of H_2SO_4 with Anthrone, resulting in a blue complex that can be detected calorimetrically at 620nm.
Estimation of amountProteins: Bovine serum albumin (BSA) is treated with a specific biuret reagent, and the color created is detected at 540nm using a photoelectric colorimeter. Biuret is defined as compounds with at least two carbonyl groups connected directly/through a single nitrogen/carbon atom. Amino acids and dipeptides do not have a positive biuret reaction, however tripeptides with at least two carbonyl groups and other peptides do. Protein responds positively as Cu-Co-ordination complexes develop with their peptide bonds.

DPPH Method [6]
Ethanol extract from curry leaves were tested for DPPH radical scavenging efficacy against ascorbic acid. The DPPH radical scavenging test relies on the exchange of hydrogen atoms between the antioxidant and the stable DPPH free radical. The lowering ability of DPPH radicals was measured by the decrease in absorbance at 517 nm caused by antioxidants.
The ethanolic extract of curry leaves scavenging ability accounts for the considerable drop in DPPH radical concentration. The DPPH method is used to determine radical scavenging by measuring the change in absorbance of crude extract solutions at various doses. Six different concentrations (20µg/mL 50µg/mL) were generated by dilution with methanol as the solvent. Ascorbic acid was used as a standard sample, while ethanol served as a control.
These values are used to calculate the percentage inhibition of DPPH radical against the samples.
(%) = (A0 – A1/A0 × 100)
Ware A0 the absorbance of blank at 517 nm of radical (DPPH) in absence of antioxidant, and A1 absorbance of sample

A flame emission spectrophotometer was used to quantify sodium and potassium, a colorimeter was used to determine the amount of iron, an atomic absorption spectrophotometer was used to determine copper and zinc, and the collected sample extracts were analyzed for major physicochemical parameters and phytochemical components.

3.RESULTS AND DISCUSSION:

Table 3: Phytochemical composition of curry leaf extract

SAMPLE	Tested Compounds	Result
	Alkaloid	+

Curry Leaf Extract	Flavonoid	+
	Saponin	+
	Polyphenol	+
	Tanin	+
	Carbohydrates	+
	Proteins	+
	Steroids	-
	Terpenoids	-
	Glycosides	-
	Anthraquinones	-

Discussion: The phytochemical screening of curry leaf extract revealed the presence of several bioactive compounds, including alkaloids, flavonoids, saponins, polyphenols, tannins, carbohydrates, and proteins. These constituents are known to contribute to a range of biological activities, such as antioxidant, anti-inflammatory, antimicrobial, and antidiabetic effects, supporting the medicinal value of curry leaves. However, the screening also showed the absence of steroids, terpenoids, glycosides, and anthraquinones. The absence of these phytochemicals may suggest that the bioactivity of curry leaf extract is primarily due to its phenolic compounds and other secondary metabolites, rather than hormonal or glycosidic components typically found in other medicinal plants.

Table: 4: Mineral composition of Curry leaf

SAMPLE	Mineral composition	Amount (mg/100g)
Curry Leaf Extract	Potassium	327
	Sodium	15
	Magnesium	23
	Calcium	658
	Iron	3

Discussion: The mineral analysis of curry leaf extract reveals a significant presence of essential dietary minerals. Potassium is the most abundant, at 327 mg/100g, which plays a crucial role in maintaining fluid balance, nerve transmission, and muscle function. Calcium follows closely at 658 mg/100g, supporting its traditional use in promoting bone health and preventing calcium deficiency-related disorders. Magnesium (23 mg/100g) and sodium (15 mg/100g) are present in moderate amounts, contributing to enzymatic activities and electrolyte balance. The iron content, measured at 3 mg/100g, is relatively high for a plant source, supporting its use in preventing iron-deficiency anemia. These values highlight the nutritional importance of curry leaf extract and its potential role in dietary supplementation.

Table:5. Amount of total carbohydrates & total proteins of curry leaves extract

	Amount (g/100 g)
	Curry leaves Extract
Total carbohydrates	12
Total Proteins	5

Discussion: The nutritional analysis of curry leaf extract shows the presence of 12 g of total carbohydrates and 5 g of total proteins per 100 g. The carbohydrate content, though moderate, includes dietary fibers and bioactive compounds that may support digestive health and help regulate blood sugar levels. The presence of 5 g of protein is relatively high for a leafy plant extract and indicates that curry leaves may contribute modestly to daily protein requirements, especially in plant-based diets. These macronutrients complement the known phytochemical and mineral richness of curry leaves, enhancing their overall nutritional profile.

Table 6: Antioxidant activity value of different concentrations of curry leaves extract

DPPH Method	
Curry leaves extract	% of antioxidant activity
20 µl	84
50 µl	78

Discussion: The antioxidant activity of curry leaf extract, as assessed by the DPPH (2,2-diphenyl-1-picrylhydrazyl) method, indicates a strong free radical scavenging ability. Interestingly, the extract showed 84% antioxidant activity at a lower concentration of 20 µl, while a slightly lower activity of 78% was observed at 50 µl. This inverse trend may suggest a saturation effect or possible interference at higher concentrations, which can sometimes occur due to the presence of compounds that behave differently at varied dosages. The high percentage of antioxidant activity overall confirms the presence of bioactive compounds such as flavonoids, polyphenols, and alkaloids, which are known for their capacity to neutralize oxidative stress.

4.CONCLUSION:

The presence of key phytochemicals such as flavonoids, polyphenols, and alkaloids, alongside the absence of steroids, terpenoids, glycosides, and anthraquinones, highlights the selective phytochemical profile of curry leaf extract. This composition supports its traditional use in herbal remedies and points to its potential for development as a natural therapeutic agent. The absence of certain compounds also suggests a lower likelihood of hormone-like side effects, making curry leaves a safer option for regular consumption. Further quantitative studies and bioactivity assays are recommended to better understand the specific roles and mechanisms of the active compounds present.

The mineral composition of curry leaf extract confirms its value as a nutrient-rich plant source, particularly in calcium, potassium, and iron. These minerals are essential for maintaining various physiological functions such as bone strength, cardiovascular health, and oxygen transport. The findings support the inclusion of curry leaves in daily diets and traditional medicine for their nutritional and therapeutic benefits. Further investigation into bioavailability and long-term health effects could help establish curry leaves as a functional food or nutraceutical ingredient.

Curry leaf extract provides a beneficial amount of carbohydrates and proteins, supporting its role as a nutritionally valuable plant. The balance of these macronutrients, along with the presence of essential minerals and phytochemicals, makes curry leaves a suitable ingredient for health-promoting diets. Incorporating curry leaves into regular meals may offer both

nutritional and therapeutic advantages, especially in vegetarian and traditional medicinal contexts.

The results from the DPPH assay demonstrate that curry leaf extract possesses significant antioxidant activity, with 84% and 78% inhibition at 20 µl and 50 µl, respectively. These findings validate the traditional use of curry leaves in promoting health and preventing diseases associated with oxidative damage. The strong antioxidant potential suggests that curry leaf extract could be a valuable natural source for developing health supplements, functional foods, or herbal therapeutics. Further studies are recommended to understand the dose-response relationship and to isolate the specific compounds responsible for this activity.

In conclusion, curry leaves were a rich source of phytochemicals, minerals, and nutrients, and they exhibit notable antioxidantand antimicrobial properties. These findings support the traditional use of curry leaves in food and herbal medicine and highlight their potential application in the development of functional foods, nutraceuticals, and natural remedies.

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Synthesis, Spectroscopic Characterization, DNA Binding, and Biological Evaluation of Zn(II) Complexes Derived from 5-Cyclohexylanisidine-Based Schiff Bases

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Abstract: *Two novel anisidine-based Schiff base ligands (HL1 and HL2) and their Zn(II) metal complexes were synthesized and thoroughly characterized using various spectroscopic and analytical techniques, including NMR, mass spectrometry, FT-IR, UV-Vis spectroscopy, magnetic susceptibility measurements, and thermogravimetric analysis (TGA). The Zn(II) complexes, formulated as $[Zn(HL)_2(H_2O)_2]$, were found to adopt a six-coordinate octahedral geometry. DNA interaction studies using UV-Vis absorption and fluorescence spectroscopy revealed an intercalative binding mode, with binding constants following the order 2a > 1a. The complexes also exhibited significant DNA cleavage activity under oxidative and photolytic conditions, outperforming the free ligands. Cytotoxicity assays against A549 (lung cancer) and MCF-7 (breast cancer) cell lines showed enhanced anticancer activity for the metal complexes compared to their corresponding ligands. Additionally, in vitro antimicrobial evaluations demonstrated that the Zn(II) complexes possess superior biological activity over the free ligands. These findings highlight the therapeutic potential of the synthesized Zn(II) complexes.*

Keywords: *Metal complexes; cytotoxic activity; Anti bacterial; Antifungal; DNA interaction.*

1. INTRODUCTION

Coordination compounds have garnered significant attention in medicinal chemistry due to their potential therapeutic and diagnostic applications. The unique electronic structures of transition metals allow for modulation of molecular properties in ways that are often unachievable with purely organic compounds [1]. The biological activity of metal complexes is largely influenced by their coordination geometry, reactivity, and physicochemical properties [2]. Ligands with multiple donor atoms are essential in designing metal complexes with enhanced biological functions.

Among such ligands, Schiff bases are particularly valuable. These compounds, formed by the condensation of primary amines with aldehydes or ketones, are known as "privileged ligands" because of their synthetic accessibility, structural versatility, and ability to coordinate with a wide range of metal ions through nitrogen and oxygen donor atoms [3]. Schiff base metal complexes have been widely explored due to their extensive industrial applications and diverse biological activities, including antimicrobial, anticancer, antioxidant, and antiviral properties [4–6]. One of the key strategies in the development of metallodrugs involves studying their interactions with DNA, which is a primary target for many anticancer agents [7]. Such

interactions can lead to the disruption of DNA replication and transcription, ultimately inducing apoptosis in cancer cells. These interactions can be evaluated through electronic absorption spectroscopy, fluorescence quenching, viscosity measurements, and DNA cleavage studies using gel electrophoresis [10].

In addition to anticancer research, transition metal complexes are being explored for their potential in treating metabolic disorders such as diabetes mellitus (DM). DM is characterized by chronic hyperglycemia due to impaired insulin secretion or action, leading to complications such as neuropathy, nephropathy, and retinopathy. Metal complexes that inhibit enzymes like α-amylase—responsible for carbohydrate breakdown—offer promising alternatives to conventional insulin therapy [8,9]. Moreover, chronic hyperglycemia promotes oxidative stress, and metal complexes may help mitigate this by enhancing antioxidant activity. Chelation of Schiff bases with biologically relevant metal ions such as Cu^{2+}, Co^{2+}, Ni^{2+}, Zn^{2+}, Mn^{2+}, Fe^{2+}, and VO^{2+} has been shown to enhance the pharmacological activity of the ligands [11–13]. This enhancement is attributed to increased lipophilicity and decreased polarity, which facilitate better cellular uptake. Platinum-based drugs such as cisplatin remain standard treatments for various cancers; however, their use is limited by toxicity and drug resistance [14,15]. As a result, there is a growing interest in developing novel metal-based therapeutics that are more effective, less toxic, and target-specific [16].

Cisplatin and similar agents exert their anticancer effects by binding to DNA and forming cross-links that inhibit cell division [17,18]. Metal complexes that bind DNA through intercalation—where planar molecules insert between DNA base pairs—exhibit stronger and more stable interactions than electrostatic or groove-binding modes [19–21]. Such intercalators are widely used as antitumor, antibacterial, and antiviral agents, making Schiff base complexes an attractive class of compounds for drug development.

In this study, we report the synthesis, characterization, and biological evaluation of novel Zn(II) complexes derived from Schiff base ligands formed by the condensation of 5-cyclohexyl-2-methoxyaniline with Salicylaldehyde and methyl substituted Salicylaldehyde. The thermal stability, antibacterial activity, and cytotoxic potential of the complexes were assessed, with particular emphasis on their interactions with DNA as a key mechanism of action.

2. Material and Methods:

2.1. Materials:

All of the preparatory materials and solvents were procured from Sigma-Aldrich, Merck, and Hi Media Ltd. The solvents used for the synthesis were thoroughly distilled and dried according to standard methods. The Supercoiled pBR322 DNA and CT-DNA were purchased from Genei in Bangalore, India, and kept at 4 ^{o}C. Double-distributed water was used to prepare all of the buffer solutions for the DNA binding and cleavage experiments.

2.2. Methods:

The elemental analysis (C, H and N) of all the synthesised compounds was performed using a Perkin-Elmer elemental analyzer. FT-IR spectra were recorded on the Perkin-Elmer Infrared Model 337 in the range 4000-250 cm^{-1}. UV-Vis spectra of compounds were analysed on a Shimadzu UV-Vis 2600 spectrophotometer in DMSO solvent in the range between 200 and 800 nm. ESI mass spectra were recorded on an HP-LC mass spectrometer (Agilent Tech,

USA). The ^{1}H-NMR and ^{13}C-NMR spectra of Schiff base were recorded on a 400 MHz Brucker NMR spectrometer in $CDCl_3$. The metal content of the complexes was determined using atomic absorption spectroscopy with the GBC Avanta 1.0 AAS. The melting points of the compounds were determined on a Polmon instrument (model No.MP-96. The thermo gravimetric analysis (TGA) of all metal complexes were carried out in a dynamic nitrogen atmosphere with a heating rate of 10 ^{o}C min^{-1} on a Shimadzu TGA-50H in the temperature range of 27–1200 ^{o}C. Fluorescence spectra were recorded on a Shimadzu RF-5301PC spectrofluorometer.

2.3. Synthesis of Schiff base Ligands (HL^1 and HL^2):

A hot methanolic solution of 5-cyclohexyl-2-methoxyaniline (10 mmol) was refluxed with methanolic solution of Salicylaldehyde (10 mM) and 2-hydroxy-4-methylbenzaldehyde(c) (10 mM) at 60–65 °C for 6 hours under magnetic stirring. The progress of the reaction and the purity of the product were monitored by thin-layer chromatography (TLC). Upon completion, an orange/brown precipitate formed, which was collected by filtration and dried in a desiccator over calcium chloride. A summary of the experimental procedure is presented in **Scheme 1** [22,23].

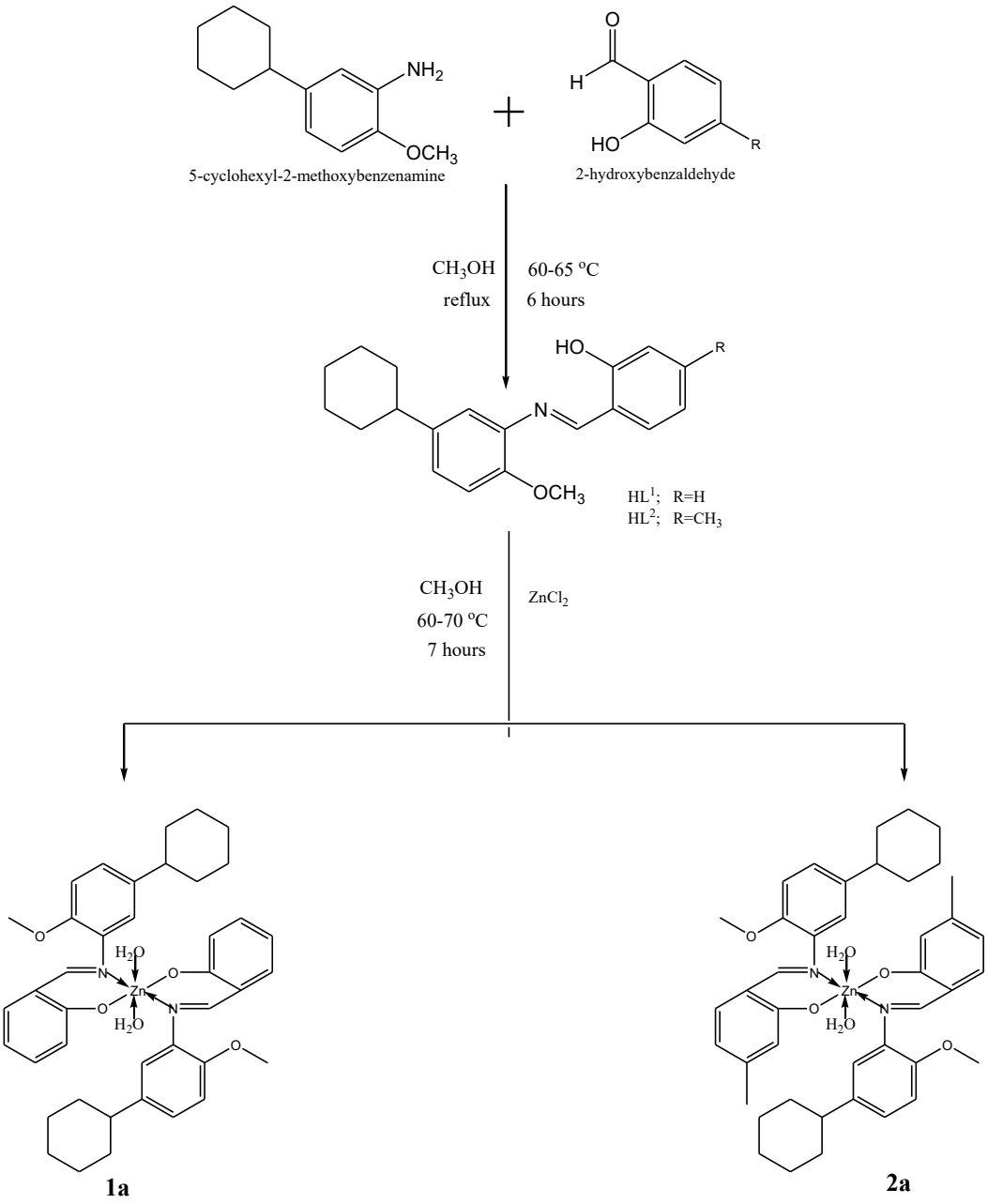
2.3.1.2-(E)-((5-cyclohexyl-2-methoxyphenylimino)methyl)phenol,

($C_{20}H_{23}NO_2$), (HL^1):

Yield:76%. M.P: 135 ^{o}C. Elamental Analysis. Calcd (%): C, 77.64; H, 7.49; N, 4.53; O, 10.34. Found: C, 77.60; H, 7.45; N, 4.58. IR (KBr): ν(O-H) 3445, ν(CH=N) 1617, ν(C-O) 1122(Fig. S1). UV-Vis; lmax/nm (cm-1): 268 (3731 cm-1), 356 (2809 cm-1) (Fig.S2). 1H NMR (400 MHz, CDCl3) δ: 13.94 (s, 1H), 8.71 (s, 1H), 7.36 (ddd, J = 8.3, 5.1, 1.6 Hz, 2H), 7.07 (dt, J = 4.9, 2.1 Hz, 2H), 7.01 (d, J = 8.3 Hz, 1H), 6.94 – 6.88 (m, 2H), 3.86 (s, 3H), 2.56 – 2.42 (m, 1H), 1.92 – 1.72 (m, 5H), 1.45 – 1.23 (m, 5H); (Fig. S3). 13C NMR (100 MHz, CDCl3) (δ); 161.92, 161.67, 151.02, 140.97, 136.67, 132.80, 131.92, 125.93, 119.58, 118.69, 118.31, 117.40, 111.86, 55.99, 43.83, 34.71,26.91, 26.14 (Fig. S4). LC-MS (m/z): Calc: 309.17: Found: 310.18 $[M+H]^+$ [22].

2.3.2.2-(E)-(5-cyclohexyl-2-methoxyphenylimino)methyl)-5-methylphenol ($C_{21}H_{25}NO_2$), (HL^2)

Yield: 75%; M.p: 138 °C; Anal. Calc (%): C, 77.98; H, 7.79; N, 4.33. Found: C, 77.95; H, 7.75; N, 4.30. IR (KBr): ν(O-H) 3446, ν(C=N) 1618, ν(C-O) 1123 (Fig. S1). UV-Vis: lmax/nm (cm-1); 274 (36496), 354 (28248) (Fig-S2). 1H NMR (400 MHz, CDCl3): δ; 13.93 (s, 1H), 8.67 (s, 1H), 7.26 (d, J = 4.0 Hz, 1H), 7.06 (d, J = 9.6 Hz, 2H), 6.90 (d, J = 8.2 Hz, 1H), 6.83 (s, 1H), 6.73 (d, J = 7.8 Hz, 1H), 3.86 (s, 3H), 2.49 (s, 1H), 2.36 (s, 3H), 1.84 (d, J = 3.4 Hz, 5H), 1.48 – 1.37 (m, 5H)(Fig. S3). 13C NMR (100 MHz, CDCl3): δ; 161.81 , 161.58 , 150.97 , 143.93, 140.95 , 136.81, 131.76, 125.63, 119.90 , 118.23 , 117.76 , 117.26 , 111.85 , 56.00 , 43.84 , 34.70 , 26.91, 26.14, 21.9 (Fig. S4). ESI–MS (m/z):Calc: 323: Found:324$[M+H]^+$ [23].



Scheme 1. Synthesis of Schiff base and corresponding 1a and 2a complexes.

2.4. Synthesis of binary metal complexes (1a-2a):

The Zink metal complexes **1a** and **2a** were synthesized by mixing of 1:2 (Metal:Ligand) molar quantities of the ligand and the metal salts using the following procedure. In a stirred hot methanolic solution containing Schiff base ligand HL^1/HL^2 (20 mM), $Zncl_2$ (10 mM) was added drop wise. The reaction mixture was then refluxed for seven hours while being heated on an oil bath at 60-70 °C. The obtained solid coloured product was isolated, filtered, and washed with hot methanol and petroleum ether. The metal complexes were dried in vacuum desiccators over anhydrous $CaCl_2$. The synthetic procedure of ligand (HL^1/HL^2) and their respective metal complexes (1a and 2a) was shown in **Scheme 1.**

2.4.1.[Zn(HL^1)$_2$(H$_2$O)$_2$]: (C$_{40}$H$_{48}$N$_2$O$_6$Zn) (1a):

Color: yellowish orange, Yield: 82%, M.pt: ~119 ^{o}C, Anal. Foun. (Cal.) C, 66.90 (66.89); H, 6.78 (6.74); Zn, 9.05 (9.10); 13.4(13.37); N, 3.5 (3.37); IR (KBr) (cm-1): ν(O-H) 3413: ν(HC=N) 1596, ν(C–O) 1119, ν(M–O) 523, ν(M–N) 429; UV-Vis (DMSO) λmax/nm (cm-1): 259 (38610), 343 (29154), 430 (23255); μeff (BM): 0; MS (ESI): m/z 717 $[M+H]^+$ (**Fig.S3.1a**).

2.4.2. :[Zn(HL^2)$_2$(H$_2$O)$_2$]: (C$_{42}$H$_{52}$N$_2$O$_6$Zn) (2a):

Color: light orange, Yield: 78%, M.pt: ~128 ^{o}C, Anal. Found. (Cal.) C, 67.56 (67.60); H, 7.18 (7.02); Zn, 8.80 (8.76); N, 3.82 (3.75); IR (KBr) (cm^{-1}): ν(O-H) 3420: ν(HC=N) 1614, ν(C–O) 1120, ν(M–O) 522, ν(M–N) 462; UV-Vis (DMSO) λmax/nm (cm^{-1}): 258 (38610), 302 (29154), 430 (23255); μeff (BM): 0; MS (ESI): m/z 745 $[M+H]^+$ (**Fig.S3.2a**).

2.5. DNA binding studies:

2.5.1. UV–Vis spectroscopic studies:

The DNA binding affinities of three monometallic complexes (1a, 1b and 1c) were assessed using the UV-visible absorption method. The complex concentration maintained constant of 10μM, while the concentration of CT-DNA varied from 0 to 10 μM. The complexes were initially dissolved in DMSO due to limited solubility in buffer solution. To prepare the CT-DNA stock solution, DNA was diluted in a Tris-HCl/NaCl buffer at pH = 7.2 (50mM NaCl/5 mM Tris-HCl). The purity of the CT-DNA was ensured by measuring UV spectra using molar extinction coefficient of 6600 M^{-1} at 260 nm [23,24]. Mixing the CT-DNA solution with the respective complex and reference solution, followed by five minutes incubation before recording the absorption spectra. By analyzing the absorption data we determined the intrinsic binding constant (K_b) for interaction of each complex with CT-DNA.

2.5.2. Fluorescence quenching study:

Using fluorescence spectrophotometer and EB-bound CT-DNA in Tris HCl/NaCl buffer (pH 7.2), the binding between metal complexes and CT-DNA was investigated. The emission spectra of CT-DNA (125 μM) bound to EB (12.5 μM) were captured in the 360–800 nm region (350 nm excitation) as complex quantities were varied from 0 to 60 μM. The comparative binding affinity of the complexes with CT-DNA was calculated using the quenching constant derived by the Stern-Volmer equation [25,26], Io/I = 1 + Ksv r. The fluorescence (emission band) intensities in the absence and presence of complexes are denoted by I_o and I, respectively; K_{sv} is a linear Stern-Volmer constant; and 'r' is the complex concentration as a proportion of the DNA concentration.

2.6. DNA cleavage:

The ability of schiff base and its monometallic metal compounds (1a, 1b and 1c) to cleave DNA was evaluated using agarosegel electrophoresis in the presence and absence of H_2O_2. Super coiled pBR322 DNA was diluted in a Tris-HCl/NaCl buffer at pH 7.2, and treated with varying concentrations of the metal complexes [27]. After a two hour incubation at room temperature, bromophenol blue (2μL) was added to the DNA sample followed by vigorous stirring. The sample was then loaded onto a 1% agarosegel containing a TAE buffer (PH 8.0) and subjected to electrophoresis at 70 V for 45 minutes. Prior to electrophoreses, the gel was

stained with ethidiumbromide. The resulting gel is photographed using the BIO-RAD Gel documentation system, and the DNA bands were observed under transilluminators.

2.7. Biological Evaluation:

2.7.1. Anti bacterial activity:

In vitro testing was using the agar well diffusion metbod to evaluate the antibacterial activity of all synthesized compounds (HL, 1a, 1b and 1c) and the standard drug Gentamycin sulphate against two Gram positive (Staphylococcus aureus and Bacillus subtilis) and two Gram negative (Escherichia coli and Klebsiella pneumonia) bacterial stains. The bacterial culture was deposited on medium dishes after 24 hours of growth. Wells with three different concentrations (25, 50 75, µg/well) were created using a 6 mm cork borer. The plates were incubated at 25 ± 2°C and inhibition zones were measured in mm and compared with the standard drug zones.

2.7.2. Anti fungal activity:

Agarwell diffusion method was used to check in vitro anti fungal activity of synthesized compounds against two fungi species are Aspergillus niger and Candida albicans. One week old fungal culture was used as inoculums. Nystatin was used as reference antifungal drug. Antifungal data of compounds were expressed from the area of their inhibitory zone.

2.7.3. Anticancer activity (MTT assay):

Synthesized substances (HL, 1a, 1b and 1c) were tested for their cytotoxicity on A-549 and MCF-7 cell lines. Cell viability was determined using the MTT assay. Tumour cells were cultured in 25 cm^2 flasks with appropriate medium at 37 °C in a CO_2 incubator. MCF-7 and A-549 cells were separately plated in a 96-well plate. After overnight growth, the cells were switched to low serum media. DMSO was used as the control. After 48 hours of exposure to different synthesized substances, the cells were treated with MTT solution for 4 hours. Then, the medium was removed. Optical density at 570 nm was measured using an ELISA plate reader, representing cell quantity. The results were reported as a percentage of cytotoxicity/viability. Every experiment was taken in triplicates, and the cytotoxicity of the test substance Doxorubicin was compared to determine the IC_{50} values.

3. Results and discussion:

The Schiff bases and its metal complexes were synthesised and characterized by spectral and elemental data. They are coloured, non hydroscopic and extremely stable at room temperature. The ligand is soluble in organic solvents like as chloroform, methanol, ethanol, dichloromethane, DMF, acetonitrile, and dimethyl sulfoxide, while the complexes are soluble in DMF and DMSO, acetonitrile and both are insoluble in water. The analytical data obtained for a set of complexes are in good agreement with the theoretical values. Additionally, it suggests that the metal-to-ligand ratio observed in these complexes is 1:2.

3.1. FT-IR Spectroscopy

FT-IR spectroscopy is an effective method for identifying functional groups in compounds and understanding how ligands bind to metal ions (chelation and denticity). The FT-IR spectra of the Schiff base ligands and their metal complexes were recorded at room temperature in the range of 4000–250 cm^{-1} using KBr pellets.

The Schiff base ligands show characteristic azomethine (C=N) stretching bands at 1610 cm^{-1} (HL^1) and 1635 cm^{-1} (HL^2). After complexation, these bands shift by approximately 14-21 cm^{-1}, indicating the involvement of the azomethine nitrogen in coordination with the metal ion [28]. A broad band observed at 3445 cm^{-1} in both HL^1 and 3445 cm^{-1} HL^2, attributed to the phenolic –OH group, disappears upon complexation. This disappearance confirms the formation of a metal–oxygen (M–O) bond through the phenolic group [29].

Additionally, the C–O stretching band appears at 1124 cm^{-1} for HL^1 and 1224 cm^{-1} for HL^2. In the metal complexes, these bands shift to slightly lower frequencies (by 4–6 cm^{-1}), further supporting coordination through the phenolic oxygen atom [30].

New bands observed around 521–522 cm^{-1} and 429–462 cm^{-1} in both complexes correspond to M–O and M–N stretching vibrations, respectively [31, 32]. A broad band at 3413-3420 cm^{-1} in both complexes 1a and 2a suggests the presence of coordinated water molecules [33], which is further supported by additional bands appeares in the region of 797 cm^{-1}.

These spectral features clearly indicate that the ligands coordinate to the metal ions in a bidentate manner through both azomethine nitrogen and phenolic oxygen atoms, as shown in **Figures S1.1a and S1.2a**.

3.2. ESI Mass Spectral Studies

ESI mass spectrometry provides useful information about the molecular structure of a compound. The mass spectra of the metal complexes 1a and 2a showed molecular ion peaks at m/z = 712.71 ($[M+H]^+$) for 1a and m/z = 675.27 ($[M+H]^+$) for 2a (Figures S3.1a and S3.2a). These peaks confirm the formation of metal complexes with a $[M(L)_2]$ composition. The mass spectral results, along with elemental analysis, support a 1:2 metal-to-ligand ratio in the complexes.

3.3. Electronic Spectra and Magnetic Moments

The electronic spectra of the synthesized Schiff base ligand (HL) and its metal complexes (1a, 1b, and 1c) were recorded at room temperature using DMSO as the solvent. The results are presented in **Table 2** and **Figures S2.1a and S2.1b**.

The free Schiff base ligand exhibited two characteristic absorption bands at 258–259 nm (3875–3861 cm^{-1}) and 302–343 nm (3311–2915 cm^{-1}), corresponding to $\pi \rightarrow \pi^*$ transitions within the aromatic rings and $n \rightarrow \pi^*$ transitions of the C=N group, respectively [34]. In the metal complexes, these bands were shifted to 258–259 nm (38759–38610 cm^{-1}) and 302–343 nm (3311–2915 cm^{-1}), indicating coordination between the ligand and metal ions.

Additionally, a new absorption band appeared in the range of 403–430 nm (2481–2325 cm^{-1}) in the metal complexes, which was absent in the free ligand. This band is attributed to ligand-to-metal charge transfer (LMCT) transitions [35]. As Zn(II) possesses a d^{10} electronic configuration, no d–d transitions were observed in its complexes. The effective magnetic moments of complexes 1a and 2a were found to be zero, suggesting their diamagnetic nature.

3.4. Thermo gravimetric analysis:

According to thermogram data, all the complexes experienced an analogous thermal breakdown pattern, often in two phases, as shown in **figure S4**. Complex 1a was stable up to 160 °C-180 °C, experiences a first-stage breakdown between 160-180 °C, likely involving the loss of two water molecules. the second stage involves rapid weight loss between 230–485 °C

due to partial breakdown of the ligand moiety. In the subsequent disintegration step, gradual weight loss was observed in a temperature range between 470 and 890 °C, indicating complete decomposition of the organic component. The final output of the transfer process is metal oxide residue [36,37].

Upon analyzing the spectral studies and analytical data the metal complexes have been proposed with the following structures: complex **1a and 2a** as $[Zn(HL)_2(H_2O)_2]$, (**Scheme I**).

3.5. DNA binding studies:

3.5.1. Electronic absorption study:

In the present study, the interactions between CT-DNA and the metal complexes 1a and 2a were examined, and the changes in absorbance with and without CT-DNA are shown in Figure 4. Complexes 1a and 2a displayed absorption bands in the range of 277–288 nm, attributed to intra-ligand π–π* transitions. Upon the addition of CT-DNA, a decrease in absorbance (hypochromism) along with a slight red shift (bathochromic shift) was observed, suggesting that the metal complexes interact with DNA through an intercalation mode [38,39]. To estimate the intrinsic binding constant (Kb) of the complexes with CT-DNA, the equation $[DNA]/(\varepsilon_a–\varepsilon_f) = [DNA]/(\varepsilon_b–\varepsilon_f)+1/K_b(\varepsilon_b–\varepsilon_f)$ was used. In this equation, [DNA] is the concentration of CT-DNA (in base pairs), Kb is the intrinsic binding constant, εa is the apparent molar absorptivity (Aobsd/[complex]), and εf and εb are the molar extinction coefficients of the free and bound forms of the complex, respectively. The calculated binding constants were $1.397 \pm 0.02 \times 10^5$ M^{-1} for complex 1a and $3.38 \pm 0.02 \times 10^5$ M^{-1} for complex 2a [40]. These findings confirm that both complexes have a strong binding affinity for CT-DNA, with complex 2a showing greater binding strength than complex 1a. (For comparison, ethidium bromide has a K_b of 7×10^7 M^{-1}) **(Figure. S6).**

3.5.2. Fluorescence quenching study:

Fluorescence analysis using the emission intensity of the probe ethidium bromide (EB) was used to study the binding strength of metal complexes 1a and 2a with CT-DNA. In Tris-HCl buffer, EB shows weak fluorescence. When EB binds to CT-DNA by inserting between DNA base pairs (intercalation), its fluorescence intensity increases significantly [41,42]. However, adding metal complexes to the EB-DNA system reduces this fluorescence, suggesting that the complexes compete with EB for DNA binding through an intercalative mode [43], as shown in Figure 4. The strongest emission of EB-DNA is observed between 590–592 nm. The Stern–Volmer quenching constants (Ksv), obtained from fluorescence quenching data, revealed that complex 2a has a higher binding affinity than 1a. The Ksv values were $9.1 \pm 0.02 \times 10^3$ M^{-1} for 1a and $1.12 \pm 0.02 \times 10^4$ M^{-1} for 2a. Figure 5 shows the emission spectra of EB bound to CT-DNA in the absence and presence of the metal complexes 1a and 2a **(Figure.S6)**.

3.6. DNA cleavage activity:

The interaction of pBR322 DNA with the newly synthesized Schiff base ligands HL1 and HL2, along with their metal complexes 1a and 2a, was studied using gel electrophoresis under oxidative (with hydrogen peroxide) and photolytic (with UV light) conditions. DNA cleavage ability was assessed by tracking the transformation of supercoiled circular DNA (Form I) into nicked (Form II) and linear (Form III) forms [65]. **Figures S.7.a and S.7.b** show the different DNA cleavage patterns observed during oxidative and photolytic treatments with HL^1, HL^2, and their metal complexes 1a and 2a. In the oxidative method (Figure 7a), the DNA control,

DNA with H_2O_2, and ligands HL^1 and HL^2 (lanes 1–4) did not cause any noticeable DNA cleavage. In contrast, lanes 5 and 6, containing complexes 1a and 2a, showed effective conversion of supercoiled DNA (Form I) into the nicked form (Form II). Similarly, in the photolytic method (Figure 7b), the DNA control and both ligands (lanes 1–3) showed no cleavage. However, the presence of metal complexes in lanes 4 (1a) and 5 (2a) resulted in clear DNA strand scission, converting Form I into Form II [44].

These findings indicate that the metal complexes exhibit stronger DNA cleavage activity than the free ligands. This enhanced activity could be due to electron transfer from the donor atoms in the ligands to the positively charged metal ion, which may increase the lipophilicity of the complexes and improve their interaction with DNA [66, 67].

3.7. Biological studies:

3.7.1. Anti bacterial activity:

The antibacterial activity of the synthesized Schiff base ligands HL1 and HL2, along with their corresponding metal complexes 1a and 2a, was evaluated using the agar well diffusion method. As shown in **Table 3** and **Figure S8**, the metal complexes exhibited significantly higher antibacterial efficacy than their respective free ligands. This enhancement can be attributed to the chelation theory proposed by Tweedy, which suggests that metal coordination increases the biological activity of ligands. Among the tested compounds, complex 2a demonstrated the most potent inhibitory effect against both Gram-positive and Gram-negative bacterial strains, although its activity was lower than that of the standard drug.

3.7.2. Antifungal activity:

The synthesized Schiff base HL^1 nd HL^2 and their metal complexes (1a and 2a) were evaluated for their in vitro antifungal efficacy against two fungal strains, Aspergillus niger and Candida albicans. Their performance was benchmarked against the well-established antifungal agent nystatin at an equivalent concentration (see **Table 4 and Figure S.9**). The results indicated that the metal complexes displayed enhanced antifungal activity relative to the free Schiff base ligand. Among them, complex 2a demonstrated notably stronger antifungal effects than complex 1a. This increased activity may be ascribed to the presence of an additional methyl group in the Schiff base ligand of complex 2a. However, it is important to note that the antifungal activity of these metal complexes remained lower than that of the standard drug, nystatin.

3.7.3. Anticancer activity (MTT assay):

The anticancer activity of the Schiff base ligands HL^1 and HL^2, along with their metal complexes 1a and 2a, was assessed using the MTT assay against MCF-7 (human breast cancer) and A-549 (human lung adenocarcinoma) cell lines. Doxorubicin, a well-established anticancer drug, served as the reference standard. The IC_{50} values of all synthesized compounds are presented in **Table 5** and **Figure S.10**. The cytotoxicity data indicated that all tested complexes exhibited significant cytotoxic effects against the MCF-7 cell line, surpassing their activity against the A-549 cell line. Among them, complex 2a exhibited the most pronounced cytotoxicity. Moreover, all metal complexes demonstrated enhanced activity compared to their corresponding free ligands, suggesting that metal coordination improved the anticancer potential of the compounds. The order of cytotoxicity was found to be $HL^1 < HL^2 < 1a < 2a$.

4. Conclusion:

Three novel Schiff base metal complexes 1a and 2a have been synthesized from a Schiff base ligands HL^1 and HL^2, which is characterized by elemental analysis and spectral analysis such as NMR, FT-IR, UV-Vis, Mass, and TGA, which revealed that the Zn(II) complexes exhibited an octahedral geometry, coordination water molecule is present in the Zn(II) complexes which were confirmed by FT-IR and TGA. DNA interaction studies revealed that two synthesized complexes bind via intercalative mode. DNA interaction studies concluded that the synthesized three complexes cleaved into nicked or linear form in both cleavage modes. Biological studies performed by antimicrobial, and cytotoxicity have shown that the 2a complex have shown enhanced activity compared to a complex and their respective ligands.

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Assessment of Fluoride Levels in Groundwater of Hasanparthy Mandal Through Spectrophotometric Analysis

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Abstract: The present study aims to demonstrate the method of fluoride determination using a spectrophotometric technique. Traditionally, ligands such as flavonoid chrysin, xylenol orange, and alizarin red-S are commonly used to form complexes with metal ions like Al^{3+} for estimating fluoride concentration in multi-element mixtures. However, these compounds are often toxic and environmentally harmful. To overcome these concerns, the current research utilizes Eriochrome **Black T (EBT)**—a well-known azo dye that is comparatively less toxic and more eco-friendly—as the complexing agent in a **complexometric titration** method. In this study, EBT is first allowed to form a complex with aluminum ions (Al^{3+}). The resulting **Al-EBT complex acts as a metallo-ligand**, which subsequently interacts with fluoride ions, leading to the development of a pink color. The fluoride concentration is then measured using **UV-Visible spectrophotometry**. This method has been effectively applied to analyze fluoride levels in **drinking water samples collected from Bheemaram, Devannapeta, Chinthagattu, Ramaram and Hasanparthy**, located in the **Hanumakonda District of Telangana State, India**. The results indicate that the fluoride concentration in the groundwater ranges between **1.50 to 1.80 mg/L**, which **exceeds the World Health Organization's recommended maximum contamination limit**. Therefore, the groundwater in this area is considered **unsuitable for consumption due to fluoride contamination**.

Key words: Fluoride estimation, Complexometric titration, Spectrophotometric method.

1. INTRODUCTION:

Fluoride is the 13th most common element on Earth and mainly comes from natural sources in the ground. It is a serious pollutant in groundwater. Fluoride is commonly found in minerals such as **fluorite (CaF_2), cryolite (Na_3AlF_6), monofluorophosphates, and fluoroapatite [$CaF_2 \cdot Ca_3(PO_4)_2$]**, which are present in the Earth's crust.Fluoride is widely used in many areas such as **medicine, water treatment, dental care, agriculture, and even in chemical industries like nuclear reactors**. People can be exposed to fluoride from **various sources like food, medicine, and cosmetics**, but the **main source of fluoride intake is groundwater**, as it contains the highest natural levels of fluoride.To protect health, the **World Health Organization (WHO)** has set the **maximum safe limit for fluoride in drinking water at 1.5 mg/L**. However, a small amount of fluoride (between **0.5 and 1.5 mg/L**) is considered **beneficial for preventing tooth decay** and maintaining good dental health.

Groundwater usually has more fluoride than surface water because it comes into more contact with rocks that contain fluoride minerals. **Drinking water with too much fluoride can cause health problems**, such as **dental fluorosis (damaged teeth)** and **skeletal fluorosis (bone issues).**Therefore, it is important to **check the amount of fluoride in drinking water** to make sure it is safe for people. **Many methods are used to measure fluoride levels** in water and other sources.

Many techniques have been developed to measure fluoride, including **chromatographic, electrochemical, titrimetric, fluorescence sensing, capillary zone electrophoresis, and spectroscopic methods** [1–5]. **Ion chromatography** gives accurate results but is **costly**, while the **ion-selective method is cheaper and more sensitive** compared to UV-Visible spectroscopy. The **ion-selective electrode method** is commonly used and works well for **industrial and field testing**, but it has some drawbacks.This method needs **special care** and uses **buffer solutions** during the chemical preparation process. These buffers include **citrate**, **Cyclohexane diamine tetraacetic acid**, **Total ionic strength adjustment buffer**, **Diethylene triamine pentaacetic acid**, and **Ethylene diamine tetraacetic acid**. Another problem is that **other ions in the water** can form **complexes with fluoride**, which can affect the accuracy of fluoride measurement using the ion-selective electrode method. Some **colored chemical compounds (called chromophore ligands)** are commonly used in **spectrophotometric methods** to measure fluoride. Ligands like **flavonoid chrysin, xylenol orange, and alizarin red-S** are often used to form complexes with **metal ions like Al^{3+}** to help detect fluoride in mixtures. However, these chemicals can be **toxic and expensive.** To avoid this, a **less toxic and more eco-friendly dye,** called **Eriochrome Black-T**—a well-known **azo dye**—is used in **complexometric titration** [6,7].In this study, we also used this method. First, **EBT dye was allowed to form a complex with aluminum (Al^{3+}).** This **Al-EBT complex** then acts like a **metal-ligand** and reacts with **fluoride,** which results in a **pink color.** Finally, the **amount of fluoride in groundwater** was measured using a **UV-Visible spectrophotometer**.

2. Materials and Methods:

Chemical reagents: All the reagents were purchased in pure form of AR grade from Sd-fine. For the synthesis of Al-EBT complex, Al $(NO_3)_3$and EBT were used and for fluoride complexation, NaF was used. H_2O was used as solvent.

Instrument: All the absorption measurements were performed using Systronics 1808 UV-Vis spectrophometer under room temperature.

Preparations of Solutions:

Al-EBT Complex Formation: **Solutions of $Al(NO_3)_3$ and EBT were prepared at a concentration of 1×10^{-3} M each**. When these two solutions were **mixed in a 1:1 ratio**, they formed an **Al-EBT complex** with a final concentration of **1×10^{-5} M**.

Stock Solution of NaF [1000mg/L]: 0.22g of NaF was dissolved in 100ml of distilled water.

Analytical Procedure: First, 2 mL of the Al-EBT complex solution was taken from the stock. Then, small amounts of fluoride solution (from **0.2 mL to 1 mL**) were gradually added. The **change in absorption** was measured using a **UV-Visible spectrophotometer at a wavelength of 450 nm**.A **standard straight-line graph** was created by plotting **absorption values against known fluoride concentrations**, which helped to calculate the **molar extinction coefficient**.To find the **fluoride concentration in groundwater samples** collected

from **Bheemaram, Devannapeta, Chinthagattu, Ramaram, and Hasanparthy** in **Hanumakonda District, Telangana**, **2 mL of each water sample** was mixed with **2 mL of the Al-EBT solution**, and the **absorbance was measured at 450 nm**.Finally, the **fluoride concentration** in each sample was calculated using the standard graph and the following formula.

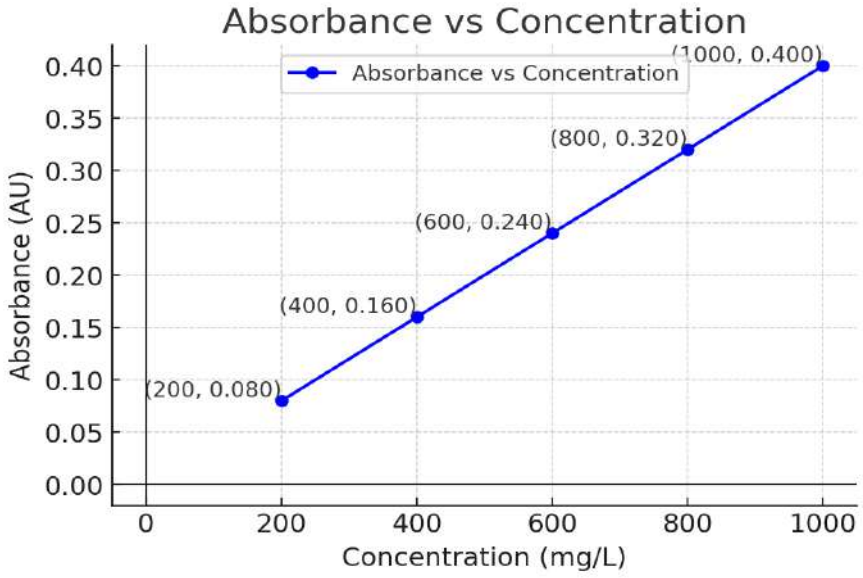
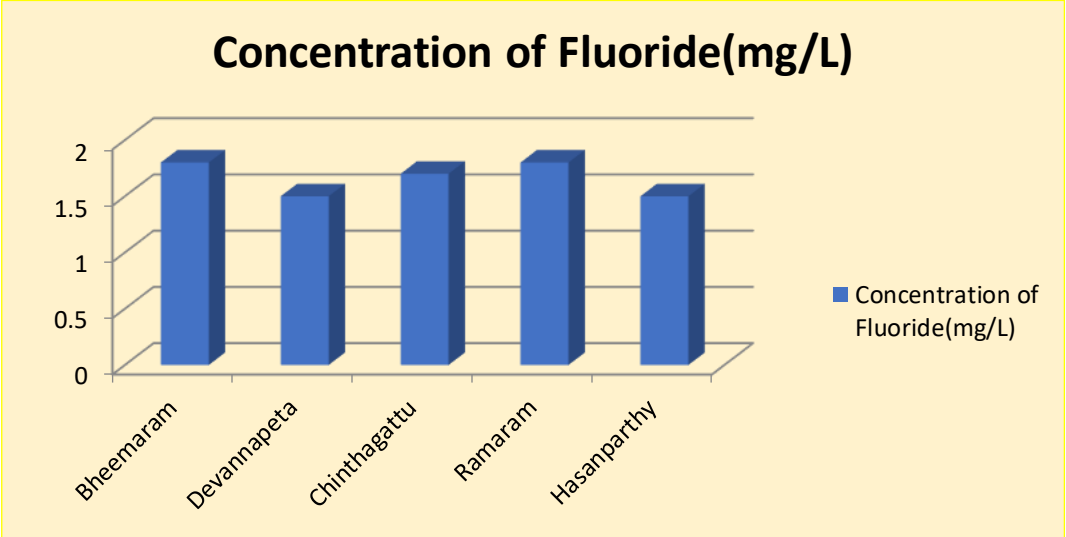


Table:

Area	Bheemaram	Devannapeta	Chinthagattu	Ramaram	Hasanparthy
Concentration of Fluoride(mg/L)	1.8	1.5	1.7	1.8	1.5



4. Result and Discussion:

The standard plot of absorption versus fluoride concentration shows a straight line with a slope. Based on this slope and the observed absorption value of the tested samples, the fluoride concentration was calculated using Equation.The estimated fluoride levels in groundwater samples collected from different villages — Bheemaram, Chinthagattu, Devannapet, Hasanparthy, and Ramaram — in the Hasanparthy Mandal region were found to range between 1.50 and 1.80 mg/L. These values exceed the World Health Organization (WHO) recommended maximum limit for fluoride in drinking water.This indicates that the groundwater in the studied areas is not suitable for consumption due to fluoride contamination.

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