Emerging Trends in Green and Innovative Chemistry

Chief Editor
Dr. Sanjay Nagarkar

Editors Ashok Pise • Namdeo Chavhan • Valmik Kapase • Vikas Bhosale • Santosh Kshirsagar • Sandip Gondake • Sagar Shinde •

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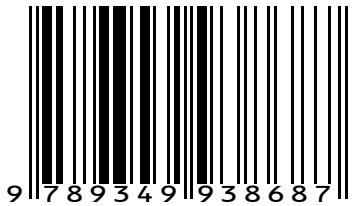

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Emerging Trends in Green and Innovative Chemistry

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Preface

The field of chemistry is undergoing a transformative shift, driven by the urgent need for sustainability, environmental responsibility, and innovative scientific approaches. The edited volume, "Emerging Trends in Green and Innovative Chemistry," is a timely contribution that brings together contemporary research, critical reviews, and novel methodologies reflecting this transition toward greener and more efficient chemical sciences.

In recent decades, the growing concerns over environmental degradation, resource depletion, and climate change have compelled the scientific community to rethink traditional chemical practices. Green chemistry has emerged as a guiding philosophy that emphasizes the design of safer chemicals, reduction of hazardous substances, energy efficiency, and the utilization of renewable resources. This volume captures these ideals by presenting a diverse range of studies focused on eco-friendly synthesis, sustainable catalysis, and innovative chemical processes.

The chapters in this book span a wide spectrum of chemical sciences, integrating both classical foundations and modern innovations. Contributions on the synthesis and biological evaluation of heterocyclic compounds highlight the continued importance of organic chemistry in pharmaceutical applications, while incorporating green methodologies such as solvent-free reactions and natural catalysts. At the same time, the volume emphasizes sustainable catalysis and synthetic strategies, including the use of eco-friendly reagents and catalysts derived from natural and renewable resources, reflecting a clear shift toward environmentally responsible chemical practices.

The integration of modern tools and interdisciplinary approaches is another key highlight of this book. Advances in computational chemistry, spectroscopy, photochemistry, and artificial intelligence are explored to enhance chemical research and industrial applications. The inclusion of topics such as artificial intelligence in the chemical industry and in silico

drug discovery approaches indicates the growing synergy between chemistry and digital technologies.

Nanotechnology and material science also form an important component of this volume. Studies on the green synthesis of nanoparticles, including zinc oxide, copper oxide, palladium, and niobium dioxide, demonstrate how plant-based and sustainable methods can be employed to develop advanced functional materials. Additionally, innovative applications such as artificial photosynthesis and the utilization of industrial waste like fly ash for catalysis reflect the broader scope of sustainable innovation.

We extend our sincere gratitude to all the authors for their scholarly contributions and commitment to advancing the field of green chemistry. Their work reflects a shared vision of sustainable scientific progress. We also acknowledge the efforts of reviewers and contributors who have helped maintain the academic rigor and quality of this publication.

This book is intended to serve as a valuable resource for researchers, academicians, students, and professionals in chemistry and allied disciplines. We hope it will inspire further research, innovation, and the widespread adoption of green and sustainable practices in chemical sciences.

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Emerging Trends in Green and Innovative Chemistry

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Biological Importance of 1-Amidoalkyl-2-Naphthols: A Critical Review

Ajit P. Ingale, Kiran D. Dhawale, Madhuri S. Pansare

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Abstract

1-Amidoalkyl-2-naphthols are a key group of naphthalene-based compounds known for their wide range of biological activities. They are usually made by combining β-naphthol, aldehydes, and amides in a single reaction. The phenolic hydroxyl group and amide in their structure help them interact with different biological targets. These compounds show many pharmacological effects, such as antibacterial, antifungal, anticancer, anti-inflammatory, and antioxidant activities. Because of their strong biological potential and flexible synthesis, they are promising starting points for developing new medicines.

Keywords: Biomimetics; Sustainable Innovation; Applied Entomology; Structural Coloration; Swarm Intelligence; Insect-Derived Biomaterials; Circular Bioeconomy; Ecosystem Services; Green Engineering; Bioinspired Robotics; Waste Bioconversion; Pollination Biology

1. Introduction

1-Amidoalkyl-2-naphthols are nitrogen-containing naphthalene derivatives that have gained ongoing interest in medicinal and synthetic organic chemistry.1 These compounds have a naphthol base with an amidoalkyl group at the C-1 position and are usually made by combining β-naphthol, aldehydes, and amides or carbamates in one reaction. Their structure includes an aromatic naphthalene core, a phenolic hydroxyl group, and an amide, all of which are important for biological activity.2 Because of this combination, 1-amidoalkyl-2-naphthols are useful building blocks with a range of biological and pharmacological effects.

2. Anti-microbial activity

A major area of research on 1-amidoalkyl-2-naphthols is their antimicrobial activity.3 Some of these compounds have shown strong antibacterial effects against both Gram-positive and Gram-negative bacteria. The phenolic hydroxyl

group helps them form hydrogen bonds with bacterial enzymes and cell walls, while the amide group improves their ability to bind to microbes. Studies on structure and activity show that adding electron-withdrawing groups to the aromatic aldehyde often makes these compounds more effective, possibly by increasing their ability to pass through cell membranes. Some have worked as well as standard antibiotics, making them promising options as new antimicrobial agents, especially as antibiotic resistance grows.

3. Antifungal Activity

Besides fighting bacteria, 1-amidoalkyl-2-naphthols also show strong antifungal effects.4 Tests against fungi like Candida albicans and Aspergillums species suggest these compounds may damage fungal cell membranes or block important enzymes. The naphthalene ring, which does not mix with water, helps these molecules interact with cell membranes and enter cells more easily. These results highlight the value of this type of compound in finding new antifungal drugs, especially as resistance to current treatments increases.

4. Anticancer Activity

Researchers are also interested in the anticancer effects of 1-amidoalkyl-2-naphthols.5 The naphthalene part of these molecules can stack with nucleic acids and proteins, which may affect processes like DNA copying and gene activity. Some versions of these compounds have killed cancer cells in lab tests, including breast, lung, and colon cancer types. They may work by triggering cell death, stopping cell division, or blocking important growth signals in tumors. The amide group can help the molecule target cancer cells more specifically. Changing the chemical groups on the molecule can also make it more effective, especially when electron-withdrawing groups are added.

5. Anti-inflammatory activity

1-Amidoalkyl-2-naphthols also have important anti-inflammatory effects.7 Ongoing inflammation is linked to many health problems, such as arthritis, heart disease, and disorders of the nervous system. Some of these compounds can block pro-inflammatory substances like tumor necrosis factor-alpha (TNF-α) and interleukins. The phenolic hydroxyl group may help control both oxidative and inflammatory processes. A few compounds also block cyclooxygenase (COX), working in a way similar to common anti-inflammatory drugs (NSAIDs). Having both antioxidant and anti-inflammatory effects makes these compounds especially useful for therapy.

6. Anti-oxidant activity

Oxidative stress is a key factor in aging and diseases like cancer and diabetes. The antioxidant power of 1-amidoalkyl-2-naphthols mainly comes from the

phenolic hydroxyl group, which can give up hydrogen atoms to neutralize harmful reactive oxygen species (ROS).8 Lab tests, such as DPPH and ABTS, show these compounds can remove free radicals. Adding electron-donating groups to the aromatic ring usually makes them better at this.9 These antioxidant effects help protect cells from oxidative damage.

7. Analgesic and antipyretic activity

Recent studies have looked at whether 1-amidoalkyl-2-naphthol compounds can relieve pain and reduce fever. Tests in animals show that some of these compounds lower pain and fever, possibly by blocking prostaglandin production.10 Because they can both reduce inflammation and pain; these compounds are promising for future drug development.

8. Anti-diabetic activity

New research suggests that 1-amidoalkyl-2-naphthols might help treat diabetes.11 Some of these compounds can block enzymes like α-glucosidase, which break down carbohydrates, helping to lower blood sugar after meals. The flexible structure of the amidoalkyl group allows for better enzyme binding and selectivity. While this research is still early, it shows promise for treating metabolic diseases.

Medicinal chemists value 1-amidoalkyl-2-naphthols for their flexible structure. The naphthalene core makes the molecule hydrophobic and helps it interact with other molecules, while the amide group allows for hydrogen bonding and increases polarity. The phenolic hydroxyl group boosts antioxidant activity and helps the molecule recognize biological targets. Studies show that changing the groups on the aromatic ring can greatly affect how the compound works. Electron-withdrawing groups often make them better at fighting microbes and cancer, while electron-donating groups can improve antioxidant effects. The size and fat-solubility of the molecule also affect how well it gets into cells and how the body processes it.

9. Conclusion

In summary, 1-amidoalkyl-2-naphthols are an important group of naphthalene compounds with many biological effects, such as fighting microbes, fungi, and cancer, as well as reducing inflammation, acting as antioxidants, relieving pain, and possibly helping with diabetes. Their structure allows them to interact with many biological targets, and studies on their structure and activity help guide new drug design. Ongoing research using new synthesis methods, computer modeling, and lab testing will help us understand their full potential. Because of their wide range of effects and flexible chemistry, these compounds are strong candidates for future medicines.

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Synthesis And Bioactivity of Dihydropyrimidinone (DHPM) Derivatives

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Abstract

Dihydropyrimidinones (DHPMs) is an main type of heterocyclic compounds whih shows biological activities. This review/article focuses on the synthetic strategies employed for the construction of DHPM frameworks and highlights their bioactivity profiles across various pharmacological targets. Several efficient synthetic protocols, including classical Biginelli multicomponent reactions, as well as modern catalytic and green chemistry approaches, have been explored to access DHPM derivatives with structural diversity and high yields. Structural modification of the DHPM core has led to compounds exhibiting antimicrobial, antiviral, anticancer, anti-inflammatory, calcium channel-blocking, and enzyme inhibitory activities. The structure–activity relationship (SAR) analysis indicates that substitutions on the dihydropyrimidinone nucleus significantly influence potency and selectivity, enabling rational design of derivatives with enhanced bio efficacy. In addition, the integration of DHPM scaffolds with other pharmacophores has yielded hybrid molecules with synergistic therapeutic effects. Overall, the versatile synthetic accessibility and promising bioactivity of DHPM derivatives underscore their significant potential in drug discovery and medicinal chemistry.

Keywords: Anti-viral Dihydropyrimidinone derivatives, Anti-bacterial Biginelli reaction, Anti-oxidant, Cytotoxic, Anti-bacterial.

1. Introduction

Heterocyclic molecule occupies a central position in medicinal chemistry due to their widespread occurrence in natural products, pharmaceuticals, and biologically active molecules. Among these, dihydropyrimidinones (DHPMs) is an important type of nitrogen-containing heterocycles with remarkable pharmacological significance. Since the discovery of the Biginelli reaction in

1893, DHPMs have attracted sustained attention because of their simple synthetic accessibility and broad spectrum of biological activities. The classical Biginelli reaction, single three-component reaction of an aldehyde, β-ketoester, and urea or thiourea under acidic conditions, provides a straightforward and efficient route to the DHPM scaffold. Over the years, numerous modifications and improvements of this multicomponent reaction was created to get around restrictions like poor yields and challenging reaction conditions. Recent advances include the use of heterogeneous catalysts, Lewis acids, ionic liquids, microwave irradiation, ultrasound-assisted synthesis, solvent-free conditions, and other green chemistry approaches. These modern strategies have significantly enhanced reaction efficiency, selectivity, and environmental compatibility while enabling structural diversification of DHPM derivatives. Biologically, DHPM derivatives shows pharmacological properties. Several DHPM-based compounds have demonstrated antimicrobial, antiviral, anticancer, anti-inflammatory, antihypertensive, and calcium channel-blocking activities. Notably, certain DHPM derivatives act as potent calcium channel antagonists and have inspired the development of clinically relevant drugs. In addition, many synthesized DHPM analogues show promising enzyme inhibitory and antioxidant properties, further expanding their therapeutic potential. Structure–activity relationship (SAR) studies have revealed that the type, position, and electronic nature of substituents on the dihydropyrimidinone nucleus strongly influence biological activity. Functionalization at specific positions of the DHPM core can modulate lipophilicity, binding affinity, and pharmacokinetic behavior, thereby enabling rational drug design. Furthermore, the incorporation of DHPM scaffolds into hybrid molecules has opened new avenues for the development of multifunctional agents with enhanced efficacy.

Figure 2 : Product Dihydropyrimidinones Derivatives.

2. Antibacterial test:

Dihydropyrimidinone (DHPM) antibacterial tests often include agar diffusion techniques (such as disc diffusion) to evaluate activity against Gram-positive and Gram-negative bacteria, such as S. aureus and E. coli, and broth microdilution to estimate Minimum Inhibitory Concentration (MIC). Additional techniques to assess compound safety and potential as antimicrobial agents include cytotoxicity assays and minimum bactericidal concentration (MBC) determination.

3. Cytotoxic test:

A cytotoxic test for dihydropyrimidinones typically involves the MTT assay, where cells are exposed to different concentrations of the compounds in a 96-well plate. Living cells metabolize the MTT substrate into purple formazan crystals, which are then dissolved and measured with a spectrophotometer, indicating cell viability. Other assays like the LDH release assay or trypan blue exclusion can also be used to assess cell membrane damage or to count live vs. dead cells, respectively.

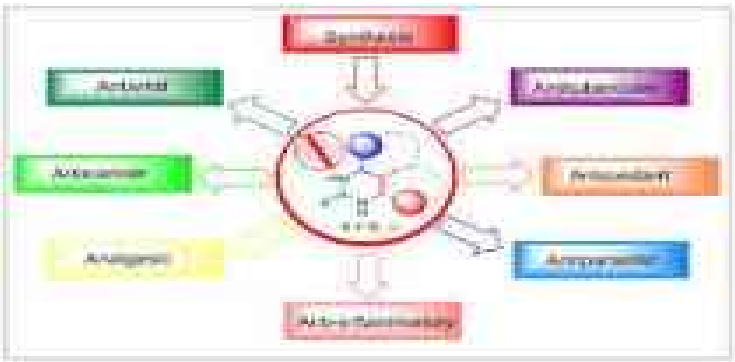


Fig. Biginelii reaction.

4. Results and Discussion:

The one-pot multicomponent reaction approach was used to synthesise DHPM derivatives utilising urea, ethyl acetoacetate, and a range of aldehydes. Heating and condensation with reflux are the methods used. We investigated the effects of pH values of 4 and 5 on a chemical reaction's outcomes. This was predicated on the idea that iminium interacts favourably at pH 4-5. Aldehyde (20 mmol), urea (40 mmol), and ethyl acetoacetate (40 mmol) were added to a round-bottom flask. H_2SO_4 was then added, and the pH was maintained at 4 or 5. The mixture was refluxed for an hour at 80 °C. Aquadest was used to rinse the mixture before it was filtered. Ethanol was then used to recrystallise the final product. This method is an advancement over one that was previously documented.

Reaction:

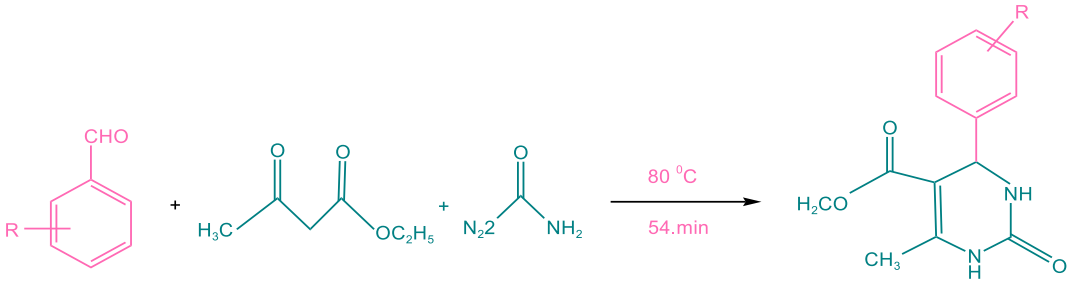
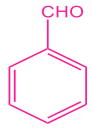
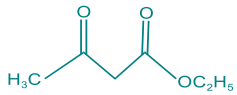
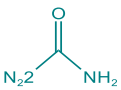
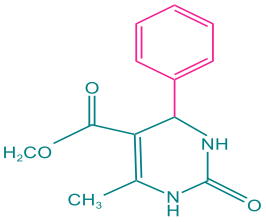
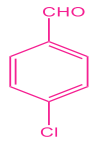
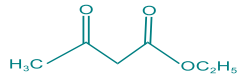
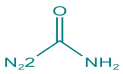
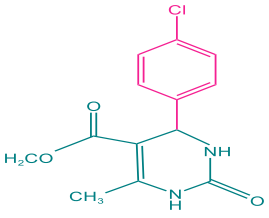
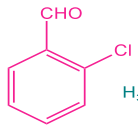
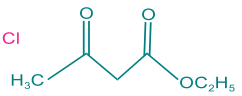
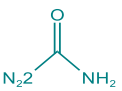
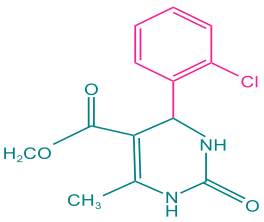
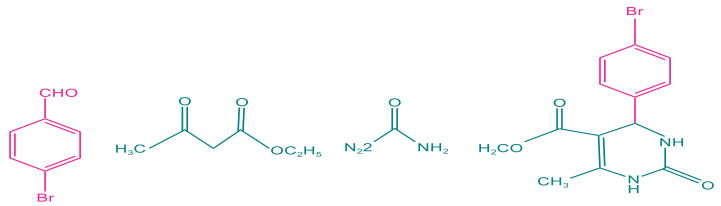
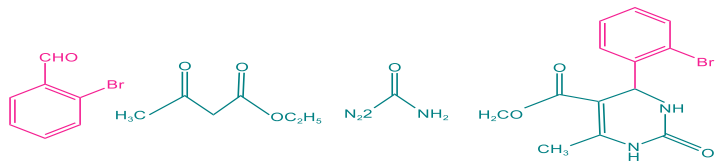
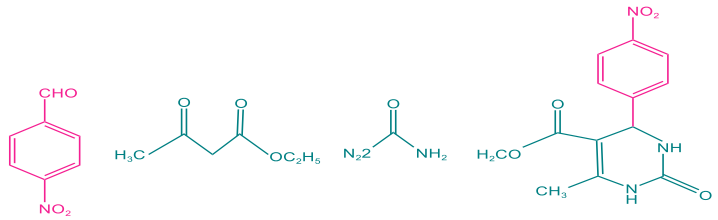
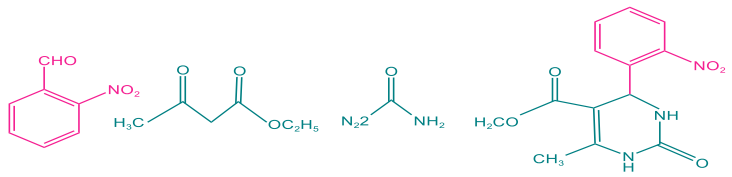
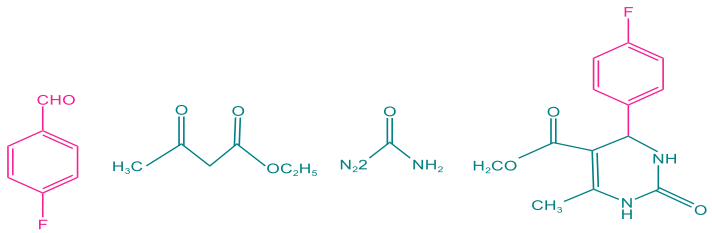
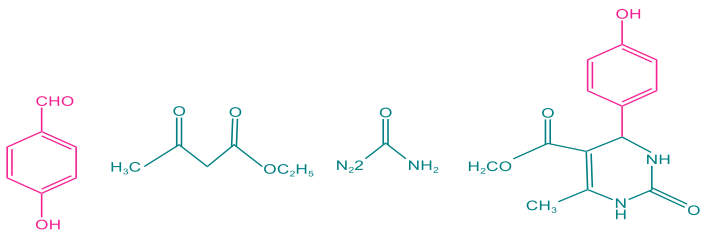
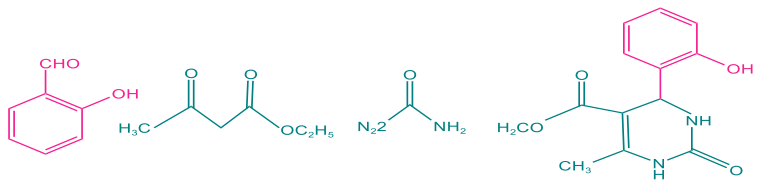
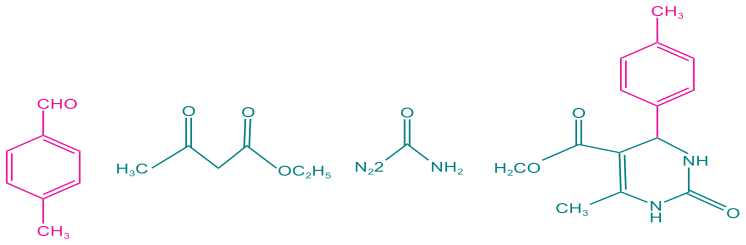
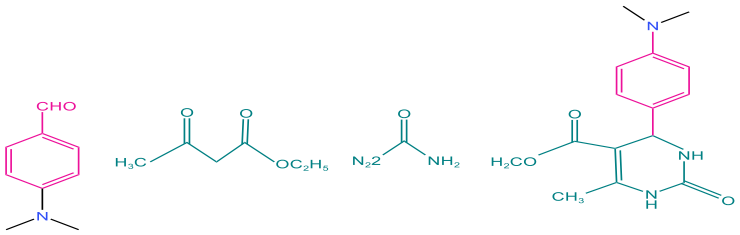


Figure 2 *: Reaction for Synthesis Dihydropyrimidinones*

Table No: 1

Sr. No	Aldehyde®	Ethyl Acetoacetate	Urea	Product®	Time (Min)	Yield (%)
1.					80	94
2.					78	92
3.					78	94

4.		80	92
5.		80	94
6.		78	95
7.		78	96
8.		78	92
9.		80	90
10		80	92

11.		80	91
12.		80	94

5. Experimental section:

A mix 1.1 g of benzaldehyde, 1.3 g of ethyl acetoacetate and 0.6 g of urea. Shake it by hand for 2 minutes. Heat the reaction mixture in the RB flask in a water bath at 80°C for one hour. Monitor the reaction using TLC.As the reaction progresses, a yellow solid will start to deposit and after an hour the flask will get full of solid. Collect the yellow solid carefully with spatula in a conical flask. Wash the yellow solid with 1 ml of cold water and recrystallize using rectified spirit; to give a colorless solid. Record the yield, M. P. and TLC. Expected M. P. of the product is 201-202°C.

6. Conclusion:

3,4-Dihydropyrimidinones have a variety of biological properties, including antiviral, anticancer, antibacterial, and antioxidant properties. As a result, they serve as a framework for the creation of numerous innovative medications. The research and development of new medications from Dihydropyrimidinone derivatives has been greatly advanced by the more recent improved synthesis techniques. According to published research, dihydropyrimidinone compounds exhibit encouraging activity. Therefore, dihydropyrimidinone research and optimisation are opening up new avenues for medicinal chemistry.

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Design, Synthesis and Biological Evaluation of Quinoline and Diazepine Based Heterocyclic Compounds: A Comprehensive Review

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Abstract

Heterocyclic compounds occupy a central position in medicinal chemistry and pharmaceutical research due to their structural diversity and wide range of biological activities. Among the numerous heterocyclic frameworks investigated for therapeutic applications, quinoline and diazepine derivatives have attracted considerable attention because of their remarkable pharmacological potential. Quinoline derivatives have demonstrated a broad spectrum of biological activities including antimalarial, antimicrobial, anticancer, antiviral, and anti-tubercular effects. Similarly, diazepine derivatives, particularly benzodiazepines, are widely used as central nervous system active agents and also exhibit promising anticancer, anti-inflammatory, and antimicrobial properties. Continuous research efforts have been directed toward the development of efficient synthetic methodologies and the design of structurally diverse derivatives with improved pharmacological profiles. This review summarizes the recent progress in the design, synthesis, and biological evaluation of quinoline and diazepine based heterocyclic compounds. In addition, important synthetic strategies, structure–activity relationships, and future perspectives in the development of these heterocyclic scaffolds for drug discovery are discussed.

Keywords: Quinoline; Diazepine; Heterocyclic compounds; Medicinal chemistry; Anticancer activity; Drug discovery

1. Introduction

Heterocyclic chemistry plays a vital role in modern drug discovery and

development. A large proportion of biologically active molecules and pharmaceutical agents contain heterocyclic frameworks that significantly influence their physicochemical and pharmacological properties. Among the various heterocyclic systems, nitrogen-containing heterocycles are particularly important due to their ability to form hydrogen bonding interactions and coordinate with biological targets.

Statistical analyses of pharmaceutical databases have revealed that nearly seventy-five percent of approved small-molecule drugs contain at least one nitrogen heterocycle. These heterocyclic structures serve as essential scaffolds for the development of therapeutic agents with diverse biological activities.

Quinoline and diazepine derivatives represent two important classes of nitrogen-containing heterocycles widely explored in medicinal chemistry. Quinoline consists of a benzene ring fused to a pyridine ring, forming a planar aromatic system that can interact effectively with biological macromolecules such as DNA and enzymes. On the other hand, diazepines are seven-membered heterocycles containing two nitrogen atoms and are commonly found in benzodiazepine drugs that act on the central nervous system.

Due to their structural versatility and pharmacological importance, quinoline and diazepine scaffolds have become attractive frameworks for the design and synthesis of novel therapeutic agents.

2. Quinoline Based Heterocyclic Compounds

Quinoline derivatives are widely distributed in nature and have been extensively investigated for their pharmacological properties. The quinoline nucleus forms the core structure of many natural products and synthetic drugs used for the treatment of various diseases. One of the most well-known natural quinoline derivatives is quinine, which has been historically used as an effective treatment for malaria.

Synthetic quinoline derivatives such as chloroquine and hydroxychloroquine have also played a crucial role in antimalarial therapy. These compounds act by interfering with the heme detoxification pathway in Plasmodium parasites, thereby inhibiting parasite growth.

Apart from antimalarial activity, quinoline derivatives have demonstrated significant antibacterial, antifungal, antiviral, and anticancer activities. Several quinoline based compounds act as DNA intercalating agents or inhibit enzymes involved in cell division, making them valuable candidates in anticancer research.

3. Diazepine Based Heterocyclic Compounds

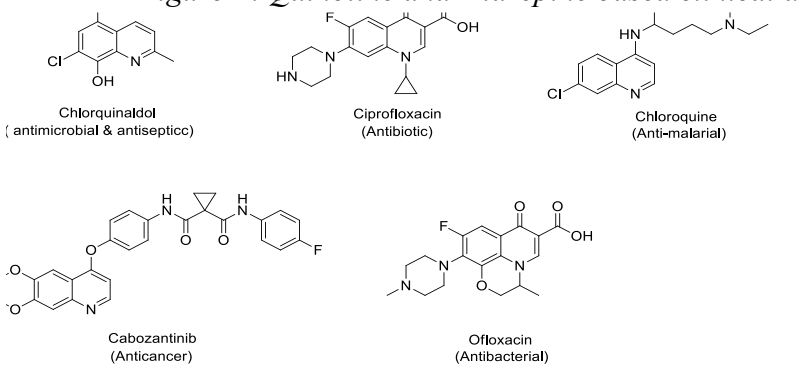
Diazepines represent another important class of heterocyclic compounds with significant pharmacological importance. These compounds contain a seven-membered ring with two nitrogen atoms and can exist in different structural forms such as 1,4-diazepines and 1,5-diazepines.

Benzodiazepines are the most widely studied members of this class and are commonly used as anxiolytic, sedative, hypnotic, anticonvulsant, and muscle relaxant drugs. These compounds act by enhancing the effect of the inhibitory neurotransmitter gamma-aminobutyric acid (GABA) in the central nervous system.

In addition to their neurological applications, recent studies have shown that diazepine derivatives possess antimicrobial, anticancer, anti-inflammatory, and antiviral activities. The ability to introduce different substituents on the diazepine ring provides opportunities for the design of new biologically active molecules.

Some of quinoline and diazepine based clinical drugs showing in Fig-1,

Figure-1. Quinoline and Diazepine based clinical drugs



4. Synthetic Approaches for Quinoline Derivatives

Several classical and modern synthetic methods have been developed for the preparation of quinoline derivatives. The Skraup synthesis is one of the earliest methods and involves the condensation of aniline with glycerol in the presence of an oxidizing agent under acidic conditions.

Another important method is the Friedländer synthesis, which involves the condensation of o-aminoaryl ketones with carbonyl compounds containing an active methylene group. This reaction provides a convenient route for the synthesis of substituted quinoline derivatives.

Other synthetic approaches include the Doebner–Miller reaction, Combes synthesis, and metal-catalyzed cross-coupling reactions. Recent advances in synthetic chemistry have also introduced microwave-assisted reactions and multicomponent reactions that significantly improve reaction efficiency and yield.

5. Synthetic Approaches for Diazepine Derivatives

The synthesis of diazepine derivatives generally involves cyclization reactions of suitable diamine precursors with aldehydes or ketones. One of the most common methods involves the condensation of o-phenylenediamine with carbonyl compounds to form benzodiazepine derivatives.

Modern synthetic strategies include multicomponent reactions, microwave-assisted synthesis, and metal-catalyzed reactions that provide efficient and environmentally friendly routes for the preparation of diazepine based heterocycles.

6. Biological Evaluation

Quinoline and diazepine derivatives have been extensively evaluated for various biological activities. Quinoline derivatives have demonstrated strong antimicrobial activity against a wide range of pathogenic microorganisms. In addition, several quinoline based compounds exhibit potent anticancer activity by inhibiting DNA replication or interfering with enzyme systems involved in cell division.

Diazepine derivatives have also shown promising biological activities including antimicrobial, anticancer, anti-inflammatory, and antioxidant effects. The biological activity of these compounds often depends on the nature and position of substituents on the heterocyclic ring.

7. Structure–Activity Relationship

Structure–activity relationship studies provide valuable insights into the influence of structural modifications on biological activity. In quinoline derivatives, substitution at specific positions of the aromatic ring can significantly enhance antimicrobial or anticancer activity.

Similarly, in diazepine derivatives, substitution on the nitrogen atoms or aromatic rings influences receptor binding affinity and pharmacological activity. Understanding these relationships helps researchers design more potent and selective drug substances.

8. Future Perspectives

Despite significant advances in the development of quinoline and diazepine derivatives, challenges such as drug resistance, toxicity, and poor bioavailability still remain. Future research should focus on the development of hybrid molecules, computational drug design, and environmentally friendly synthetic methodologies.

Integration of molecular modeling, artificial intelligence and green chemistry approaches may further accelerate the discovery of new heterocyclic drugs based on quinoline and diazepine scaffolds.

9. Conclusion

Quinoline and diazepine based heterocyclic compounds continue to attract considerable attention in medicinal chemistry due to their diverse biological activities and therapeutic potential. Numerous synthetic methodologies have been developed for the preparation of these compounds, and many derivatives have demonstrated promising pharmacological properties. Continued research in this field is expected to contribute significantly to the discovery of new therapeutic agents for the treatment of various diseases.

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Malic Acid Catalyzed Reductive Amination of Aldehydes Under Solvent-Free Condition

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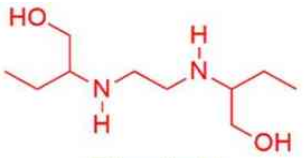
Abstract

Using malic acid as a catalyst, a new, efficient, green, and solvent-free technique for the one-pot reductive amination of carbonyl compounds has been created. Reductive amination has been applied to a variety of functionalised amines and aldehydes, including aliphatic, aromatic, and heteroaromatic ones, using this technique. The carbonyl compounds underwent a single, side-reaction-free reductive amination. This method's main advantages were its simplicity, green protocol, quick transformation, range of substrates, high yield, metal-free operation, and catalyst recyclability. This contributes to the process's affordability, practicality, and biodegradability.

Keywords: Amines, Malic acid, Sodium borohydride, solvent-free condition.

1. Introduction

The manufacture of biomaterials, medications, insecticides, and pesticides requires a range of secondary amine molecules as building blocks (Figure 1). Amines are frequently utilised for both biological and pharmacological objectives due to their immense significance. Reducing aldehyde groups by reductive amination or imine reduction remains the most straightforward process for producing substituted amines. For this reaction, a variety of expensive metal catalysts have been used, such as palladium gold, platinum, iridium, rhodium, rhenium, and ruthenium. These metal catalysts were highly toxic, costly, and non-recyclable.



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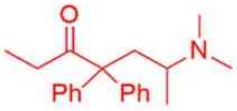

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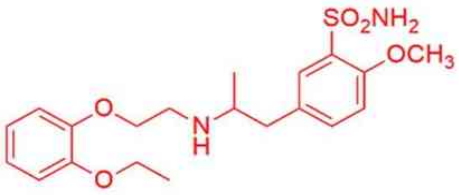
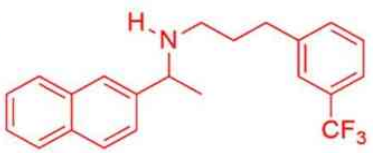


Flomax/Tamsulosin



Cinacalceta

Reductive amination of carbonyl compounds or reduction of imines are the simplest ways to produce secondary amines. For the reductive amination reaction, metal-assisted hydrogenation and hydride attack on imine derivatives were documented. The catalytic hydrogenation of compounds containing an alkene, acetylene, and certain other functional groups including cyano, nitro, nitro, and furyl is limited by the reducible capacities of certain imine substances. nBu_2SnClH, nBu_3SnH/SiO_2, nBu_2SnIH, $NaBH_4$/Brønsted acidic ionic liquid diborane/MeOH, $NaBH(OAc)_3$, ammoniaborane/$Ti(OiPr)_4$, hydrioiridium(III) complex, $PMHS/ZnCl_2/H_2SO_4$, $Ti(OiPr)_4$/wet clay, $NaBH_4/H_2SO_4$, $NaBH_4/Fe(OTf)_3$, and solid acid activated $NaBH_4$ have been used. Eco-friendly catalysts are required to replace them. An environmental science approach aims to decrease or even eliminate the use and manufacturing of harmful substances.

Thus, employing solvent-free methods and nontoxic catalysts is a great option. Due to the widespread use of solvents in practically all commercial processes and the anticipated scarcity of fossil fuels, research into ways utilising recyclable and ecologically acceptable catalysts has recently advanced. Additionally, it has been observed that the catalysts used are typically not environmentally friendly, which has a substantial ecological impact.

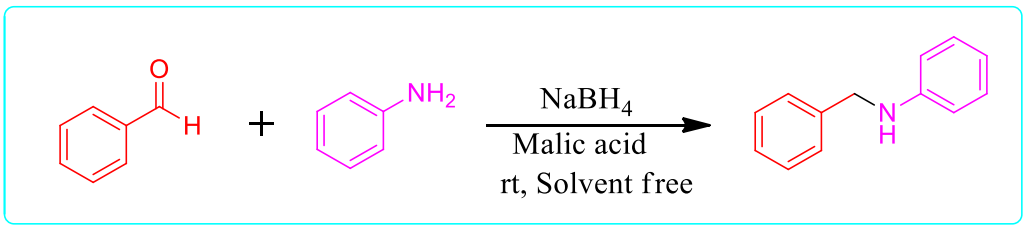
Malic acid has recently been shown to be useful in that framework to accelerate chemical reactions. The use of thiamin hydrochloride as a green catalyst in organic processes has lately expanded due to its unique combination of pharmacological actions, including acidity, low toxicity, in flammability, water solubility, recyclability, and availability from recyclable raw materials. The use of innovative, nontoxic, reasonably priced, efficient, environmentally

acceptable, recycling catalytic levels of high performance is currently being driven by a number of scientific needs for environmental improvement for both commercial advantages.

We create a new, eco-friendly methodology for the solvent-free reductive amination process (Scheme 1). Thiamin hydrochloride is a catalyst that is recyclable, economical, efficient, sustainable, and less dangerous (Figure 2). We looked at the best-performing electron-donating and electron-withdrawing substrates for a number of heterocyclic, aromatic, acyclic, aliphatic, and cyclic amines. Amine (10 mmol), Aldehyde (10 mmol), and sodium borohydride ($NaBH_4$) (12 mmol) were added to the reaction together with malic acid (0.3 g) at room temperature without the use of a solvent.

Results and discussion:

Our investigations begin with a model reaction using 10 mmol of benzaldehyde, 10 mmol of aniline, and 12 mmol of sodium borohydride in the presence of catalyst malic acid (0.33 mmol) at room temperature without the use of a solvent (Scheme 1). At normal temperature, the reductive amination reaction using benzaldehyde substrate yields 98% in under two minutes. In order to comprehend how thiamin hydrochloride affects the reductive amination reaction, we



Scheme 1. Malic acid catalyzed reaction

Table 1: Catalytic investigation for the reductive amination reaction[a]

Sr. No.	Catalyst (mmol)	Time (min)	Yield (%)
1	**0.03**	**60**	**16**
2	**0.06**	**60**	**32**
3	**0.09**	**60**	**45**
4	**0.12**	**60**	**67**
5	**0.33**	**60**	**75**
6	**0.28**	**4**	**97**
7	**0.32**	**2**	**97**

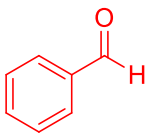
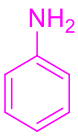
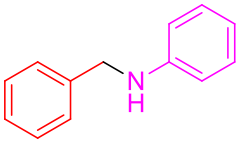
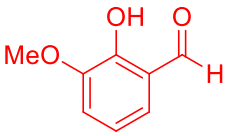
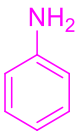
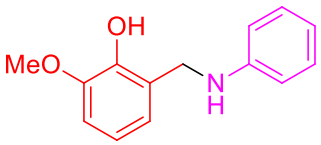
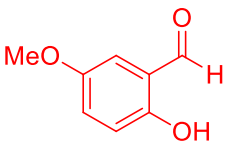
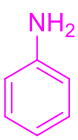
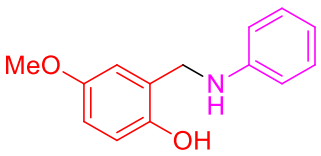
Investigated at room temperature under the solvent-free conditions of benzaldehyde, sodium borohydride, and aniline reactions. After 6 hours, the yield

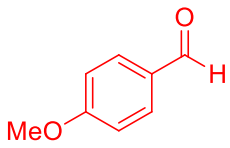
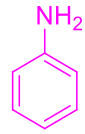
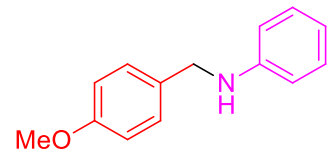
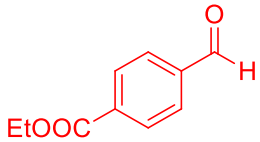
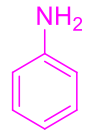
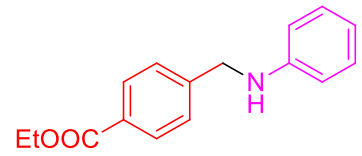
increases by 12%, but after 10 hours, the productivity only increases by 16%. At room temperature and without metals or solvents, the reaction was unsuccessful. When malic acid is present during the process, a greater yield is seen.

0.03 mg of malic acid catalyst, administered in 16% after one hour of reaction time, was used for the reaction (Table 1, Sr. No. 1). The catalyst concentration then increases from 0.06 to 0.33 mg as the yield increases (Table 1, Sr. No. 2–5). A yield of almost 98% was obtained when the catalyst was used at 0.28 mg (Table 1, Sr. No. 6). Lastly, there is no discernible difference in the reaction when the catalyst is increased by 0.32 mg once again (Table 1, Sr. No. 7).

Results are compared and displayed in Table 2 to better understand the efficacy of our method in solvent-free conditions and various solvents used for reductive amination, such as methanol, water, ethanol, DCM, chloroform, tetrahydrofuran, dimethyl formamide, and 1, 4-dioxane. The results showed that both the current methodology and the eco-friendly approach had advantages in terms of synthesis technique, reaction speed, and reaction rates. Furthermore, the results demonstrate that the most efficient method is the solvent-free reductive amination of an aldehyde using the malic acid catalyst described here (Scheme 1). The reaction result of various aromatic aldehydes interacting with amines in the presence of sodium borohydride under the catalyst malic acid was detailed by concentrating on the ideal scenario.

Table 2. Various substrate study for the reductive amination reaction

Sr. No.	Aldehydes	Amines	Products	Time(min)	Yield (%)
1				1	98
2				2	95
3				2	97

4				3	96
5				2	94

Experimental sections:

Materials and methods

Aldrich and Alfa Aesar supplied all reagent-grade compounds, which were employed without purification. The open glass capillary method was used to determine melting points, which were not adjusted. A Shimadzu FTIR Affinity-1 Fourier Transform Infrared spectrophotometer was used to record the IR spectra. Using tetramethylsilane (TMS) as the internal standard and $CDCl_3$ and DMSO as the solvent, NMR spectra were acquired on a BRUKER AVANCE 11 400 FT spectrometer (400 MHz for ^{1}H NMR, 100 MHz for ^{13}C NMR"). Using precoated sheets of silica gel G/UV-254 plates, TLC was used to monitor each reaction. FTIR, H NMR, and C NMR spectroscopy are used to characterize each product.

General procedure for reductive amination:

Aniline (10 mmol or 0.93 mL), benzaldehyde (10 mmol or 1.06 mL), and sodium borohydride (12 mmol or 0.4 g) were combined with malic acid (0.33 mmol) and rapidly agitated at room temperature for the required amount of time (Table 2 Sr. No. 1). TLC was used to track the reaction's development. Diethyl ether (10 mL) was used to extract the reaction mixture once the reactions were finished. To obtain a pure product, the organic layer was dried over anhydrous sodium sulphate and concentrated at lower pressure. Column chromatography techniques have been used to purify all of the chemicals. Without losing its catalytic activity, the catalyst was gathered and repurposed.

Conclusion:

To sum up, a very effective and chemoselective solvent-free technique for reductive amination of aldehydes is presented. Because of the moderate conditions, high yields, great chemoselectivity, and ease of product isolation and purification all of which meet the requirements for a green chemical practice the approach is both highly efficient and environmentally benign.

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Modern Approaches in Green Catalysis for Pharmaceutical Manufacturing

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Abstract

Green catalysis is revolutionizing chemical synthesis by replacing traditional, waste heavy stoichiometric processes with a holistic, "cradle-to-gate" sustainable model. By leveraging the convergence of Single-Atom Catalysts (SACs) for maximum atom economy, Biocatalysis through directed evolution, and Photocatalysis to harness visible light, the industry is significantly reducing energy consumption and environmental impact. This shift is further supported by the integration of Earth-abundant metals and green reaction media, such as supercritical fluids and aqueous systems, which eliminate the need for toxic volatile organic compounds (VOCs). Enhanced by modern tools like AI and computational chemistry, these advancements facilitate the transition toward circular chemistry, enabling the pharmaceutical, biomass, and fine chemical sectors to achieve high-efficiency, zero-waste production. Ultimately, these innovations address the critical challenges of catalyst stability and scalability, aligning modern chemical manufacturing with global sustainability goals.

Keywords: Biocatalysts, Green catalysis, Nano catalysts, Sustainable chemistry, N-heterocycles, metal-catalysis, Sustainable Pharmaceutical Synthesis, Eco-friendly Manufacturing, Waste Minimization, Atom Economy, Renewable Feedstocks, Supercritical Carbon Dioxide (CO_2), Ionic Liquids, Enzymatic Catalysis, Asymmetric Synthesis, Lipases, Iron-based Catalysts, Environmental Sustainability, Drug Manufacturing

1. Introduction

Sustainable catalysis serves as the technological engine driving the pharmaceutical and chemical industries toward a circular economy. By adhering

to the 12 Principles of Green Chemistry, researchers are replacing energy-intensive, waste-heavy traditional methods like the resource-depleting Haber-Bosch process with efficient alternatives. These modern strategies focus on maximizing atom economy and minimizing the E-factor by utilizing Earth-abundant materials, nano catalysts, and precision biocatalysis.

A critical application of these advances is the synthesis of Nitrogen-containing heterocycles (N-heterocycles). These structural components are essential to global health, appearing in approximately 59% of FDA-approved small-molecule drugs, including blockbusters like Lipitor and targeted therapies like Pemigatinib. Both saturated (piperidines, pyrrolidines) and unsaturated (indoles, quinazolines) frameworks are vital for treating conditions ranging from ADHD to cancer.

To produce these complex molecules sustainably, the industry is transitioning from hazardous classical reactions to "green" catalytic pathways. These include one-pot reactions, microwave irradiation, and the use of recyclable catalysts. Such innovations not only reduce toxic waste and energy consumption but also ensure that drug manufacturing aligns with 2026 climate strategies. While scalability remains a challenge, green catalysis is effectively establishing a safer, more efficient standard for drug discovery and environmental remediation.

2. Methodology

The methodology of this study is based on a systematic literature review of recent research on green catalytic methods for sustainable chemical and pharmaceutical synthesis. The authors analysed peer-reviewed journal articles, scientific reports, and experimental studies focusing on green catalysis and the synthesis of medicinally important N-heterocyclic compounds, with particular attention to research published in the last five years. Various catalytic strategies were examined, including homogeneous and heterogeneous catalysis, recyclable catalysts, nano catalysts, and transition-metal catalysts such as palladium, copper, nickel, and iron systems.

The review also evaluates sustainable reaction techniques such as microwave irradiation, one-pot reactions, and acceptor less coupling reactions. In addition, the study investigates the use of green solvents such as water, supercritical CO_2, bio-based solvents, and ionic liquids, along with biocatalytic methods using enzymes like lipases, oxidases, and dehydrogenases. All approaches were assessed according to green chemistry principles, including atom economy, waste reduction, energy efficiency, and reduced toxicity, to highlight environmentally friendly strategies for efficient pharmaceutical

synthesis.

3. Analysis of Green Synthesis:

The analysis demonstrates how green chemistry and green catalysis are transforming modern pharmaceutical and chemical synthesis by replacing traditional hazardous and energy-intensive processes with more sustainable alternatives. A major focus of the analysis is solvent efficiency and life-cycle impact. Conventional volatile organic solvents such as dichloromethane and acetonitrile contribute significantly to environmental pollution, toxicity, and waste generation. The study shows that replacing these solvents with greener alternatives including water, supercritical CO_2, and ionic liquids can significantly reduce environmental footprints. These solvents not only lower toxicity but also improve downstream processing by simplifying product separation and purification, thereby reducing energy consumption and waste production.

Another key aspect of the analysis is biocatalytic precision and selectivity. The paper highlights the role of enzymes such as lipases and oxidases in enabling highly selective chemical transformations. Biocatalysis operates under mild reaction conditions, typically at moderate temperatures and neutral pH, which minimizes energy requirements and prevents the formation of unwanted by-products. Because enzymes possess strong chemo selectivity and stereoselectivity, they are particularly valuable in asymmetric synthesis, a crucial step in producing chiral pharmaceutical compounds. As a result, biocatalytic processes often achieve higher atom economy, a concept introduced by Barry Trost, which emphasizes maximizing the incorporation of reactant atoms into the final product while minimizing waste.

The analysis also evaluates catalytic sustainability, particularly in the context of transition-metal catalysis. While metals such as palladium, copper, and nickel remain essential for forming carbon-carbon bonds in organic synthesis, the study identifies a growing shift toward more sustainable catalytic systems. Recyclable catalysts and catalysts based on earth abundant metals, such as iron, copper, and zinc, are increasingly being explored as alternatives to expensive and toxic noble metals. Iron-based catalysts are especially promising due to their low toxicity, high abundance, and cost-effectiveness, making them attractive for large scale industrial applications.

A significant portion of the analysis focuses on the structural importance of N-heterocyclic compounds, which are present in approximately 59% of FDA-approved small-molecule drugs. Because of their importance in pharmaceutical chemistry, the development of greener synthetic pathways for these compounds

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is a major research priority. The study highlights modern synthetic approaches such as one-pot reactions, microwave-assisted synthesis, and nano catalysis, which reduce reaction time, minimize intermediate purification steps, and improve overall yield and efficiency. These methods significantly lower the E-factor, which measures the ratio of waste generated to product formed.

Finally, the analysis provides a comparative evaluation of classical versus green synthetic methodologies. The findings suggest that modern green catalytic strategies outperform traditional methods by combining high synthetic performance with environmental responsibility. By integrating principles such as atom economy, waste reduction, energy efficiency, and safer chemical processes, green catalysis offers a sustainable pathway for producing complex pharmaceutical compounds-including anti-inflammatory drugs, antibiotics, and anticancer agents-while minimizing ecological impact and supporting global public health goals.

4. Conclusion

The study concludes that green catalysis and green chemistry are playing a transformative role in modern chemical and pharmaceutical synthesis by promoting environmentally responsible and sustainable manufacturing practices. By replacing conventional energy-intensive and waste-generating methods with catalytic systems based on biocatalysts, nano catalysts, and earth-abundant metal catalysts, the chemical industry can significantly reduce environmental impact while maintaining high reaction efficiency and selectivity. The adoption of green solvents such as water, supercritical CO_2, and ionic liquids further minimizes toxicity and simplifies purification processes.

Modern techniques including one-pot reactions, microwave-assisted synthesis, and recyclable catalysts enhance atom economy, reduce the E-factor, and lower energy consumption. These advancements are particularly important for the sustainable synthesis of N-heterocyclic compounds, which form the structural backbone of many pharmaceutical drugs.

Overall, integrating green chemistry principles with advanced catalytic technologies provides an effective pathway toward sustainable drug manufacturing, reduced chemical waste, and improved environmental protection. Although challenges such as catalyst stability, cost, and industrial scalability remain, continued research and technological innovation will further strengthen the role of green catalysis in achieving long-term sustainability in chemical and

pharmaceutical industries.

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A Sustainable Route Towards Organic Transformations Using Catalysts Derived from Natural Feedstock

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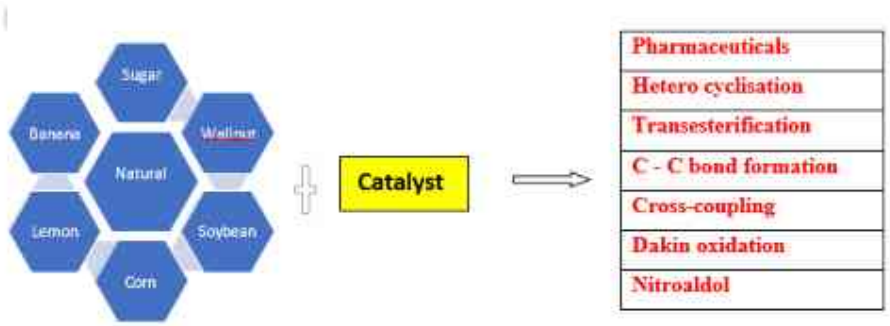
1. Introduction

Catalysts are the jewel in the crown of the chemical industry, accelerating reaction kinetics and augmenting the efficiency of desired reaction paths. Natural feedstock is a renewable resource capable of providing valuable functional products; in addition, it confers an opportunity to create catalysts [1]. As an alternative to stoichiometric reagents, and as a part of a sustainable approach, the implications of using natural feedstocks as a source of new catalysts has attracted considerable interest [1]. Natural feedstock-derived catalysts can promote chemical transformations more efficiently. Recent reports have highlighted the significant role of these biogenic, cost-effective, innocuous, biodegradable materials as catalysts in many biologically and pharmacologically important protocols [1]. This review outlines the decisive organic transformations for which feedstock-derived catalysts have been employed effectively and successfully, along with their economic and environmental benefits over traditional catalytic systems [1]. Sustainability has become a watchword and guiding principle for modern society, and with it a growing appreciation that anthropogenic 'waste', in all its manifold forms, can offer a valuable source of energy, construction materials, chemicals and high value functional products. In the context of chemical transformations, waste materials not only provide alternative renewable feedstocks, but also a resource from which to create catalysts serve to improve the overall energy and atom-efficiency of existing and novel chemical processes [2]. This review outlines key chemical transformations for which waste derived heterogeneous catalysts have been developed, spanning biomass conversion to environmental remediation, and their benefits and disadvantages relative to

conventional catalytic technologies [3]. Feedstock plays a vital role in sustainable petrochemical production. It is a renewable resource that can be used as a source of new catalysts, promoting chemical transformations more efficiently [4]. The use of natural feedstocks as catalysts offers economic and environmental benefits over traditional catalytic systems [5]. Additionally, feedstocks can be used in the production of biosurfactants, which are biodegradable and biocompatible, reducing the cost of waste treatment and providing an opportunity for profit [6].

Furthermore, the use of low-cost substrates as feedstocks for biosurfactant production can significantly reduce manufacturing costs and contribute to cleaner production [6]. Renewable feedstocks derived from biomass, waste oils, and fats can also be used as a source for fuels and chemicals, addressing environmental concerns and reducing greenhouse gas emissions [7]. Overall, feedstocks are essential for sustainable petrochemical production as they offer alternative and environmentally friendly solutions [8].



2. Study Background (Literature Review) and Significance of Study:

Most chemical processes require 80% of heterogeneous catalysts, 15% of homogeneous catalysts, and about 5% of bio- catalysts. To protect the environment and maintain standards of living, the demand for environmental catalysts has been increasing since about 1970. The industrial sector is always engaged in searching for innovative catalysts that will alleviate environmental pollution, reduce production costs, and be energy-efficient, free from catalytic poisoning, and reusable.

In general, the feedstock (commonly referred to as the raw material) is any naturally available, unprocessed, or minimally processed material that is the primary material used in manufacturing or processing to produce goods, high-value energy fuel, finished products, or intermediate materials that are then the feed- stock for future finished products. As feedstock materials are bottleneck assets and are highly relevant to the production of other products. Feedstock

materials include wood, rocks, ore, seawater, coal, stones, sand, as well as renewable bio- logical substances such as crops, cotton, woody plants, algae, raw biomass, petroleum, and natural gas. In the chemical industry, oil is a feedstock for a host of chemicals, including methane, propylene, and butane.

3. National Status

In the last few decades, significant progress has been made in the development of fuels, chemicals, and materials from naturally available renewable feedstock. Currently, plastics, foams, and thermosets from lignin and plant oils, electronic materials from chicken feathers, biodiesel from plant oils, and algae as well as many more useful products have been developed using natural feedstock. Most literature reviews demonstrating the utilization of plant-material-derived catalysts have focused on the production of biodiesel. The implication of such catalysts in the synthesis of fine chemicals, intermediates, pharmaceutical products, and many other chemicals has not been extensively studied. Plant material has enormous value, not only as a renewable resource in the production of value-added products but also as a catalyst in organic synthesis. In the recent literature, some synthetic methods incorporating the use of plant material-derived catalysts have been reported.

4. International Status

Huge tons of waste are generated daily worldwide from different sectors such as agriculture, the food industry, fruit, and the pulp industry, and from dead animal and plant material. Waste disposal is a universal issue and deposition of waste can be of great concern if not managed properly. Recently, considerable attention has been focused on the conversion of waste into useful products. In the context of organic transformations, waste materials provide not only alternative renewable feedstock but also a resource from which to create catalysts. Such waste-derived catalysts can improve the overall energy and atom efficiency of existing and novel chemical processes

The current demand from the industrial sector for environmentally friendly catalysts has led to catalytic substances developed from natural resources becoming an alternative to conventional catalytic systems. The investment of natural feedstock material for the development of productive catalysts or catalyst supports or solvents can considerably reduce the substantial waste disposal problem and mitigate possible environmental pollution. Another benefit of this raw material is that, due to its natural abundance, synthetic processes may become economically viable.

5. Research Methodology

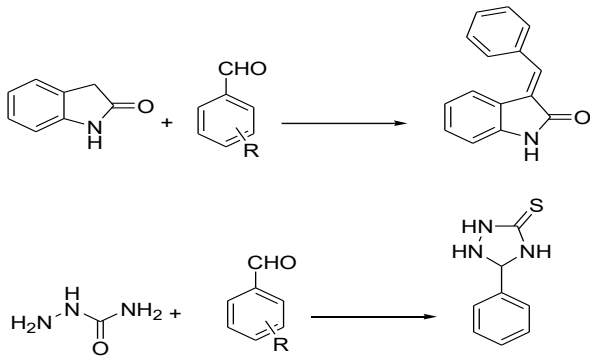
a) Synthesis of Catalyst

This catalyst is made from the shell of the natural feedstock like wall nut, banana, lemon, soybean etc. To make it, the first step is to make ash from shells of natural feedstock. A muffle furnace in the lab was used to produce ash. After hitting 500°C for five hours, the ash was formed. A 10% saturated solution i.e. 10 gm of ash sample dissolve in 100 ml of water was made from the resulting ash the filtrate of this prepared sample was used as a catalyst for the reaction. In modern era chemistry this catalyst is used as green catalyst. This catalyst is an example of ecofriendly catalyst.

b) Synthesis of Organic compound

The work up plant material will be used as catalyst in the synthesis of organic compound. In a further study, we will do characterization using various techniques like FTIR, NMR, Mass spectroscopy etc. and bio-evaluation of synthesized organic compound like anticancer, antifungal, antibacterial, antioxidant activity etc. is done.

Proposed Scheme:



6. Conclusion

The development of catalysts derived from natural feedstock represents a promising and sustainable route for advancing organic transformations. Utilizing renewable, biodegradable, and abundantly available resources such as plant extracts, biopolymers, agricultural waste, and naturally occurring minerals significantly reduces dependence on fossil-based and toxic catalytic systems. These bio-derived catalysts not only align with the principles of green chemistry but also contribute to minimizing environmental impact, energy consumption, and hazardous by-products. Natural feedstock–based catalysts often exhibit remarkable catalytic efficiency, selectivity, and reusability in various organic

reactions including oxidation, reduction, coupling, condensation, and multicomponent reactions. Their ease of preparation, cost-effectiveness, and potential for large- scale application further enhance their industrial relevance. Additionally, the integration of nanotechnology with biomass-derived materials has opened new avenues for designing high- surface-area, highly active, and stable catalytic systems.

Overall, sustainable catalyst development from natural resources provides an eco-friendly alternative to conventional synthetic catalysts, promoting cleaner production processes and supporting the global transition toward sustainable chemical manufacturing. Continued research focusing on improving catalytic performance, recyclability, mechanistic understanding, and scalability will further strengthen the role of natural feedstock–derived catalysts in modern organic synthesis.

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Exploring Advances in Chemical Sciences: A Comprehensive Guide to Modern Methods and Techniques

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Abstract

The field of chemical sciences is continuously evolving, driven by groundbreaking discoveries and innovative technologies that reshape how we understand and manipulate matter. From cutting-edge analytical techniques to sustainable synthesis methods, modern advancements are opening new frontiers in research, industry, and everyday applications. The field of chemical sciences has undergone remarkable transformations over the past few decades, Modern chemical sciences encompass a wide range of disciplines, from organic and inorganic chemistry to physical, analytical, and materials chemistry.

Keywords: Chemical Sciences, Traditional to Modern Methods, Analytical Techniques, Spectroscopy, Microscopy, Computational Chemistry, Molecular Modelling.

1. Introduction to Modern Chemical Sciences

The field of chemical sciences has undergone remarkable transformations over the past few decades, driven by groundbreaking research and innovative technologies. Modern chemical sciences encompass a wide range of disciplines, from organic and inorganic chemistry to physical, analytical, and materials chemistry. These advances have not only deepened our understanding of molecular structures and reactions but have also paved the way for practical applications that impact everyday life from developing new pharmaceuticals and sustainable energy solutions to creating advanced materials with unique properties [1]. In this comprehensive guide, we will explore the latest methods and techniques that are shaping the future of chemical research, highlighting how

modern tools such as spectroscopy, chromatography, computational chemistry, and nanotechnology are revolutionizing the way scientists approach complex chemical problems.

2. Historical Perspective: From Traditional to Modern Methods

The evolution of chemical sciences provides valuable insight into how modern methods and techniques have come to revolutionize the field. Historically, chemistry began as alchemya blend of mysticism, philosophy, and early experimentation aimed at transforming base metals into gold and discovering the elixir of life. While alchemy lacked scientific rigor, it laid the groundwork for systematic experimentation and observation.

These tools allow for detailed molecular insights, real-time reaction monitoring, and the design of novel materials with tailored properties. Additionally, green chemistry principles and automated synthesis methods exemplify the shift toward more sustainable and efficient practices [2]. By tracing this journey from traditional alchemical roots to contemporary innovations figure.1., we can appreciate the transformative impact of evolving methodologies. This historical perspective sets the stage for exploring the latest advances that continue to push the boundaries of chemical research and application [3].

3. Analytical Techniques in Contemporary Chemistry

In the rapidly evolving field of chemical sciences, analytical techniques play a pivotal role in advancing research, quality control, and industrial applications. Modern analytical methods allow chemists to identify, quantify, and characterize substances with unprecedented precision and accuracy. Techniques such as chromatography, spectroscopy, and mass spectrometry have become indispensable tools in laboratories worldwide.

Chromatography, including gas chromatography (GC) and high-performance liquid chromatography (HPLC), enables the separation of complex mixtures into individual components, facilitating detailed analysis. Spectroscopic methods, such as nuclear magnetic resonance (NMR) and infrared (IR) spectroscopy, provide insights into molecular structure and functional groups, while ultraviolet-visible (UV-Vis) spectroscopy is widely used to study electronic transitions in molecules. Mass spectrometry (MS) has revolutionized analytical chemistry by allowing the determination of molecular weights and structural information through fragmentation patterns. Coupled techniques like GC-MS and LC-MS combine separation and identification, offering powerful solutions for

analyzing intricate samples in pharmaceuticals, environmental monitoring, and forensic science [4].

4. Advances in Spectroscopy and Microscopy

Simultaneously, advancements in microscopy especially with the advent of techniques like atomic force microscopy (AFM), scanning tunneling microscopy (STM), and super-resolution fluorescence microscopy have enabled researchers to visualize surfaces and molecular arrangements with extraordinary precision. These cutting-edge tools provide three-dimensional imaging at the nanoscale, offering insights into molecular interactions, crystal structures, and dynamic processes in real time. Together, these innovations in spectroscopy and microscopy are not only expanding the frontiers of chemical research but also driving progress in related fields such as materials science, pharmaceuticals, and nanotechnology [5].

5. Breakthroughs in Synthetic Chemistry

chemistry has experienced remarkable advancements in recent years, transforming the way chemists design and construct complex molecules. Breakthroughs in this field are not only accelerating drug discovery and materials science but are also enabling more sustainable and efficient chemical processes.

One of the most significant developments is the rise of catalytic methods that allow for precise control over chemical reactions. Transition metal catalysis, for example, has been refined to facilitate the formation of carbon-carbon and carbon-heteroatom bonds with unprecedented selectivity and yield. This precision reduces waste and energy consumption, aligning synthetic chemistry with green chemistry principles. Additionally, the integration of automation and machine learning is revolutionizing synthetic route planning [6].

6. Role of Computational Chemistry and Molecular Modelling

In recent years, computational chemistry and molecular modelling have revolutionized the field of chemical sciences by providing powerful tools to predict, visualize, and analyse molecular structures and reactions with unprecedented accuracy. These techniques leverage advanced algorithms, high-performance computing, and quantum mechanical principles to simulate the behavior of molecules at the atomic level, enabling researchers to explore complex chemical phenomena without the need for time-consuming and costly laboratory experiments.

Computational chemistry encompasses a range of methods, including ab initio calculations, density functional theory (DFT), and molecular dynamics

simulations, each offering unique insights into molecular properties such as energy states, reaction pathways, and electronic distributions. Molecular modelling, on the other hand, allows scientists to construct three-dimensional representations of molecules and predict their interactions with other compounds, which is particularly valuable in drug design, materials science, and catalysis [7].

7. Emerging Techniques in Material Chemistry

Material chemistry is undergoing a transformative phase, driven by innovative techniques that are expanding the boundaries of what's possible in designing and manipulating materials at the molecular and atomic levels. Emerging methods such as advanced spectroscopy, high-throughput screening, and machine learning-assisted material design are revolutionizing how scientists discover and optimize new materials with tailored properties.

One of the most exciting developments is the integration of computational chemistry with experimental approaches [8-9]. By leveraging powerful algorithms and artificial intelligence, researchers can predict the behavior and characteristics of novel compounds before they are synthesized in the lab, significantly accelerating the development process. Techniques like automated synthesis platforms and in situ characterization tools enable real-time monitoring and rapid iteration, leading to more efficient and sustainable material development.

8. High-Throughput Screening and Automation in Chemistry

High-throughput screening (HTS) and automation have revolutionized the way chemical research is conducted, enabling scientists to accelerate the discovery and optimization of new compounds, materials, and reactions. Traditionally, chemical experimentation involved labor-intensive, manual processes that limited the number of tests researchers could perform within a given timeframe. With the advent of HTS technologies, it's now possible to rapidly evaluate thousands of chemical samples simultaneously using automated platforms.

HTS integrates robotics, data processing software, and sensitive detection methods to systematically test a vast array of chemical reactions or biological interactions under varied conditions. This approach not only speeds up the identification of promising candidates but also enhances the reproducibility and accuracy of experimental results. Automation minimizes human error and frees researchers to focus on data analysis and hypothesis-driven experimentation [10].

9. Conclusion:
The Impact of Advances on Industry and Society

The rapid advances in chemical sciences over recent decades have profoundly transformed both industry and society. Innovative methods and cutting-edge techniques have enabled the development of new materials, more efficient catalysts, and sustainable processes that were once thought impossible. Industries ranging from pharmaceuticals and energy to agriculture and manufacturing have benefited immensely, witnessing increased productivity, reduced environmental footprints, and enhanced product quality.

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Emerging Trends in Chemical Sciences

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Abstract

The chemical sciences have undergone tremendous change as a result of scientific innovation, which has made it possible to create highly accurate analytical methods, environmentally friendly procedures, and improved materials. Chemistry is essential for bridging the gap between basic science and technology. Chemical research and commercial development have advanced more quickly in recent years thanks to interdisciplinary approaches that integrate nanotechnology, computational chemistry, catalysis, and green chemistry. Global issues, including energy sustainability, environmental preservation, and better healthcare, have all benefited from these developments. Major developments in contemporary chemical sciences are covered in this chapter, including advanced analytical techniques, computational methodologies, sustainable chemistry practices, nanomaterials, and catalytic technologies. It also emphasises the increasing impact of data-driven research and artificial intelligence on chemical innovation. Future ideas on how developing technologies will continue to transform chemical research and its applications in society are presented in the chapter's conclusion.

Keywords: Chemical innovation, Green chemistry, Nanotechnology, Catalysis, Computational chemistry, Analytical techniques, Sustainable technology.

1. Introduction

The quick development of the chemical sciences has been fuelled by scientific and technological innovation. Because it links fields like physics, biology,

environmental science, and engineering, chemistry is frequently referred to as the central science[1]. The advancement of contemporary technology has greatly improved chemists' capacity to study material qualities, molecular structures, and reaction mechanisms[2,3].

The scope of chemical research has increased during the last few decades due to technological advancements in instruments, computational methodologies, and experimental approaches. In addition to comprehending chemical reactions, modern chemistry today focuses on creating environmentally friendly materials and procedures[4,5].

Chemical sciences now provide more opportunities for innovation thanks to the integration of cutting-edge technologies like biotechnology, nanotechnology, and artificial intelligence[6]. These advancements are making it possible for academics to tackle difficult global issues, including disease treatment, pollution control, energy scarcity, and climate change[7].

2. Innovations in Catalysis

2.1 Importance of Catalysis in Chemical Processes

In both industrial and laboratory chemical processes, catalysis is essential. Catalysts speed up chemical reactions without changing their chemical composition at the conclusion of the reaction. Catalytic reactions are thought to be involved in a significant amount of commercial chemical manufacturing.

Catalytic technologies are now crucial for increasing reaction efficiency, cutting down on energy use, and minimising waste production. Therefore, one of the key goals of chemical innovation continues to be the creation of sophisticated catalytic systems.

2.2 Homogeneous and Heterogeneous Catalysts

Homogeneous and heterogeneous catalysts are the two main types into which catalysts are often divided. Heterogeneous catalysts function in a distinct phase, frequently as solid materials interacting with liquid or gaseous reactants, whereas homogeneous catalysts reside in the same phase as the reactants, typically in solution.

Highly selective transition metal catalysts that are widely employed in organic synthesis and pharmaceutical manufacture have been developed as a result of recent research. Furthermore, the efficiency of industrial chemical processes has been greatly increased by heterogeneous catalysts based on metal oxides and supported metal nanoparticles.

2.3 Emerging Catalytic Technologies

New fields of catalytic research, such as photocatalysis and electrocatalysis, have emerged. Photocatalytic systems, which are used in solar fuel production and environmental cleaning, employ light energy to propel chemical reactions. Conversely, energy technologies like carbon dioxide reduction, fuel cells, and hydrogen production depend heavily on electrocatalysis.

3. Nanotechnology and Advanced Materials

3.1 Development of Nanomaterials

One of the most revolutionary developments in chemical research is nanotechnology. Materials with structural dimensions between one and one hundred nanometres are known as nanomaterials. Materials have distinct chemical and physical characteristics at this scale that set them apart from their bulk counterparts.

Carbon nanotubes, graphene, metal nanoparticles, and quantum dots are typical examples of nanomaterials. These substances have remarkable mechanical, electrical, and catalytic qualities.

3.2 Applications of Nanotechnology

Applications for nanomaterials can be found in many different sectors, including as environmental research, electronics, medicine, and energy storage. Nanoparticles are employed in biomedical research for targeted drug delivery systems, which improve the effectiveness of medication distribution to particular tissues or cells.

Nanomaterials are utilised in environmental applications to remove pollutants and purify water. Nanostructured materials are also being investigated for application in sophisticated electronic gadgets, solar cells, and high-performance batteries.

4. Green Chemistry and Sustainable Chemical Processes

4.1 Concept of Green Chemistry

Green chemistry is a contemporary method for creating chemical reactions that cause the least amount of damage to the environment. Its main objectives include lowering dangerous materials, preserving resources, and increasing energy efficiency.

The idea was created to solve environmental issues related to conventional chemical production methods. Researchers hope to develop safer and more sustainable chemical technologies by utilising the concepts of green chemistry.

4.2 Principles and Applications

Green chemistry promotes the use of energy-efficient processes, ecologically friendly solvents, and renewable raw materials. Catalytic reactions, solvent-free synthesis, and the utilisation of biodegradable materials are common components of sustainable chemical processes.

Green chemistry is used in industry to provide safer pharmaceutical manufacturing methods, ecologically friendly fuels, and biodegradable polymers. These developments support sustainable growth and lessen industrial pollution.

5. Advances in Computational Chemistry

5.1 Molecular Modelling and Simulation

In order to comprehend chemical processes at the molecular level, computational chemistry has become a crucial technique. Researchers can examine how molecules behave and forecast chemical reactions by utilising computer simulations and mathematical models.

Scientists can examine molecule geometry, electrical structures, and reaction pathways using molecular modelling tools. These computational methods eliminate the need for expensive and time-consuming experiments.

5.2 Artificial Intelligence in Chemical Research

Chemical research is increasingly using machine learning and artificial intelligence (AI) to examine complicated information and forecast chemical behaviour. AI-driven models can help with chemical reaction optimisation, material design, and the identification of possible medication candidates. These technologies are increasing the effectiveness of chemical research and quickening the speed of scientific discovery.

6. Innovations in Analytical Techniques

6.1 Modern Instrumental Methods

Chemists are now much better equipped to analyse chemicals with high precision and accuracy because of the development of sophisticated analytical tools. Molecular structures and chemical compositions can be identified at very low concentrations thanks to modern analytical techniques. Nuclear magnetic resonance spectroscopy (NMR), mass spectrometry (MS), gas chromatography (GC), and high-performance liquid chromatography (HPLC) are significant analytical techniques.

6.2 Applications of Analytical Innovations

Pharmaceutical research, environmental monitoring, food safety analysis, and forensic investigations all make extensive use of advanced analytical techniques.

With the use of these technologies, scientists may reliably assess chemical purity and find pollutants at trace levels.

7. Role of Chemical Innovation in Modern Technology

Chemical sciences play a major role in the advancement of technology across a range of industries. Chemistry advancements have made it possible to produce cutting-edge materials for application in medical equipment, electronics, and renewable energy systems.

For instance, high-capacity lithium-ion batteries, effective solar cells, and innovative medications have all been made possible by chemical research. Chemical technologies are also necessary for pollution control techniques and water purification systems. These advancements show how chemical innovation has a direct impact on both societal well-being and technical advancement.

8. Future Perspectives in Chemical Innovation

Technology integration and interdisciplinary cooperation will probably define the future of chemical sciences. Chemistry's significance in addressing global issues will continue to grow as new research fields like nanomedicine, smart materials, and sustainable energy technologies emerge.

Chemical discovery is anticipated to be significantly accelerated by automation, artificial intelligence, and sophisticated computational techniques. Environmentally friendly chemical manufacturing techniques will also receive more attention. These advancements will guarantee that chemistry continues to be a major force behind scientific and technological progress.

9. Conclusion

Chemical science advancement has been greatly aided by scientific and technological innovation. The capabilities of contemporary chemical research have been greatly increased by advancements in catalysis, nanotechnology, green chemistry, computational chemistry, and analytical methods.

Energy technology, healthcare, industrial production, and environmental protection have all benefited from these developments. The influence of chemical sciences in tackling global scientific and technological challenges will be further enhanced by sustained investment in research and multidisciplinary collaboration.

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Advances in Photochemistry, Spectroscopy and Catalytic Materials

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Abstract

Recent developments in photochemistry, spectroscopic techniques, and catalytic materials have significantly expanded the scope of chemical research. Photoredox catalysis, time-resolved spectroscopy, and advanced analytical techniques provide new insights into chemical mechanisms and enable innovative applications in energy conversion and sustainable chemistry. This paper reviews the progress in photochemistry, photocatalysis, spectroscopic methods, and modern catalytic materials used in energy and environmental applications.

Introduction

Photochemistry and advanced analytical techniques have become essential tools in modern chemical sciences [1 - 3]. Light-driven reactions enable unique chemical transformations that are difficult to achieve using traditional thermal methods [4-6]. At the same time, modern spectroscopic techniques allow scientists to observe short-lived intermediates and study reaction mechanisms in real time [7-9]. These developments have led to breakthroughs in solar energy conversion, artificial photosynthesis, and catalytic material design [10,11].

Photocatalysis and Photo-redox Chemistry

Photocatalysis involves the acceleration of chemical reactions through the absorption of light. Photo-redox catalysis uses light-activated catalysts to drive redox reactions.

Applications include:

- Organic synthesis
- Pharmaceutical production
- Environmental remediation

- Solar energy conversion

Photo-redox catalysis has enabled many previously difficult transformations in organic chemistry.

Multi-Photon Photo-redox Catalysis

In traditional photochemical reactions, a single photon drives the reaction. However, some reactions require more energy than one photon can provide.

Multi-photon processes combine the energy of two photons, allowing:

- Stronger redox reactions
- Activation of inert molecules
- More efficient chemical transformations

This approach has opened new opportunities in photochemical research.

Photochemical Hydrogen Production

It is considered a clean and sustainable energy carrier. Photochemical hydrogen production uses light energy to generate hydrogen from water or other sources.

Transition metal complexes such as iridium and nickel hydride catalysts have shown promising results in photochemical hydrogen evolution. These systems play an important role in developing renewable energy technologies.

Advances in Spectroscopic Techniques

Time-Resolved Spectroscopy

Time-resolved spectroscopy allows scientists to observe chemical reactions occurring in extremely short time scales. It helps identify:

- Reaction intermediates
- Excited-state dynamics
- Reaction pathways

Nuclear Magnetic Resonance (NMR) Spectroscopy

NMR spectroscopy is widely used to study molecular structures and reaction kinetics. It is particularly useful in studying metal hydride complexes and catalytic systems.

Electrochemical Methods

Electrochemical techniques such as cyclic voltammetry provide valuable information about electron transfer reactions and catalytic processes.

Catalytic Materials for Energy Applications

Electrocatalysts for Water Splitting

Water splitting produces hydrogen and oxygen using electrical energy. Efficient electrocatalysts are required for the oxygen evolution reaction (OER).

Materials such as cobalt-iron catalysts have shown high catalytic activity and stability.

CO_2 Conversion Catalysts

Layered Double Hydroxides (LDHs) are promising catalysts for converting carbon dioxide into useful chemicals and fuels. These materials can help reduce greenhouse gas emissions and promote sustainable chemical processes.

Artificial Photosynthesis

Artificial photosynthesis mimics natural photosynthesis to convert sunlight into chemical fuels. This technology integrates:

- Light-absorbing materials
- Catalysts for water oxidation
- Systems for hydrogen or fuel production

Artificial photosynthesis represents one of the most promising approaches for sustainable energy generation.

Conclusion

Photochemistry, spectroscopy, and advanced catalytic materials are transforming modern chemical sciences. Photoredox catalysis and artificial photosynthesis provide new pathways for energy conversion and chemical synthesis. Meanwhile, spectroscopic techniques allow detailed investigation of reaction mechanisms at the molecular level. Continued research in these fields will contribute significantly to sustainable chemistry, renewable energy, and environmental protection.

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Advances in Computational Chemistry and Catalysis

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Abstract

Computational chemistry has emerged as one of the most powerful tools in modern chemical sciences. The integration of theoretical models with experimental studies has enabled chemists to understand reaction mechanisms, predict catalytic behavior, and design efficient catalysts. This paper reviews the development of computational catalysis, highlighting the role of density functional theory (DFT), molecular dynamics simulations, and quantum mechanical approaches in studying catalytic systems. Special attention is given to transition metal catalysis, enzyme modeling, and machine learning potentials for large-scale simulations. These advances have significantly enhanced the ability of scientists to design catalysts for energy conversion, sustainable chemistry, and industrial applications.

Introduction

Chemical sciences have undergone significant transformations due to the development of theoretical and computational tools [1, 2]. Traditionally, chemical reactions were studied mainly through experimental observations [3]. However, the introduction of quantum mechanics and computer-based modeling has enabled researchers to study molecular structures, electronic properties, and reaction mechanisms at the atomic level [4]. Computational chemistry now plays an essential role in catalyst design, mechanistic analysis, and materials development [5,6]. This paper discusses the evolution of computational catalysis, its methodologies, and its applications in modern chemical research [7,8].

Development of Computational Catalysis

Computational catalysis has expanded rapidly over the past few decades Early theoretical models were limited due to insufficient computational power, but modern high-performance computing has enabled accurate simulations of

complex catalytic systems.

Computational catalysis combines quantum chemical calculations, kinetic modeling, and molecular simulations to understand catalytic mechanisms and optimize catalyst performance.

Density Functional Theory (DFT)

Density Functional Theory (DFT) is one of the most widely used computational methods in chemistry. It allows scientists to study electronic structures, reaction pathways, and energy profiles of chemical systems.

Advantages of DFT include:

- Good balance between accuracy and computational cost
- Ability to analyze reaction mechanisms
- Applicability to large molecular systems

DFT is particularly useful for studying transition metal catalysts, where complex electronic structures influence catalytic activity.

Computational Modelling of Transition Metal Catalysts

Transition metals play a central role in many catalytic processes due to their versatile oxidation states and coordination geometries. Computational modelling helps in understanding:

- Active catalytic sites
- Reaction intermediates
- Selectivity of catalytic reactions
- Energy barriers of catalytic cycles

However, modelling these systems can be challenging due to electron correlation and multiple spin states. Advanced quantum mechanical methods are often required for accurate predictions.

Computational Studies of Enzymatic Catalysis

Biological catalysts such as enzymes have inspired the development of highly efficient synthetic catalysts. Computational studies help researchers understand enzyme mechanisms at the molecular level.

One important example is [FeFe]-hydrogenase, an enzyme that catalyzes hydrogen production. Computational methods such as QM/MM (Quantum Mechanics/Molecular Mechanics) allow researchers to model large biological systems while maintaining accuracy near the active site.

First-Principles Molecular Dynamics

First-principles molecular dynamics (MD) simulations track the movement of atoms in real time based on quantum mechanical calculations.

Applications include:

- Studying catalytic reactions under realistic conditions
- Understanding temperature-dependent reaction mechanisms
- Investigating dynamic changes in catalytic active sites

Despite its advantages, MD simulations are computationally expensive and often limited to short time scales.

Machine Learning in Computational Chemistry

Machine learning methods are increasingly used to accelerate chemical simulations. Machine learning potentials can reproduce quantum-mechanical accuracy while enabling simulations over larger time and length scales.

These approaches are expected to play a major role in future catalyst design and reaction prediction.

Conclusion

Computational chemistry has revolutionised the study of catalytic systems. Techniques such as DFT, molecular dynamics simulations, and hybrid quantum methods allow scientists to understand complex reaction mechanisms with unprecedented detail. The integration of machine learning with computational chemistry promises even greater advancements in catalyst design, sustainable energy research, and industrial chemistry. As computational power continues to increase, computational catalysis will become an even more essential component of chemical research.

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Biological Importance of Quinoxaline Derivatives: A Critical Review

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Abstract

Quinoxaline derivatives are an important group of nitrogen-containing compounds that have been widely studied in medicinal chemistry for their range of biological activities. The quinoxaline structure, made up of a benzene ring joined to a pyrazine ring, allows these compounds to interact with many biological targets. Many quinoxaline derivatives have shown strong pharmacological effects, such as antibacterial, antifungal, antiviral, anticancer, anti-inflammatory, and antioxidant activities. Notably, quinoxaline-based compounds have shown promise as antimicrobial and anticancer agents by working through enzyme inhibition, DNA interaction, and changes in cell signaling. Because of their wide range of biological effects and flexible structure, quinoxaline derivatives remain a focus in the search for new therapeutic agents.

1. Introduction

Nitrogen-containing heterocycles are a key group of structures in modern medicinal chemistry. Among them, quinoxaline is a bicyclic aromatic system formed by joining a benzene ring with a pyrazine ring, and it has become an important scaffold with a wide range of pharmacological uses.1 Its flat structure, electron-deficient nature, and two nitrogen atoms allow quinoxaline derivatives to take part in different interactions, such as hydrogen bonding, pi-pi stacking, dipole interactions, and metal coordination. These features help explain their broad range of biological activities.

For many years, quinoxaline-based compounds have received a lot of attention because they are found in natural products, medicines, agrochemicals, and other useful materials.2 By changing the structure at different points on the quinoxaline core, researchers have created compounds with strong antibacterial,

antifungal, antiviral, antitubercular, anticancer, anti-inflammatory, antioxidant, antiparasitic, and central nervous system (CNS) effects.3 In particular, quinoxaline 1,4-di-N-oxide derivatives have shown unique properties that target low-oxygen environments, which adds to their potential as treatments.4 This review looks at the biological importance of quinoxaline derivatives, focusing on how their structure relates to their activity, how they work, and their possible uses.4

2. Antibacterial Activity

Quinoxaline derivatives exhibit potent antibacterial activity against both Gram-positive and Gram-negative bacteria. Early investigations revealed that quinoxaline 1,4-di-N-oxides act as bioreductive agents, generating reactive intermediates under anaerobic conditions that damage bacterial DNA and essential biomolecules.5

Mechanisms of antibacterial action include:

- DNA strand breakage
- Inhibition of DNA gyrase and topoisomerases
- Generation of reactive oxygen species (ROS)

3. Disruption of bacterial redox balance

Electron-withdrawing substituents at the C-2 position generally enhance adding an electron-withdrawing group at the C-2 position usually increases antibacterial strength. Some derivatives have worked against resistant bacteria like Staphylococcus aureus and Escherichia coli, showing their promise as future antimicrobial agents species remain a global health concern, particularly in immune compromised patients. Substituted quinoxalines have demonstrated promising antifungal properties, attributed to membrane destabilization and interference with ergosterol biosynthesis.6

Lipophilic derivatives display improved penetration into fungal cell membranes, resulting in enhanced antifungal efficacy. Some compounds exhibit comparable activity to standard antifungal drugs, suggesting their potential as alternative therapeutic agents.

4. Antitubercular Activity

Tuberculosis (TB), caused by Mycobacterium tuberculosis, remains a serious treatment challenge because of multidrug resistance. Quinoxaline derivatives, especially quinoxaline 1,4-di-N-oxides, have shown strong activity against TB.7

Proposed mechanisms include:

- DNA gyrase inhibition

- Interference with mycobacterial respiration
- Bioreductive activation under hypoxic conditions

These compounds are toxic mainly to mycobacteria, which makes them good candidates for developing new TB drugs.

5. Antiviral Activity

Several quinoxaline derivatives exhibit antiviral activity against HIV, herpes simplex virus, and influenza viruses. Their antiviral effects are often associated with inhibition of viral enzymes such as reverse transcriptase or protease.8 Certain quinoxaline analogues function as non-nucleoside reverse transcriptase inhibitors (NNRTIs), blocking viral replication by preventing DNA synthesis from viral RNA templates. Structural optimization has improved potency and reduced cytotoxicity.

6. Anticancer Activity

One of the most studied features of quinoxaline derivatives is their potential to fight cancer. Their flat aromatic structure helps them insert into DNA, which blocks replication and transcription in fast-growing cancer cells.9

Mechanisms include:

- Topoisomerase inhibition
- Induction of apoptosis
- Cell cycle arrest
- Kinase inhibition
- Hypoxia-selective cytotoxicity (quinoxaline 1,4-di-N-oxides)

Activation in low-oxygen conditions is especially important because tumors often have areas with little oxygen. Bioreductive activation creates toxic radicals mainly in these low-oxygen tumor cells, which increases selectivity and lowers side effects.10

7. Anti-inflammatory Activity

Chronic inflammation is a factor in many diseases, like arthritis and heart disease.11 Quinoxaline derivatives have shown anti-inflammatory effects by lowering levels of cytokines such as TNF-α and IL-6. Some compounds also block cyclooxygenase (COX) enzymes, which reduces prostaglandin production. Studies show that where substitutions are made on the molecule affects how well they target COX and how strong their anti-inflammatory effects are.12

8. Antioxidant Activity

Oxidative stress plays a role in aging and diseases that cause degeneration. Quinoxaline derivatives with hydroxyl or methoxy groups are good at neutralizing free radicals.13

Their antioxidant action involves:

- Neutralization of ROS
- Chelation of transition metal ions
- Prevention of lipid peroxidation
- These abilities make them more useful for treating disorders related to oxidative stress.

9. Central Nervous System (CNS) Activity

Researchers have studied quinoxaline derivatives for different uses in the central nervous system (CNS).14 Some derivatives can prevent seizures caused by chemicals, possibly by affecting GABA or glutamate pathways. Others may act as antidepressants or anti-anxiety agents by changing levels of monoamine neurotransmitters, which could help treat mood disorders.15 By reducing excitotoxicity and oxidative stress, quinoxaline derivatives might help treat neurodegenerative diseases.16

10. Conclusion

Quinoxaline derivatives are a very versatile group of compounds with many biological activities. Their flexible structure and ability to interact in different ways make them valuable in drug discovery. These compounds show promise as antimicrobial, anticancer, CNS, and metabolic agents. Continued research is likely to produce new quinoxaline-based drugs that are more effective, safer, and better suited for clinical use.

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Itaconic Acid is Used as A Green Catalyst in A One-Pot Technique for the Solvent-Free Acylation of Amines

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Abstract

Nanocatalysis is used as a green approach in organic biosynthesis. In the last few years, these have been widely used in the manufacturing industry. In equivalence to heterogeneous catalysts, homogeneous catalysts are not efficient due to their byproducts, hard work up and not recovered. Heterogeneous catalysts are used in organic reactions using metal oxides, clay particles, zeolites and heteropolymer acid, which reduces the generation of hazardous material. Green catalysts are required for organic products and their synthesis. Green methodology is developed for the synthesis of organic compounds using safer chemicals and solvents.

Keywards: Amines, Itaconic acid, Acetic anhydride, solvent-free condition.

1. Introduction

The green chemistry viewpoint states that in order to create a cleaner process, pollution can be managed by lowering and eliminating dangerous substances from the reaction mixture. The synthetic method for sustainable organic transformations uses a variety of solvents, including water, glycerol, polyethylene glycol, and waste biodiesel.

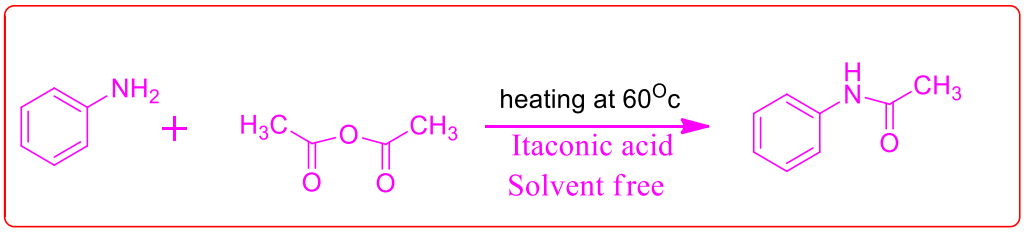
A sustainable and eco-friendly approach is necessary for an organic transformation to be successful inside the atom economy. These many techniques have been applied without a homogenous catalyst or solvent to produce the less stable. Another crucial component that is connected to lower effluent loads and cheaper costs is the recycling process of the catalysts without significant loss of catalytic activity or productivity, which eventually results in greener reactions with the right yield and production. Consequently, the researcher creates novel

chemicals using reusable, eco-friendly nanoparticles that are more effective catalysts. In recent years, magnetite nanoparticles have been a significant area of study in chemical and medicinal research to enhance peptide synthesis during coupling processes. Previous research has shown the acylation of alcohol and phenols utilising acetic anhydride or acetyl chloride in the presence of various functionalised nanoparticles, acid and base catalysts, and varied reaction conditions. Each of the aforementioned catalysed processes has some disadvantages, like a harsh solvent, a longer reaction rate, challenging handling, etc. because an environmentally friendly catalyst is used to carry out the extremely effective reaction in a solvent-free environment.

We create a new, eco-friendly way for the solvent-free acylation procedure (Scheme 1). Itaconic acid is a catalyst that is recyclable, inexpensive, efficient, sustainable, and less dangerous. We looked at the best-performing electron-donating and electron-withdrawing substrates for a number of heterocyclic, aromatic, acyclic, aliphatic, and cyclic amines. Amine (10 mmol), acetic anhydride (10 mmol), and itaconic acid (0.33 g) were added to the process and heated to 60^{O}C without the use of a solvent.

2. Results and discussion

Our studies begin with a model reaction between 10 mmol of acetic anhydride and 10 mmol of aniline, heated at 60 degrees Celsius without the use of a solvent and catalysed by 0.33 mmol of itaconic acid (Scheme 1). In 20 minutes at 60^{O}C, the acylation procedure using aniline substrate yields a 98% yield. In order to comprehend how malic acid affects the acylation reaction, we examined in an acetic anhydride and aniline process heated at 60^{O}C with



Scheme 1: Acylation of amines catalysed by itaconic acid

Table 1: Catalytic investigation for amine acylation

Sr. No.	Catalyst (mmol)	Time (min)	Yield (%)
1	0.04	60	22
2	0.08	60	40
3	0.12	60	45

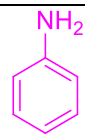
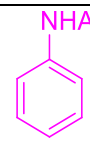
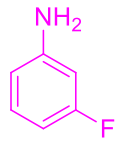
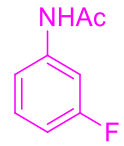
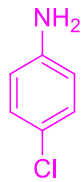
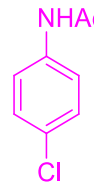
4	**0.16**	**60**	**62**
5	**0.20**	**60**	**75**
6	**0.28**	**23**	**97**
7	**0.33**	**20**	**96**

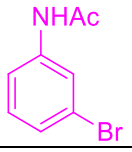
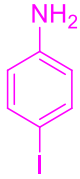
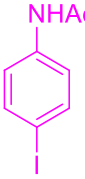
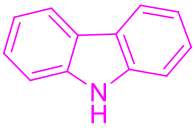
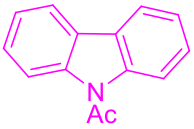
Without the use of a solvent. We discovered that after six hours, the yield increases by 12%, while the resulting productivity only increases by 16% after ten hours. At room temperature and without any metals or solvents, the reaction was unsuccessful. When itaconic acid is present during the process, a greater yield is seen.

After one hour of reaction time, 0.05 mg of malic acid catalyst was added in 20% to carry out the reaction (Table 1, Sr. No. 1). The catalyst concentration then increases from 0.10 to 0.25 mg as the yield increases (Table 1, Sr. No. 2–5). A yield of almost 97% was obtained using 0.28 mg of the catalyst (Table 1, Sr. No. 6). Finally, there is no discernible difference in the reaction when the catalyst quantity is increased by 0.33 mg once again (Table 1, Sr. No. 7).

Results are compared and displayed in Table 2 to better understand the efficacy of our method in solvent-free circumstances and various acylation solvents, such as methanol, water, ethanol, DCM, chloroform, tetrahydrofuran, dimethyl formamide, and 1, 4-dioxane. The results showed that both the current methodology and the eco-friendly approach had advantages in terms of synthesis technique, reaction speed, and reaction rates.

Table 2 Different substrate study in acylation reaction

Sr. No.	Amines	Products	Time(min)	Yield (%)
1			19	97
2			18	96
3			20	98

4			18	93
5			21	95
6			20	96

3. Experimental Section:

Materials and methods

Aldrich and Alfa Aesar supplied all of the reagent-grade compounds, which were employed without purification. The open glass capillary method was used to determine melting points, which were not adjusted. A Shimadzu FTIR Affinity-1 Fourier Transform Infrared spectrophotometer was used to record the IR spectra. Using tetramethylsilane (TMS) as the internal standard and CDCl and DMSO-d as the solvent, NMR spectra were acquired on a BRUKER AVANCE 11 400 FT spectrometer (400 MHz for "H NMR, 100 MHz for "C NMR"). Using precoated sheets of silica gel G/UV-254 plates, TLC was used to monitor each reaction. All of the products are known compounds that were identified structurally using FTIR and "H NMR and "C NMR spectroscopy," as well as by comparing their melting points to values found in the literature.

General Procedure for Acylation Reaction

Aniline (10 mmol or 0.93 mL), acetic anhydride (10 mmol or 1.06 mL), and itaconic acid (0.33 mmol) were combined and heated strongly at 60°C for the proper amount of time (Table 2 Sr. No. 1). TLC was used to track the reaction's development. Diethyl ether (10 mL) was used to extract the reaction mixture once the reactions were finished. To obtain a pure product, the organic layer was dried over anhydrous sodium sulphate and concentrated at lower pressure. Column chromatography techniques have been used to purify all of the chemicals. Without losing its catalytic activity, the catalyst was gathered and repurposed.

4. Conclusion

Finally, a very effective and chemoselective solvent-free acylation technique for amines is described. Because of the moderate conditions, high yields, great chemoselectivity, and ease of product isolation and purification all of which meet the requirements for a green chemical practice the approach is both highly efficient and environmentally benign.

Acknowledgements

We are thankful to Department of Chemistry and college for constant support.

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Synthesis and Biological Activities of Chalcones: Review

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Abstract

Chalcones are a family of organic compounds whose fundamental and versatile chemical structure is formed by joining two aromatic rings with a three-carbon (α, β-unsaturated carbonyl system). These compounds have attracted a lot of attention due to their diverse range of biological effects and potential applications in various disciplines, including medicine. Chalcones can be altered to produce a range of derivatives with distinctive properties due to their special structure. Chalcones exhibit a range of biological effects, including as antioxidant, antibacterial, anti-inflammatory, anti-cancer, and antidiabetic qualities.

Keywords: Chalcone, Biological Activity, Anti-inflammatory Activity, Anti-Cancer Activity, Antifungal, Antibacterial Activity.

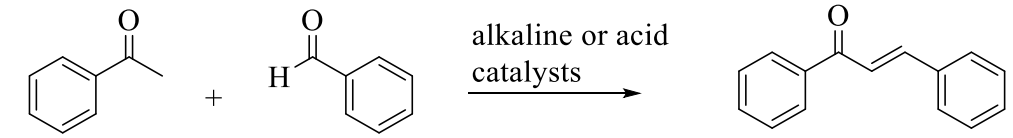
Introduction

Medicinal chemistry is the only academic field that directly affects people's growth, well-being, and health. Medicinal chemistry functions at the nexus of synthetic organic chemistry and biology, with a primary focus on medication development. Heterocyclic chemistry is one of the most prevalent and important subfields in organic chemistry. It has been a vast area of research for over a century. In recent years, organic chemistry has paid more attention to the synthesis and biological development of bioactive compounds. [1,2]

Chalcones have a conjugated double bond and a fully delocalized π electron system on the phenyl ring [3-8]. Molecules with such a structure have a comparatively low redox potential and are more likely to experience an electron

transfer reaction.Chalcones are sometimes referred to as beta-phenyl-alpha-benzoyl-ethylene or benzalacetophenone. 1, 2 Chalcones and their natural or synthetic derivatives (by changing the structure of the chalcone rings) are known to have a range of pharmacological effects, such as anti-inflammatory [9], anti-oxidant [10], antitumor [11], anti-tubercular [12], anti-viral [13], anti-malarial [14], anti-fungal [15], and antibacterial activities.[16] Due to their effects on a variety of targets, a number of natural, synthetic, and semi-synthetic chalcones have demonstrated strong therapeutic bioactivity.[17]

Scheme 1. Claisen−Schmidt Condensation: Synthesis of Chalcone from Acetophenone Derivatives. Benzaldehyde and acetophenone derivatives are treated at 50–100° with an acid catalyst or in an alkaline environment.Chalcone 10 was caused by the presence of a liquid solvent.



acetophenone benzaldehyde chalcone

Scheme 2. Construction of Chalcone Derivative, **Synthesis of Chalcone from Phenyl Halide:** Chalcone is made from phenyl halide. Phenyl halide and styrene reacted with carbon monoxide and a Pd catalyst to produce chalcone.

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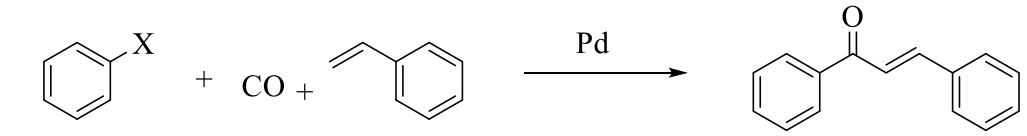
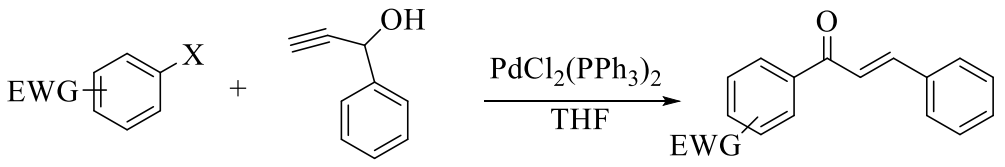


phenyl halide carbon monixide styrene chalcone

Scheme 4. Synthesis of Chalcone (I): Using PdCl2(pph3)2 in THF, propargyl alcohol and phenyl halide were reacted using microwave irradiation to create the chalcone derivative (1).



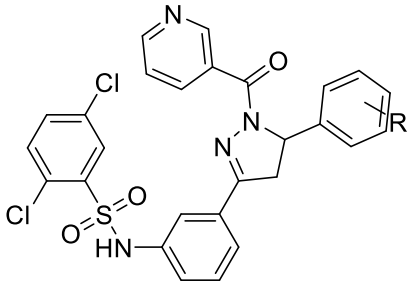
Phenyl Halide Propagyl alcohol chalcone

(I)

Biological Activity

1) Antibacterial and Anti-inflammatory:

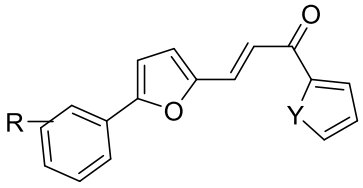
The antibacterial and anti-inflammatory properties of newly synthesized chalcone derivatives were evaluated in vitro against gram-positive Bacillus pumilis and Bacillus subtilis as well as gram-negative Escherichia coli and Proteus vulgaris. The reference medication used for the antibacterial assessment was chloramphenicol. Interestingly, several compounds showed weak inhibitory action against P. vulgaris but strong inhibitory effects against B. pumilis, B. subtilis, and E. coli. Compounds 1a and 1b, two of the produced compounds, showed exceptional antibacterial activity against the tested bacterial species.



Compound 1a R= Pyridin-3-yl
Compound 1b R= 3,4,5-trimethoxy

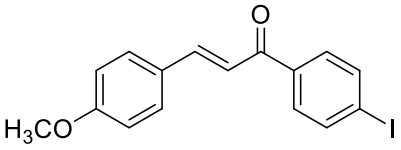
Compound 1

The in vitro antibacterial activity of a novel sequence of synthetic chalcone derivatives was evaluated. Escherichia coli and Klebsiella spp. (gram-negative bacteria) and Staphylococcus aureus and Enterococcus faecalis (gram-positive bacteria) were used to test the synthetic compounds' antibacterial efficacy. The antibacterial activity was assessed using the well diffusion method.



X= 4-Cl, Y = O

Compound 2

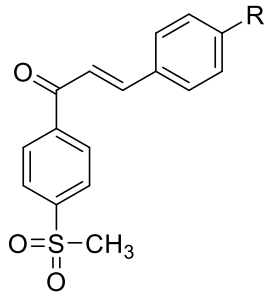


Compound 3

2) Analgesic and Anti-Inflammatory Activity:

The in vitro analgesic and anti-inflammatory properties of a novel sequence of synthetic chalcone derivatives were evaluated. The standard was 10 mg/kg b.w.IP of indomethacin. The anti-inflammatory properties of sulfur-based chalcones

with different substitution groups at the para position of the benzene ring were evaluated. Compound 4 shown strong anti-inflammatory efficacy among the produced compounds.

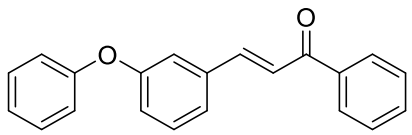


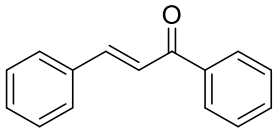
Where: R= H, 2-F,4-F, 4-Br,4-CH_3, 4-OCH_3, 2-Cl, 4Cl, 2,4Cl

Compound 4

3) Antimicrobial and Antioxidant:

The antibacterial and antioxidant properties of a novel sequence of synthetic chalcone derivatives were evaluated in vitro. Gram-positive bacteria like Staphylococcus aureus and Bacillus subtilis, gram-negative bacteria like Pseudomonas aeruginosa, Salmonella typhi, and Escherichia coli, and fungi like Candida albicans and Aspergillus niger were among the microorganisms against which the synthesized compounds' antimicrobial efficacy was examined. Since Ofloxacin, Ciprofloxacin, and Fluconazole were used as reference standards for antibacterial and antifungal comparisons. Compound 5a had significant antibacterial activity, particularly against Pseudomonas aeruginosa, among the produced compounds. Compound 5b also showed impressive antioxidant activity. The typical reference medication for evaluating antioxidant capacity was ethylenediaminetetraacetic acid (EDTA).[34–37].



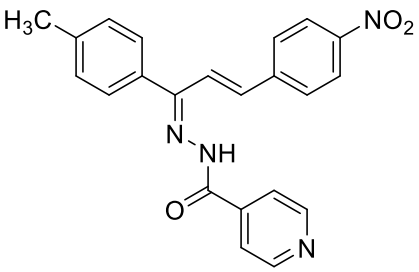


Compound 5a **Compound 5b**

4) Antifungal:

The anti-inflammatory properties of a novel series of synthetic chalcone derivatives were evaluated. The solvent used to prepare the test compounds was dimethyl sulfoxide (DMSO). Indomethacin was used as the standard medication in order to create a reference point. Interestingly, the measured inhibition

percentage increased to 53.23% after two hours. These chalcone hydrazide compounds showed substantial anti-inflammatory effects. The chemical known as compound 6,



Compound 6

Candida albicans, Escherichia coli, Pseudomonas aeruginosa, and Staphylococcus aureus were among the test organisms used to evaluate the in vitro antifungal efficacy of a novel sequence of produced chalcone derivatives. Inhibition zone diameters were measured in millimeters and compared to control standards. A modified Kirby-Bauer diffusion technique was used to test for antibiotic susceptibility. Using a saline suspension of each strain, Mueller-Hinton agar plates were swabbed.

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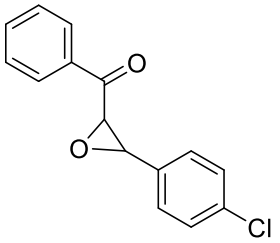

Compound 7

Conclusion

Chalcones are noteworthy for their versatile synthetic methods and a broad spectrum of biological functions within the realm of medicine. Numerous biological effects, including anticancer, anthelmintic, antitubercular, antimicrobial, antibacterial, antidiabetic, antioxidant, anti-inflammatory, and antifungal qualities, are exhibited by chalcone derivatives. Because of their intrinsic variety of activities, chalcone derivatives have attracted a lot of interest as a promising area for research in the hunt for new lead compounds.

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Synthesis and Characterization of Some Chromone Derivatives by Non-Conventional Approach

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Abstract

By cyclizing the oxidative reaction of alpha beta unsaturated carbonyl compounds or chalcones (3o-t) with iodine crystals, the new synthetic chromone derivatives (4o-t) series were produced using an unconventional approach that produced an excellent yield in dimethyl sulfoxide. IR, mass, and 1HNMR spectroscopy were used to validate these synthetic compounds.

Keywords: o-hydroxy acetophenones, derivatives of chalcones and chromones, fluorinated aromatic aldehyde,

Introduction

In the fields of medicine, biochemistry, and chemistry, fluorine atoms are crucial. According to a review of the literature, fluorine is the second most hetero element in life science-oriented study, behind nitrogen. Additionally, the literature review revealed that roughly 30% of newly registered agrochemicals and over 20% of newly available medicinal medicines contain atom1. Fluorinated heterocycles have been linked to anticancer2, antibacterial3, anti-inflammatory, and psychopharmaceutical4 properties. They also function as highly selective inhibitors of amineric neurotransmitter5 production.

There are many fascinating biological activities associated with chromones and other similar ring structures. According to a review of the literature, chromone compounds are used in medicine because they have a variety of physiological and biological characteristics.

In recent decades, chromone compounds have attracted a lot of attention. Carbonic anhydrase is inhibited by a number of sulfonamide6 isolated

chromones, which also show in vitro antibacterial7 and antifungal8 action. Derivatives of 2 and 4 chromones have antioxidant9 and antibacterial properties.

Chalcones are a significant class of natural products, and some of them have been shown to have a variety of biological properties, including antibacterial, antitumor, anticancer, antimalarial, and antitubercular properties. Chalcones13 have a wide range of actions, including anti-inflammatory14, insecticidal15, antiviral16, antimicrobial17, and more, according to a review of the literature.

Chalcones are both synthetic and naturally occurring substances that can be found in a variety of plants. Because they serve as precursors in the synthesis of numerous heterocyclic compounds18, these molecules are of tremendous interest. The primary intermediates in the synthesis of natural products are α-β-unsaturated carbonyl molecules, or chalcones.

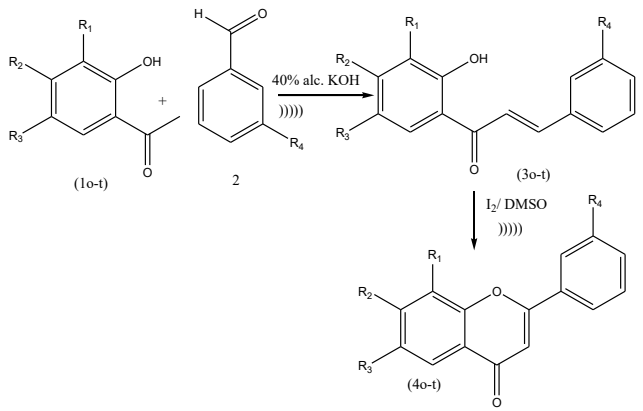
Results and Discussion

Scheme I illustrates the preparation of 2-(3-fluorophenyl)-8-methy-4H-chromen-4-one. The Claisen-Schmidt condensation of different aromatic substituted ortho hydroxyl acetophenones with substituted aromatic aldehydes in the presence of ethanol and potassium hydroxide was used to create the starting molecules (E)-3-(3-fluorophenyl)-1-(2-hydroxy-5-methylphenyl) prop-2-en-1-one.

1HNMR, IR, and mass spectrometry were used to characterise the chalcones derivatives (3o-t). Important distinguishing feature peaks in the 1H NMR spectra of chalcone 3p indicate the existence of olefinic proton αH dd at 5.85 δ, J = 14.98 Hz, and βH dd at 6.40 δ, J ∼ 14.98 Hz trans geometry.

Additionally, the chromones displayed the significant 1HNMR distinctive feature peaks of olefin αH at 5.55 δ.

Scheme-I



Experimental Section

The melting points of the synthetic compounds were measured in liquid paraffin capillaries and are not adjusted. Thin layer chromatography was used to track the reaction's conclusion. A Perkin Elmer Spectrum Version 10.4.2 FTIR Spectrophotometer was used to record the infrared spectra.Using CDCl3 as a solvent and TMS as an internal standard, 1HNMR spectra were captured on a Bruker Avance-II 400 MHz NMR spectrophotometer. The peak values were displayed in δ (ppm). A Waters, Q-TOF Micromass (LC-MS) mass spectrometer was used to record the mass spectra.

Synthesis of (E)-3-(3-fluorophenyl)-1-(2-hydroxy-5-methylphenyl) prop-2-en-1-one (3q) 3-fluorocarbaldehyde 1 (0.05 mol) and substituted 2-hydroxy acetophenone 2 (0.05 mol) were dissolved in 20 millilitres of ethyl alcohol in a 100 millilitre beaker. Twelve millilitres of 50% potassium hydroxide were added to this reaction mixture. For a few minutes, the material was sonicated. Concentrated hydrochloric acid was used to neutralise the reaction mixture after it was placed on crushed ice. To obtain pure compound 3o, the resulting product was filtered, dried, and crystallised from an appropriate solvent. Table 1 provides a summary of the compounds that were created using the above method.

3o: IR (cm-1): 3354 (O-H), 1692 (Conj. C=O), 1617, (C=C), 1400 (C-F).

1H NMR (δ): 11.15 (s, O-H), 7.17 to 8.20 (7 H Ar-H), 6.97 (dd, 1H, 16.12Hz), 5. 4 (dd, 1H, 15.2Hz), 2.36 (s, Ar-CH3).

MS :(m/z): 250 (M+1).

3q: IR (cm-1): 3173 (O-H), 1647 (Conj. C=O), 1580 (C=C), 785(C-F).

1H NMR (δ): 13.25 (s, O-H), 7.17 to 7.96 (8H Ar-H and –CH=CH-).

MS :(m/z): 304 (M+1).

Synthesis of 2-(3-fluorophenyl-8-methyl-4H-chromen-4-one(4o-t)

Chalcone (0.005 mol) was dissolved in 12–15 millilitres of DMSO. A catalytic quantity of iodine (about two crystals) was added to this reaction mixture. The reaction mixture was sonicated for half an hour. To complete the reaction, thin layer chromatography is utilised. One to three grams of sodium thiosulphate were added to the content, which was then poured over crushed ice. To obtain a pure compound of chromone derivatives, the products were filtered, cleaned with cold water, dried under an infrared lamp, and refined by recrystallisation from an appropriate solvent.

4q: IR (cm-1): 1692 conj. (C=O), 1617 (C=C), 1112 (C-O).

1HNMR (400 MHz, CDCl3, δ): 7.17-8.20 (m, 7H aromatic), 5.40 (s, 1H, chromone), 2.36 (s, Ar-CH3).

MS: (M+1) : 248.

Table-1: The physical constants of prepared compounds (3o-t) and (4o-t)

Compound	R_1	R_2	R_3	R_4	M.P. (^{0}C)	Yield (%)
3o	H	H	Br	F	152	70
3p	Cl	H	Cl	F	188	72
3q	H	H	CH_3	F	165	60
3r	H	H	Cl	F	176	73
3s	H	CH_3	Cl	F	230	74
3t	H	H	H	F	110	69
4o	H	H	Br	F	138	68
4p	Cl	H	Cl	F	165	64
4q	H	H	CH_3	F	168	79
4r	H	H	Cl	F	177	73
4s	H	CH_3	Cl	F	156	67
4t	H	H	H	F	144	77

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Design, Synthesis and Biological Applications of Nitrogen-Containing Heterocyclic Compounds: Recent Advances and Future Perspectives

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Abstract

Heterocyclic compounds constitute one of the most significant classes of organic molecules due to their structural diversity and broad spectrum of biological activities. The incorporation of heteroatoms such as nitrogen, oxygen, and sulfur into cyclic frameworks profoundly influences physicochemical properties, reactivity, and pharmacological behaviour. Nitrogen-containing heterocycles, in particular, are privileged scaffolds in medicinal chemistry and form the core structure of numerous clinically approved drugs. This chapter presents a comprehensive overview of the design, classification, synthetic methodologies, and biological applications of heterocyclic compounds, with emphasis on nitrogen-containing systems such as triazoles, thiazoles, imidazoles, tetrazoles, and benzothiazoles. Classical synthetic approaches, cyclization strategies, transition-metal-catalysed methods, multicomponent reactions, and green synthetic protocols are discussed in detail. The biological potential of heterocycles including anticancer, antimicrobial, anti-inflammatory, and antioxidant activities is critically analysed with structure–activity relationship (SAR) insights. Recent developments from the past decade are summarized to highlight emerging trends in heterocyclic chemistry. Finally, future perspectives including computational drug design, hybrid molecule development, and

sustainable synthesis are addressed. The chapter aims to provide researchers and academicians with a consolidated understanding of modern heterocyclic chemistry and its expanding role in drug discovery and industrial application.

Keywords: Heterocyclic compounds; Nitrogen heterocycles; Triazole; Thiazole; Multicomponent reactions; Green synthesis; Medicinal chemistry etc.

Introduction

Heterocyclic compounds are cyclic organic molecules containing at least one atom other than carbon within the ring system. These heteroatoms—commonly nitrogen, oxygen, or sulfur—modify the electronic distribution and reactivity of the ring, leading to unique structural and biological properties. Heterocyclic frameworks are ubiquitous in natural products, pharmaceuticals, agrochemicals, dyes, polymers, and advanced materials.

Nitrogen-containing heterocycles represent a particularly important subclass due to their hydrogen-bonding ability, tunable basicity, and enhanced solubility. A significant proportion of FDA-approved drugs contain at least one nitrogen heterocycle. For example, Metronidazole contains an imidazole ring responsible for antimicrobial activity, while Fluconazole possesses a 1,2,4-triazole moiety essential for antifungal efficacy.

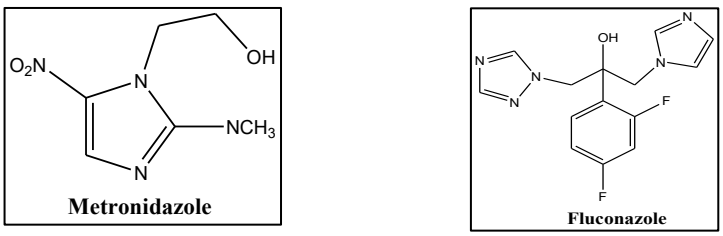

Fig.1: Drugs contains Nitrogen heterocycle

Industrially, heterocyclic compounds are utilized in corrosion inhibitors, catalysts, pesticides, and optoelectronic materials. Their synthetic versatility and biological relevance make heterocyclic chemistry a cornerstone of modern organic and medicinal chemistry.

2. Classification of Heterocycles

Heterocyclic compounds can be classified based on ring size, nature of heteroatom, and degree of saturation.

2.1 Based on Ring Size

- **Three-membered rings:** Aziridine, oxirane

- **Four-membered rings:** Azetidine
- **Five-membered rings:** Pyrrole, furan, thiophene, imidazole, thiazole
- **Six-membered rings:** Pyridine, pyrimidine
- **Fused systems:** Benzothiazole, quinoline, indole

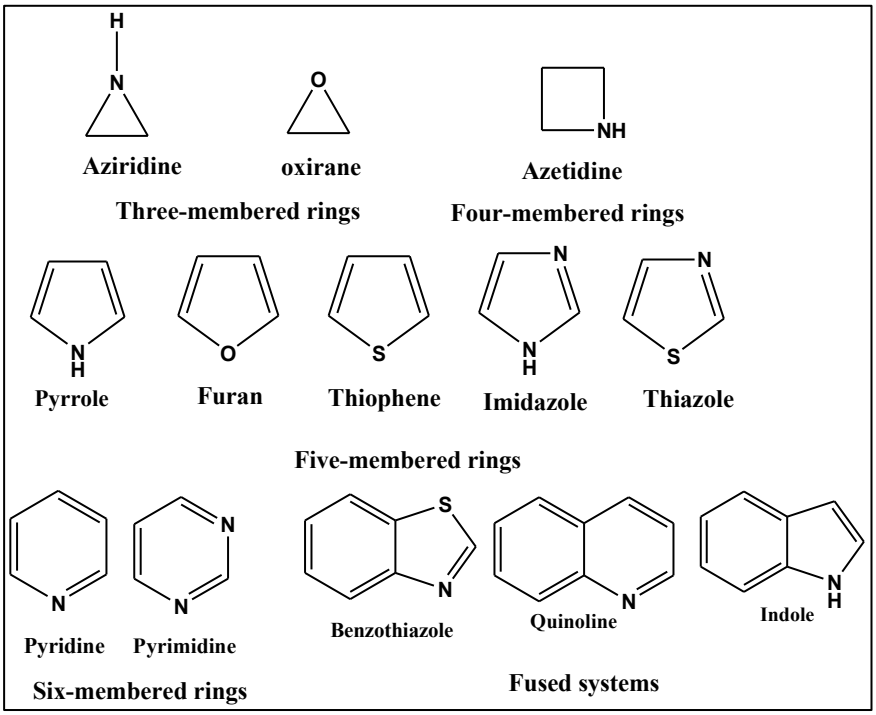

Fig.2: Classification of heterocycles Based on Ring Size

Five- and six-membered heterocycles are the most stable and widely studied due to aromatic stabilization.

2.2 Based on Heteroatom

- **Nitrogen heterocycles:** Pyridine, triazole, tetrazole
- **Oxygen heterocycles:** Furan
- **Sulfur heterocycles:** Thiophene
- **Mixed heterocycles:** Thiazole (N and S), oxazole (N and O)

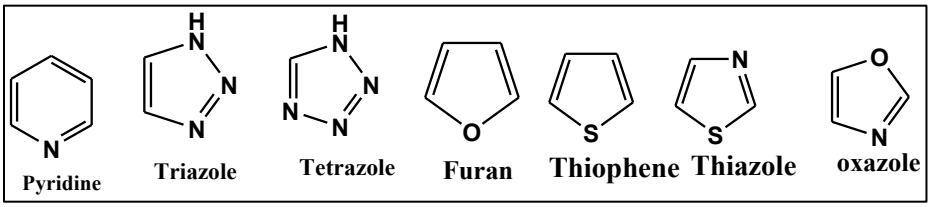

Fig. 3: Classification of heterocycles based on Heteroatom

Nitrogen heterocycles dominate medicinal chemistry because nitrogen atoms contribute to receptor binding interactions.

2.3 Based on Saturation

- **Aromatic heterocycles:** Pyridine, imidazole
- **Saturated heterocycles:** Piperidine
- **Partially saturated heterocycles:** Dihydro derivatives

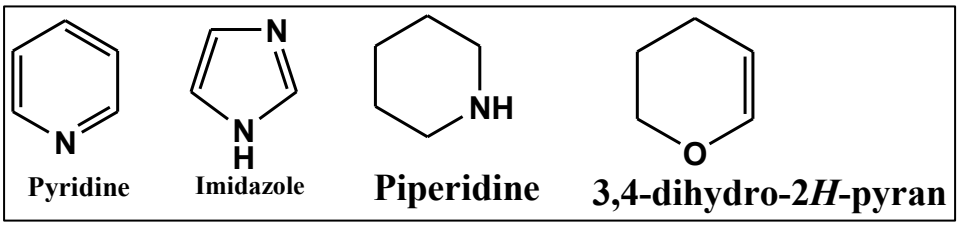

Fig. 4: Classification of heterocycles based on Saturation

Aromatic heterocycles exhibit enhanced stability due to delocalized π-electrons.

3. Biological Applications of Heterocycles

Heterocyclic compounds demonstrate diverse pharmacological properties.

3.1 Anticancer Activity

Triazole, imidazole, and thiazole derivatives exhibit cytotoxic effects through inhibition of kinases, tubulin polymerization, and DNA interaction. Substituent effects significantly influence activity; electron-withdrawing groups often enhance cytotoxic potential.

3.2 Antimicrobial Activity

Nitrogen heterocycles disrupt microbial enzyme systems and membrane integrity. The presence of halogens or nitro groups can enhance antimicrobial efficacy.

3.3 Anti-inflammatory Activity

Heterocycles modulate inflammatory pathways by inhibiting cyclooxygenase (COX) enzymes and cytokine production. SAR studies indicate that heteroatom positioning affects binding affinity.

3.4 Antioxidant Activity

Phenolic and heterocyclic systems containing conjugated double bonds exhibit radical scavenging ability. Electron-donating substituents improve antioxidant potential.

4. Structure–Activity Relationship (SAR) Insights

- Electron-withdrawing groups increase antimicrobial activity.
- Bulky substituents may improve anticancer selectivity.

- Increased lipophilicity enhances membrane permeability.
- Heteroatom position influences hydrogen bonding capacity.

Hybridization of two pharmacophores often improves potency.

5. Recent Literature Review (Last 5–10 Years)

Recent research trends include:

- Development of triazole-based anticancer hybrids
- Metal-free click chemistry protocols
- C–H activation for direct heterocycle functionalization
- Design of benzothiazole derivatives as antimicrobial agents
- Use of computational docking for activity prediction

The integration of synthetic chemistry with computational modeling has accelerated drug discovery.

6. Conclusion

Heterocyclic compounds, particularly nitrogen-containing systems, remain central to modern organic and medicinal chemistry. Advances in synthetic methodologies, including transition metal catalysis, multicomponent reactions, and green chemistry techniques, have significantly expanded structural diversity and efficiency. Their broad spectrum of biological activities—anticancer, antimicrobial, anti-inflammatory, and antioxidant—demonstrates their immense therapeutic potential. Continued integration of synthetic innovation with computational tools and sustainable practices will shape the future of heterocyclic chemistry and drug discovery.

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Artificial Intelligence Transforming the Chemical Industry

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Abstract

Artificial Intelligence (AI) is increasingly reshaping the chemical industry by accelerating research, optimizing manufacturing processes, and improving sustainability. This paper explores key AI applications in chemical research and industrial operations, including molecular design, process optimization, quality control, and predictive maintenance. The study also examines benefits such as reduced costs, faster innovation cycles, and improved safety, while addressing challenges related to data quality, interpretability, and ethical concerns. Artificial Intelligence (AI) is emerging as a transformative force in the chemical industry, reshaping traditional approaches to research, development, manufacturing, and supply chain management. By leveraging machine learning, data analytics, and automation, AI accelerates molecular discovery, optimizes chemical processes, and enhances operational efficiency while reducing costs and environmental impact. AI-driven tools enable predictive maintenance, real-time process control, and the development of sustainable and high-performance materials. Despite challenges related to data quality, and regulatory considerations, the integration of AI offers significant competitive advantages. This transformation positions AI as a key enabler of innovation, sustainability, and resilience in the evolving chemical industry. In recent years, the chemical industry has undergone significant transformation due to technological advancements, globalization, and increasing environmental regulations. Sustainability has become a major focus, with companies adopting green chemistry principles, waste minimization techniques, and energy-efficient production systems. Digitalization, automation, and advanced data analytics are improving process efficiency, safety, and supply chain management.

Introduction

Chemistry industry plays a crucial role in pharmaceuticals, materials science,

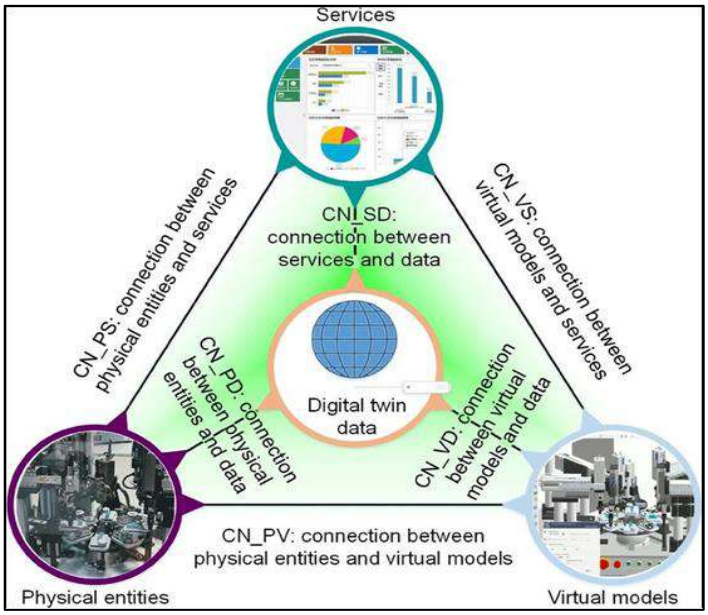
energy, and manufacturing. Traditional chemical research and production methods are often time-consuming and resource-intensive. AI technologies—such as machine learning, deep learning, and neural networks—offer new approaches to handling complex chemical data and enhancing decision- making. Artificial Intelligence (AI) is rapidly reshaping the chemical industry, driving innovation, efficiency, and sustainability across the entire value chain—from research and development to manufacturing, supply chains, and customer engagement.

Key Applications of AI in the Chemistry Industry

- **Drug and Molecule Discovery:** AI models predict molecular properties and reactions Generative models design novel compounds Reduces time and cost of experimental trials
- **Process Optimization:** AI control's reaction conditions (temperature, pressure, catalysts) Improves yield and energy efficiency Enables real-time process adjustments
- **Quality Control and Safety:** Computer vision detects defects and impurities Predictive analytics prevent equipment failure Enhances workplace and environmental safety 4 Materials Science AI accelerates discovery of polymers, catalysts, and batter Simulates material behavior before synthesis
- **Benefits of AI Adoption Faster research and development, Lower operational costs:** Increased accuracy and reproducibility, Improved sustainability and waste reduction
- **Challenges and Limitations:** Limited availability of high-quality chemical data, Lack of model interpretability ("black-box" issue), High implementation costs, Need for interdisciplinary expertise
- **Conclusion:** AI is transforming the chemistry industry by enabling smarter research, safer operations, and sustainable practices. While challenges remain, continued advancements in AI algorithms and data infrastructure will further expand its impact.

Digital Twin / Simulation Module

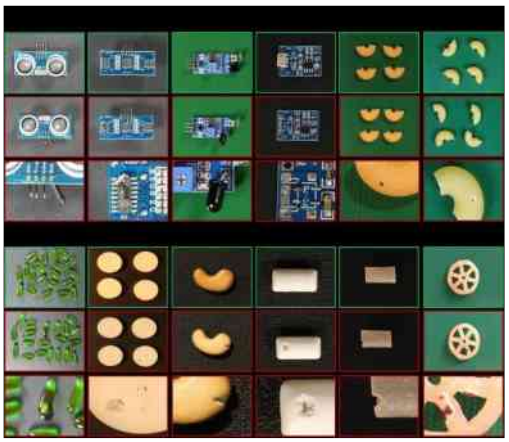
A Digital Twin is a real-time virtual replica of a chemical process, unit operation, or entire plant. It combines process simulation + live plant data + AI models to mirror how the real system behaves. Think of it as a "living simulator" of your plant.



Detection Component

The Detection Component continuously monitors process, equipment, and safety data to identify abnormalities, faults, or early warning signs before they become failures or incidents.

Think of it as the plant's early-warning nervous system.

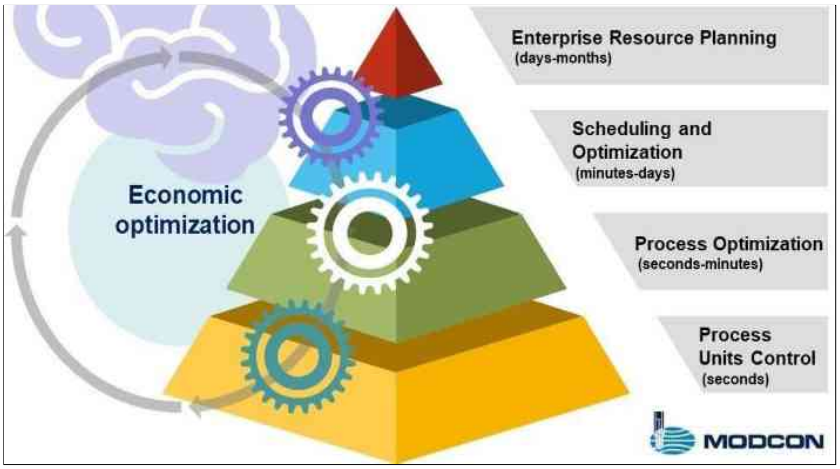


Real-Time Control Systems

Real-Time Control Systems (RTCS) continuously measure, decide, and act on process conditions within strict time limits to keep chemical operations stable, safe, and optimal.

Economic Optimization Layer

The Economic Optimization Layer is the top decision-making layer that continuously adjusts plant targets to maximize profit or minimize total cost, while respecting safety, quality, and operational constraints.



Artificial Intelligence in the Pharmaceutical Industry

Artificial Intelligence (AI) is revolutionizing the pharmaceutical sector by transforming drug discovery, development, manufacturing, and quality control. By integrating AI with chemical and biological data, pharmaceutical companies can innovate faster, reduce costs, and improve patient outcomes.

1. AI in Drug Discovery and Design

AI significantly accelerates early-stage pharmaceutical research.

- Molecular modeling and screening: Machine learning predicts chemical structures, biological activity, and toxicity, enabling rapid identification of promising drug candidates.
- De novo drug design: AI generates novel molecules with desired therapeutic properties.
- Target identification: AI analyzes biological and chemical data to identify new drug targets.

2. AI in Process Development and Manufacturing

AI improves efficiency and consistency in pharmaceutical production.

- Process optimization: AI models optimize reaction conditions, formulation parameters, and scale-up processes.
- Predictive maintenance: AI anticipates equipment failures, reducing downtime and ensuring compliance with Good Manufacturing Practices (GMP).
- Continuous manufacturing: AI supports real-time monitoring and control for consistent product quality.

3. Quality Control and Regulatory Compliance

AI enhances quality assurance in pharmaceutical chemistry.

- Real-time quality monitoring: AI detects deviations during synthesis and formulation.
- Data integrity and compliance: AI helps ensure adherence to regulatory standards such as FDA and EMA guidelines.
- Automated documentation: AI streamlines reporting and validation processes.

4. AI in Formulation and Delivery Systems

AI enables the design of advanced drug formulations.

- Optimization of excipients and dosage forms
- Controlled and targeted drug delivery
- Stability prediction and shelf-life estimation
- Benefits and Challenges Benefits
- Skilled workforce requirements
- Faster drug development timelines
- Reduced R&D and manufacturing costs

- Improved product quality and patient safety

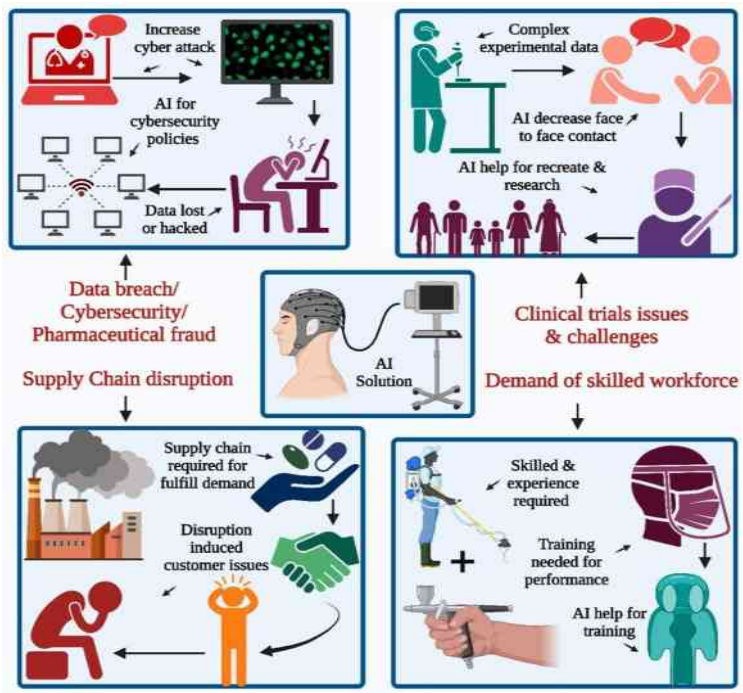
Challenges

- Limited high-quality data
- Validation and regulatory acceptance

Conclusion

AI is becoming a critical enabler in pharmaceutical chemistry, bridging chemical engineering, data science, and biology. Its adoption enhances innovation, ensures manufacturing excellence, and supports the development of safer, more effective medicines. If you want, I can also provide a short abstract, research paper format, or case studies focused on AI in pharmaceutical chemistry.

Pharmaceutical diagram



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Artificial Photosynthesis: Reimagining Solar Energy Through Chemistry

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1. Introduction: Learning from Nature's Blueprint

For billions of years, nature has perfected a chemical process that sustains nearly all life on Earth: photosynthesis. Through this elegant system, plants, algae, and certain bacteria convert sunlight, water, and carbon dioxide into oxygen and energy-rich organic molecules. The simplicity of the inputs and the sophistication of the molecular machinery have inspired generations of scientists. In recent decades, chemists have pursued one of the most ambitious innovations in modern science: artificial photosynthesis—a technology designed to replicate and improve upon nature's method of storing solar energy in chemical bonds.

2. The Chemical Foundation of Natural Photosynthesis

To appreciate the innovation of artificial photosynthesis, one must first understand the natural process. In plants, photosynthesis occurs in chloroplasts, where pigment molecules absorb sunlight. The overall reaction can be summarized as:

Carbon dioxide + Water + Light energy → Glucose + Oxygen

In the light-dependent stage, sunlight excites electrons in chlorophyll molecules. These high-energy electrons travel through a series of protein complexes embedded in membranes. Water molecules are split in a reaction known as water oxidation, releasing oxygen, protons, and electrons. This reaction is particularly significant because splitting water requires breaking strong chemical bonds. The energy harvested during this stage is temporarily stored in energy-rich molecules.

In the second stage, carbon dioxide is chemically reduced and assembled into carbohydrates. The process involves carefully controlled electron transfers and enzyme-mediated steps. Natural photosynthesis is efficient, self-repairing, and environmentally benign. However, its overall energy conversion efficiency is relatively modest. Artificial systems aim to surpass these limitations while retaining the sustainability of the natural model.

3. Concept and Goals of Artificial Photosynthesis

Artificial photosynthesis seeks to create man-made systems that mimic key features of natural photosynthesis: light absorption, charge separation, and catalytic fuel formation. At its core, the technology involves three essential components:

- A light-absorbing material
- A catalyst for water oxidation

A catalyst for fuel formation (such as hydrogen evolution or carbon dioxide reduction)

The overarching goal is to convert sunlight, water, and carbon dioxide into fuels without producing harmful by-products. Hydrogen gas is often a primary target fuel because it burns cleanly, producing only water. Alternatively, carbon-based fuels such as methanol or methane can be generated through carbon dioxide reduction, creating a circular carbon economy.

4. Water Splitting: The Central Chemical Challenge

One of the most significant achievements in artificial photosynthesis research is the development of catalysts capable of splitting water efficiently. Water splitting involves two half-reactions:

- Oxidation of water to produce oxygen
- Reduction of protons to produce hydrogen

The oxidation step is particularly challenging because it requires the removal of four electrons and the formation of an oxygen-oxygen bond. In natural systems, this reaction is carried out by a manganese-containing cluster embedded in a protein complex. Replicating this complexity in a synthetic material has required decades of research.

A major breakthrough came in the early 21st century when researchers led by Daniel G. Nocera demonstrated a cobalt-based catalyst capable of efficiently evolving oxygen in water under mild conditions. This discovery showed that relatively abundant elements could perform complex redox reactions

previously thought to require rare and expensive metals.

5. Photoelectrochemical Cells: Integrating Light and Catalysis

A central device in artificial photosynthesis research is the photoelectrochemical (PEC) cell. This system integrates light absorption and catalytic reactions within a single platform. In a typical PEC cell, a semiconductor material absorbs sunlight and generates excited electrons and holes (positive charge carriers). These charge carriers drive the water-splitting reactions at separate electrodes.

6. Hydrogen as a Clean Energy Carrier

Hydrogen production is one of the most promising outcomes of artificial photosynthesis. Hydrogen gas has a high energy content per unit mass and produces only water when combusted or used in fuel cells. Unlike fossil fuels, hydrogen does not emit carbon dioxide during use. Traditional hydrogen production relies heavily on natural gas reforming, a process that emits significant amounts of carbon dioxide. Artificial photosynthesis offers a cleaner alternative by using only sunlight and water. When integrated with renewable energy infrastructure, this approach could support a sustainable hydrogen economy.

However, hydrogen storage and transportation remain technical challenges. Hydrogen molecules are small and can leak easily. Additionally, compressing or liquefying hydrogen requires energy. Researchers are exploring chemical carriers such as ammonia and liquid organic hydrogen carriers to improve practicality.

7. Carbon Dioxide Reduction: Closing the Carbon Cycle

Beyond hydrogen production, artificial photosynthesis can convert carbon dioxide into useful fuels and chemicals. This process addresses both renewable energy storage and carbon capture. By using captured carbon dioxide as a raw material, chemists can create methanol, carbon monoxide, methane, or even multi-carbon compounds.

8. Materials Innovation and Nanotechnology

The progress of artificial photosynthesis is closely tied to materials innovation. At the nanoscale, materials exhibit unique properties that enhance catalytic activity and light absorption. Nanoparticles, quantum dots, and layered materials can be engineered to control electron flow with extraordinary precision. Design hetero structures combinations of different materials to optimize

performance. For example, pairing a light-absorbing semiconductor with a robust catalyst improves overall efficiency. Surface modifications and molecular linkers enhance charge transfer between components.

9. Economic and Environmental Implications

Artificial photosynthesis has the potential to reshape global energy systems. By providing a renewable pathway to fuel production, it could reduce dependence on fossil fuels and lower greenhouse gas emissions. Decentralized fuel generation systems could empower remote communities and reduce energy inequality.

From an environmental perspective, artificial photosynthesis produces minimal pollution when designed properly. The primary inputs—sunlight, water, and carbon dioxide—are abundant and renewable. Unlike fossil fuel extraction, this process does not require destructive mining or drilling.

Economically, large-scale implementation could create new industries cantered around solar fuel production, catalyst manufacturing, and carbon utilization technologies. However, significant investment in infrastructure, research, and policy support is necessary for commercialization.

10. Challenges and Future Directions

Despite promising advances, artificial photosynthesis faces several challenges:

- Improving overall energy conversion efficiency
- Enhancing long-term stability of materials
- Reducing production costs
- Scaling laboratory prototypes to industrial systems

Durability is particularly important. Devices must operate for years under sunlight exposure without significant degradation. Researchers are developing self-healing materials and corrosion-resistant coatings to address this issue. Another frontier is the integration of biological and synthetic systems. Hybrid approaches combine engineered microorganisms with inorganic catalysts, merging the selectivity of biology with the robustness of synthetic materials.

Looking forward, continued interdisciplinary collaboration among chemists, physicists, engineers, and environmental scientists will be essential. International research initiatives and funding programs are accelerating innovation in this field.

11. Ethical and Societal Considerations

As with any transformative technology, artificial photosynthesis raises ethical

and societal questions. Equitable access to clean energy technologies must be prioritized to prevent widening economic disparities. Environmental impacts of material extraction and device disposal must also be carefully managed.

Policymakers play a crucial role in supporting sustainable innovation. Incentives for renewable energy adoption, carbon pricing, and international cooperation can facilitate large-scale deployment. Public education is equally important. Understanding the chemistry behind renewable fuels empowers citizens to make informed decisions about energy use and sustainability.

12. Conclusion: Chemistry at the Heart of a Sustainable Future

Artificial photosynthesis stands as one of the most visionary innovations in modern chemistry. By harnessing sunlight to produce clean fuels, it embodies the principles of sustainability, efficiency, and environmental responsibility. This technology does not merely imitate nature—it builds upon natural inspiration to design systems capable of meeting global energy demands.

The journey from laboratory discovery to global infrastructure is long and complex. Yet each breakthrough in catalyst design, semiconductor engineering, and carbon conversion brings the vision closer to reality. Artificial photosynthesis demonstrates how chemistry, often viewed as an abstract science of molecules and reactions, can directly address pressing global challenges.

In redefining how humanity captures and stores solar energy, artificial photosynthesis represents more than a scientific achievement. It is a testament to human creativity and the power of chemical innovation to shape a cleaner, more sustainable world.

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Study of Green Synthesis of Zinc Oxide nanoparticles using Pentalinon Luteum Plant Extract

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Abstract

Aquatic ecosystems and human health are seriously threatened by the textile industry's excessive water consumption and consequent release of hazardous dye effluents. This study describes the environmentally benign, biogenic manufacturing of zinc oxide nanoparticles (ZnO NPs) utilizing Pentalinon luteum leaf extract. Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), and Energy Dispersive X-ray Analysis (EDAX) were used to analyze the produced NPs. The generation of spherical, somewhat agglomerated ZnO NPs with crystallite diameters ranging from 16.24 nm to 28.33 nm was confirmed by the results. The green synthesis approach turned shown to be an economical, safe, and effective substitute for traditional chemical synthesis.

1. Introduction

Significant water pollution has resulted from industrialization, especially in the tannery, paper, and textile industries. Because textile effluents include complex dyes that lower dissolved oxygen (DO) and sunlight penetration, they increase biological oxygen demand (BOD) and interfere with aquatic photosynthesis, making them especially dangerous. Metal oxide nanoparticle-based photocatalytic degradation has become a highly sought-after remedy to counter this. Zinc Oxide (ZnO) is favored above other options because of its high surface area, effective electron carrier capabilities, and chemical durability. We can create these nanoparticles without the use of hazardous reducing chemicals by

applying "Green Chemistry" principles, particularly with plant extracts like Pentalinon luteum.

2. Materials and Methods

2.1 Preparation of Leaf Extract

The leaves of Pentalinon luteum were gathered from Karjat Taluka in Ahilyanagar, India. After being cleaned with deionized (DI) water, the leaves were left to air dry for six days. After dispersing 10 g of the resultant leaf powder in 300 mL of DI water, the mixture was heated to 70°C for 30 minutes. Whatman No. 41 filter paper was used to collect the filtrate, which was then kept at room temperature.

2.2 Green Synthesis of ZnO NPs

A wet chemical method was applied: 2.875 g of zinc sulphate (0.1M) was combined with 100 mL of the leaf extract. To create a precipitate, the mixture was shaken at 70°C for an hour after being stirred for a full day. The mixture was repeatedly washed with ethanol after being centrifuged at 5000 rpm and dried for 12 hours at 100°C. The final product was calcined at 400°C for two hours in order to create pure ZnO NPs.

3. Results and Discussion

3.1 FTIR Analysis

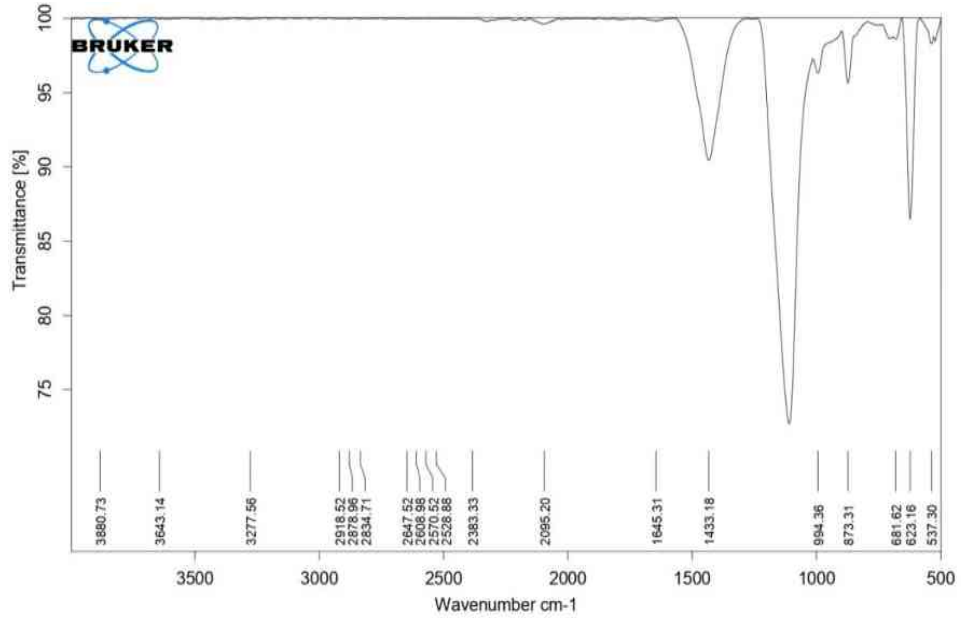

Fig. 1. FT-IR spectra of synthesized Zinc oxide nanoparticles

The biomolecules (carbohydrates, phenols, and flavonoids) in charge of the reduction and capping of the NPs were identified using FTIR. Zn-O Stretching: The development of the metal oxide framework is confirmed by distinct peaks at 537.30, 623.16, and 681.62 cm^{-1}.C-C Bands: Organic residues from the extract are indicated by a peak at 1433.18 cm^{-1}. Adsorbed Water: The O-H bending vibrations are associated with the peak at 1645.31 cm^{-1}.

3.2 SEM and Morphology

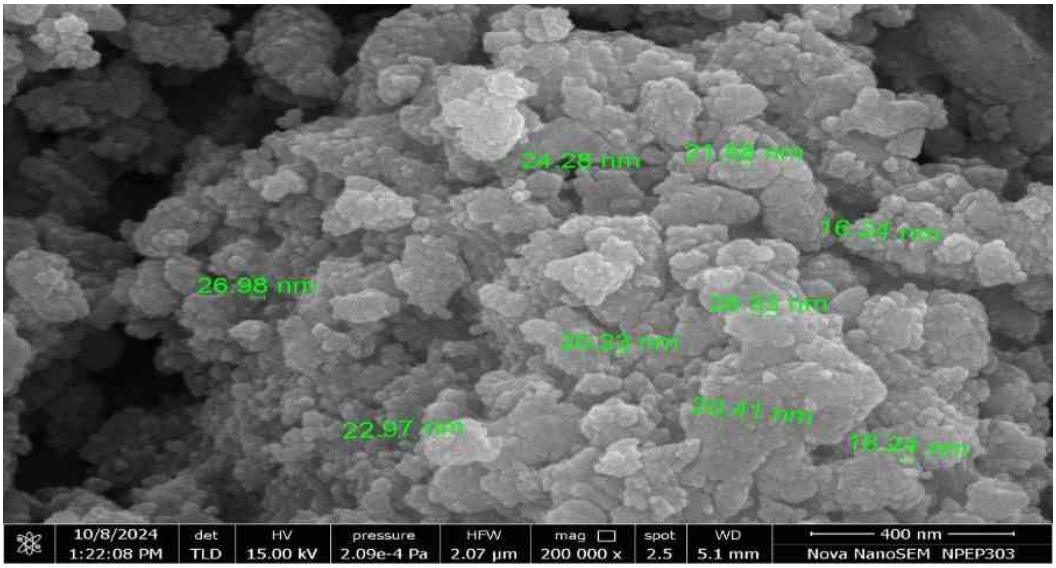

Fig. 2. SEM images of zinc oxide nanoparticles

The ZnO NPs are mostly spherical but have some irregular shapes because of aggregation, according to SEM images. The synthetic material's nanoscale scale was confirmed by the particle size measurements, which ranged from 16.24 nm to 28.33 nm.

3.3 EDAX and Elemental Mapping

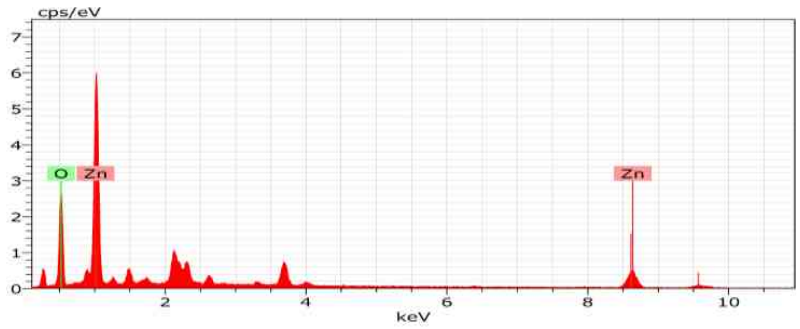

Figure3.EDAX Spectra of ZnO nanoparticles

The sample's excellent purity was validated by EDAX analysis. The composition of elements revealed: • Zinc (Zn): Weight percentage: 73.47% • Weight percentage of oxygen (O): 26.53% .Although the ratio indicates a slight oxygen shortfall relative to zinc, which is common in biogenic ZnO formation, the mapping showed a uniform distribution of elements.

4. Conclusion

The simple, affordable, and "green" production of ZnO nanoparticles was carried out using Pentalinon luteum. Characterization confirmed the crystallinity and nanostructure of the particles. Because of these qualities, these NPs show great promise as catalysts for the photocatalytic degradation of industrial dyes, providing a sustainable way to remediate waste water.

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Green and Sustainable Ionic Liquid Catalyzed Synthesis of Pyrimidinone Derivatives: Mechanistic Insights, Scope and Applications

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Abstract

Pyrimidinone derivative comes under a crucial class of heterocyclic compounds due to their wide-ranging biological, pharmaceutical and material science applications. Conventional methods for their synthesis often involve hazardous solvents, strong mineral acids, prolonged reaction times, and high energy requirements, resulting in significant environmental and economic drawbacks.

Keywords: Green chemistry; Ionic liquids; Pyrimidinone derivatives; Multicomponent reactions; Sustainable catalysis; Heterocyclic synthesis.

Introduction

Heterocyclic compounds represent a fundamental class of chemical entities that are widely encountered in biologically active molecules, pharmaceuticals, agrochemicals, dyes, and advanced functional materials [16–18]. Among these, pyrimidinone derivatives are particularly significant due to their notable pharmacological properties. These compounds exhibit a wide range of biological activities, including antibacterial, antifungal, antiviral, anticancer, antitubercular, anti-inflammatory, and antioxidant effects [16,17]. Owing to such diverse therapeutic potential, pyrimidinones have attracted sustained attention in medicinal chemistry, synthetic organic chemistry, and drug discovery research.

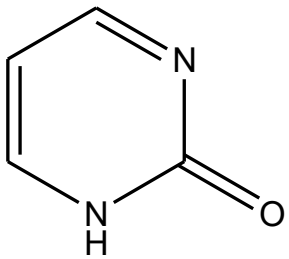
Traditional approaches for the synthesis of pyrimidinones are primarily based on the classical Biginelli reaction, which involves an acid-catalyzed three-component condensation of aldehydes, β-ketoesters, and urea or thiourea [1–3]. Despite its simplicity and synthetic utility, this method suffers from several limitations, such as slow reaction rates, moderate yields, harsh reaction

conditions, and the extensive use of organic solvents [2,3]. These drawbacks adversely affect both the environmental sustainability and economic feasibility of the process. Growing concerns regarding environmental pollution, depletion of natural resources, and climate change have encouraged the adoption of green chemistry principles, which emphasize the reduction or elimination of hazardous substances in chemical processes [5]. In this context, ionic liquids have been established as efficient and environmentally sustainable reaction media and catalysts, offering a promising alternative to conventional volatile organic solvents [6–8].

Ionic liquids possess unique physicochemical properties, including negligible vapor pressure, high thermal stability, non-flammability, tunable polarity, and excellent solvating ability [6,7,9]. These characteristics make them highly suitable for environmentally benign chemical transformations. Therefore, this chapter focuses on the application of ionic liquids as green catalytic systems for the efficient synthesis of pyrimidinone derivatives, highlighting their mechanistic aspects, synthetic versatility, environmental benefits, and potential industrial applications.

Pyrimidinone Derivatives: Structural Features and Biological Importance

Pyrimidinones are six-membered heterocyclic compounds containing two nitrogen atoms and a carbonyl group within the ring. The presence of multiple functional groups and heteroatoms allows extensive structural modification, enabling fine-tuning of biological properties.



Pyrimidinone

The significant pharmacological importance of pyrimidinone frameworks has driven considerable research toward the development of efficient, cost-effective, and environmentally sustainable synthetic methodologies. Green synthesis of these compounds not only reduces ecological impact but also improves their acceptability for pharmaceutical applications.

Conventional Synthetic Methods and Their Limitations

The Biginelli reaction is one of the most widely utilized methods for the synthesis of dihydropyrimidinone derivatives [1–3]. Conventionally, this transformation is carried out in organic solvents using strong mineral acids, such as hydrochloric acid, sulfuric acid, or various Lewis acids, as catalysts [2-3].

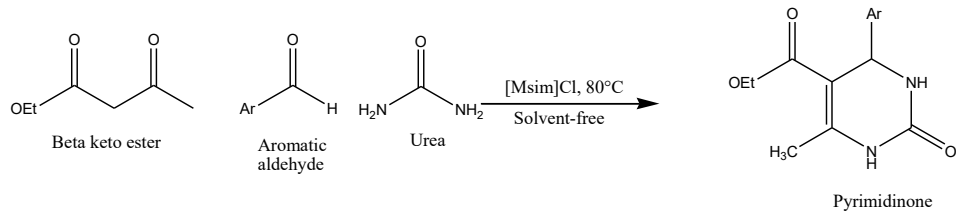
Green Synthesis of Pyrimidinones using Ionic Liquid

1. Catalyst Selection and Design

Among the various ionic liquids investigated, 3-methyl-1-sulfonic acid imidazolium chloride ([Msim]Cl) has been identified as a highly efficient catalyst for the synthesis of pyrimidinone derivatives [10–13]. The presence of the sulfonic acid group imparts strong Brønsted acidity, facilitating efficient activation of carbonyl substrates and promoting rapid cyclization. [Msim]Cl exhibits excellent thermal stability, high solubility in reaction mixtures, and outstanding recyclability. These properties make it an ideal candidate for sustainable catalytic applications in heterocyclic synthesis.

2. General Experimental Procedure

An equimolar mixture of aromatic aldehyde (1 mmol) and ethyl acetoacetate (1 mmol), along with urea (1.2 mmol), was introduced into a round-bottom flask. Subsequently, 10 mol% of the ionic liquid catalyst [Msim]Cl was added to the reaction mixture. The contents were stirred at 80°C under solvent-free conditions. The progress of the reaction was monitored by thin-layer chromatography using a hexane:ethyl acetate (7:3) solvent system. After completion (15–30 minutes), the mixture was allowed to cool to ambient temperature and then poured onto crushed ice.



The ionic liquid catalyst was recovered from the aqueous filtrate by evaporation and successfully reused for up to six successive cycles with only negligible reduction in catalytic efficiency, demonstrating its excellent recyclability [23–25].

Catalyst Recyclability and Process Sustainability

Catalyst recyclability represents a key advantage of ionic liquid catalysis. The catalyst can be conveniently recovered from the reaction system and reused

repeatedly with minimal decline in activity. In this work, [Msim]Cl was recycled up to six consecutive runs with negligible loss in yield, confirming its high operational stability [23–25]. The solvent-free nature of the reaction minimizes solvent waste and reduces the environmental footprint. Furthermore, the short reaction time and moderate temperature requirements significantly lower energy consumption, making the process highly sustainable.

Green Chemistry Metrics and Environmental Assessment

The developed methodology conforms to green chemistry principles, with key performance indicators such as atom economy, reaction mass efficiency and e-factor exhibiting marked enhancement compared to traditional approaches [5, 20]. High product yield and minimal waste generation contribute to superior process efficiency. The absence of volatile organic solvents eliminates atmospheric emissions and reduces health hazards. Additionally, the recyclability of the ionic liquid catalyst further enhances material efficiency and economic feasibility.

Pharmaceutical and Industrial Applications

Green synthesized pyrimidinone derivatives find extensive applications in pharmaceutical research, particularly in the development of antimicrobial, anticancer, antiviral, and anti-inflammatory agents. Their environmentally benign synthesis enhances regulatory compliance and supports sustainable drug manufacturing. Beyond pharmaceuticals, pyrimidinones are employed in agrochemical formulations, corrosion inhibitors, dyes, and advanced functional materials. The scalability of ionic liquid catalyzed synthesis makes it highly attractive for industrial adoption.

Conclusion

Ionic liquid catalyzed synthesis represents a powerful and sustainable approach for the preparation of pyrimidinone derivatives. The methodology offers significant advantages over conventional protocols, including enhanced reaction efficiency, operational simplicity, catalyst recyclability, and minimal environmental impact. Continued advancements in ionic liquid design and green process engineering are expected to further expand their role in sustainable chemical manufacturing.

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Identification of Potential Phytocompounds Against Multidrug-Resistant Tuberculosis (MDR TB) and Methicillin-Resistant *Staphylococcus aureus* (MRSA): In Silico Approaches

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Abstract

A serious concern to world health is the quick rise of methicillin-resistant Staphylococcus aureus (MRSA) and multidrug-resistant tuberculosis (MDR-TB). Due to the emergence of resistance, conventional antibiotics are becoming less and less effective, which calls for the creation of new therapeutic medicines. In order to find possible phytocompounds from medicinal plants with antibacterial action, the current study used an integrated in-silico drug discovery approach. The Protein Data Bank provided validated protein targets, whereas PubChem and ChEMBL provided phytochemicals. Auto Dock Vina and Schrödinger Glide were used for high-throughput molecular docking, and GROMACS was used for molecular dynamics simulations. Drug-likeness and pharmacokinetic characteristics were assessed using pharmacophore modeling and ADMET prediction. The investigation found interesting phytocompounds with stable protein-ligand interactions and high binding affinities.

Keywords: Phytocompounds, Multidrug-resistant tuberculosis, Pharmacophore model, Pharmacokinetic, Molecular Docking

Introduction

The effectiveness of existing medications is threatened by antimicrobial resistance (AMR), with methicillin-resistant Staphylococcus aureus (MRSA) and

multidrug-resistant tuberculosis (MDR-TB) being two of the most pressing worldwide priorities (Abebe et al., 2023). Resistance to first-line medications (rifampicin, isoniazid) restricts treatment options for MDR-TB, while MRSA is the cause of chronic infections acquired in hospitals and the community. Novel phytocompounds with antibacterial action can be found in medicinal plants; these compounds frequently work through numerous routes, reducing the likelihood that resistance would evolve (Alara et al., 2024). Plant-derived compounds can be quickly identified, screened, and optimized using in-silico methods prior to experimental testing thanks to advancements in computational drug discovery (Das et al., 2024).

Phytocompounds in Medicinal Chemistry:

Alkaloids, terpenoids, flavonoids, phenolics, lignans, and saponins are examples of plant secondary metabolites that cover uncharted chemical space. They provide unique scaffolding, three-dimensional geometries, and stereochemical richness that can result in superior ligand-target interactions. Many have polypharmacology, which modulates several bacterial targets or pathways (e.g., cell wall synthesis + membrane integrity + efflux), which can enhance synergy with current antibiotics and prevent the development of resistance. Additionally, scaffold hopping and medicinal chemistry optimization are made easier by their chemodiversity (Shoaib et al., 2022).

Obstacles and our approach to mitigation. Dereplication (re-discovering known actives), uneven sample composition, poor solubility/permeability, metabolic instability, and liabilities like PAINS or pan-assay aggregators are common problems in natural product research. Strict data curation and standardization (tautomer/protomer handling, charge states, duplicate removal), the application of liability filters (PAINS/BRENK/aggregator alerts) and synthetic accessibility scoring, early-stage ADME/Tox triage (e.g., hERG/Ames/CYP risk), and the prioritization of vendor-available or readily synthesizable scaffolds to ensure downstream feasibility are how this project tackles these issues (Rallabandi et al., 2020).

Materials and Methods

1. Selection of Medicinal Plants and Phytocompounds

Ethnopharmacological reports and a survey of the literature were used to choose medicinal plants with proven antibacterial qualities. Phytochemical components were obtained in SDF format from the PubChem and ChEMBL databases. Compounds were transformed into suitable formats for docking investigations

after being screened for structural integrity.

2. Protein Target Selection and Preparation

From the Protein Data Bank, validated protein targets linked to treatment resistance in MRSA and MDR-TB were chosen. Structural completeness and biological significance were taken into consideration while selecting high-resolution crystal structures.

In order to prepare proteins, water molecules and heteroatoms were removed, missing hydrogen atoms were added, bond ordering were assigned, energy was minimized, and ligands were optimized using charge assignment and geometry minimization to guarantee precise docking.

3. Virtual Screening and Molecular Docking

Schrödinger Glide and Auto Dock Vina were used for high-throughput virtual screening. The binding affinity between phytocompounds and target proteins was assessed using docking simulations. Binding energy (kcal/mol), interaction with active site residues, stability of docking pose, detailed interaction analysis that included hydrogen bond interactions, hydrophobic interactions, π–π stacking, and electrostatic interactions were used to rank the compounds. The top-ranked compounds were then shortlisted for additional analysis.

4. Molecular Dynamics Simulations

GROMACS was used to run molecular dynamics simulations in order to verify docking stability. Force field selection, solvation in an explicit water box, counter-ion addition, energy minimization, equilibration (NVT and NPT ensembles), production run (50–100 ns), trajectory analysis, root mean square deviation (RMSD), root mean square fluctuation (RMSF), hydrogen bond stability, radius of gyration (Rg), and solvent accessible surface area (SASA) are all included in the simulation protocol. To determine thermodynamic stability, binding free energy calculations were performed using MM-PBSA techniques.

5. Pharmacophore Modeling

The following structural characteristics of active chemicals were found to be common: Ionizable groups, aromatic rings, hydrophobic centers, hydrogen bond donors, and acceptors. In order to find new molecules with comparable essential properties, a pharmacophore model was created and used to other compound libraries.

6. ADMET Prediction

Swiss ADME was used to estimate pharmacokinetic and toxicity characteristics. Intestinal absorption, blood–brain barrier permeability, cytochrome P450 interactions, water solubility, lipophilicity, and toxicity hazards were among the parameters assessed. Lipinski's Rule of Five and Veber's Rule were used to evaluate drug-likeness, and compounds that met these standards were regarded as possible drug candidates.

Results

Several phytocompounds with notable binding affinities (≤ –8.0 kcal/mol) against MDR-TB and MRSA targets were found using high-throughput docking. A thorough docking investigation showed: stable hydrogen bonds with important catalytic residues, Strong hydrophobic contacts inside binding pockets, favorable electrostatic complementarity, stable RMSD profiles, minimal active site residue fluctuations, consistent hydrogen bond interactions, favorable radius of gyration, and SASA values were all validated by molecular dynamics simulations. For the best compounds, MM-PBSA free energy estimates showed significant binding stability. Common structural characteristics that are in charge of biological activity were found using pharmacophore analysis. For a few substances, ADMET predictions demonstrated acceptable pharmacokinetic characteristics and adherence to drug-likeness guidelines.

Discussion

Phytocompounds with potent inhibitory activity against MDR-TB and MRSA targets were successfully found using the integrated computational approach. By confirming binding affinity and pharmacokinetic feasibility, the combination of docking, molecular dynamics, and ADMET analysis improves reliability. Strong thermodynamic stability of specific compounds is suggested by stable MD trajectories and advantageous free energy values. The eligibility of the chosen compounds for additional experimental validation is further supported by drug-likeness filters. These results demonstrate the potential of substances derived from plants as substitute antimicrobial agents in the fight against infections that are resistant to drugs.

Conclusion

The current study shows that promising phytocompounds against MRSA and MDR-TB can be successfully found using computational drug development techniques. A few compounds showed: These compounds may be used as lead candidates for additional in-vitro and in-vivo validation investigations due to

their strong binding affinity, stable protein–ligand interactions, favorable pharmacophore characteristics, and acceptable ADMET profiles. The integrated approach offers a strong foundation for the development of antimicrobial drugs based on natural products.

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Modern Synthetic Organic Chemistry

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Introduction

Modern synthetic organic chemistry stands at the forefront of molecular innovation [1], enabling the precise construction of complex organic molecules for pharmaceuticals [2], agrochemicals [3], materials science [4] and chemical biology [5]. Over the past few decades, the discipline has evolved from classical functional group transformations to highly efficient, selective, and sustainable synthetic methodologies [6]. Central to this progress is the concept of retrosynthetic analysis, introduced by E. J. Corey, which provides a logical framework for deconstructing complex target molecules into simpler, accessible precursors [1].

Contemporary synthetic strategies emphasize step economy, atom economy, and environmental responsibility [7]. The development of transition metal–catalyzed cross-coupling reactions, such as the Suzuki–Miyaura coupling, has revolutionized carbon–carbon bond formation [2], while asymmetric catalysis has enabled the selective synthesis of enantiomerically pure compounds essential for modern drug development [8, 9]. Emerging approaches, including C–H activation, organ catalysis, photo-redox chemistry, and flow synthesis, further expand the synthetic toolbox by improving efficiency and reducing waste[10,11].

This chapter explores the principles, methodologies, and innovations that define modern synthetic organic strategies, highlighting their theoretical foundations, practical applications, and growing importance in sustainable chemical research and industrial production [12,13].

Transition Metal-Catalyzed Cross-Coupling Reactions

Transition metal-catalyzed cross-coupling reactions have revolutionized modern organic synthesis by providing robust and versatile strategies for forming carbon–carbon and carbon–heteroatom bonds. Since the pioneering work on palladium-catalyzed reactions in the late 20th century, these transformations have become

indispensable tools for the construction of complex molecules, ranging from pharmaceuticals and natural products to advanced materials. At the core of these reactions lies the ability of transition metals—such as palladium, nickel, and copper—to facilitate bond formation through well-defined catalytic cycles involving oxidative addition, transmetalation, and reductive elimination. This mechanistic versatility allows for high efficiency, broad substrate scope, and remarkable selectivity, making cross-coupling reactions a central component of synthetic strategy.

Over the past decades, significant advancements have been made in expanding the types of coupling partners, developing milder and more sustainable reaction conditions, and exploring asymmetric and stereoselective variants. The integration of novel ligands, heterogeneous catalysts, and innovative activation modes continues to push the boundaries of what can be achieved synthetically. This chapter provides a comprehensive overview of transition metal-catalyzed cross-coupling reactions, highlighting their mechanistic principles, key catalytic systems, and modern applications in complex molecule synthesis. Emphasis is placed on both classical methodologies and emerging innovations, providing a foundation for understanding and applying these reactions in contemporary chemical research.

Asymmetric Synthesis

Asymmetric synthesis, also known as enantioselective synthesis, is a cornerstone of modern organic chemistry, enabling the selective formation of chiral molecules with a defined three-dimensional arrangement. The ability to control stereochemistry is crucial because the biological, physical, and chemical properties of chiral compounds can differ dramatically between enantiomers. This is particularly important in pharmaceuticals, agrochemicals, and natural product synthesis, where one enantiomer often exhibits the desired activity while the other may be inactive or harmful.

Emphasis is placed on both classical approaches and cutting-edge developments, highlighting their applications in complex molecule construction and their significance in contemporary chemical research.

Organocatalysis

Organocatalysisis a rapidly growing field in modern organic synthesis, defined by the use of small, purely organic molecules to accelerate chemical reactions with high selectivity. Unlike traditional catalysis that relies on metals, organocatalysts are metal-free**,** environmentally friendly, and often compatible

with mild reaction conditions, making them highly attractive for sustainable and green chemistry applications.

The power of organocatalysis lies in its ability to control stereochemistry**,** enabling asymmetric transformations that produce enantiomerically enriched compounds. Common organocatalysts include chiral amines, cinchona alkaloids, ureas, thioureas, and phosphoric acids, which operate through various activation modes such as enamine, iminium, hydrogen-bonding, or Brønsted acid catalysis. These interactions allow precise control over reaction pathways, regioselectivity, and stereoselectivity, expanding the synthetic toolbox for constructing complex molecules.

Over the past two decades, organocatalysis has revolutionized the synthesis of natural products, pharmaceuticals, and fine chemicals, providing alternatives to metal-based catalysis while often offering simpler operational protocols and higher functional group tolerance.

Multicomponent Reactions (MCRs)

Multicomponent reactions (MCRs) are powerful synthetic strategies in organic chemistry in which three or more reactants combine in a single reaction vessel to form a product that incorporates substantial portions of all starting materials. This approach offers exceptional efficiency, atom economy, and step-economy, making it highly attractive for the rapid construction of complex molecular architectures.

MCRs are particularly valuable in the synthesis of heterocycles, natural product analogs, pharmaceuticals, and functional materials, as they enable the generation of molecular diversity with minimal purification steps. By integrating multiple bond-forming events into a single operation, MCRs reduce reaction time, waste, and energy consumption, aligning with the principles of green and sustainable chemistry. Over the past few decades, advances in catalyst design, reaction conditions, and mechanistic understanding have expanded the scope of MCRs. Modern strategies include isocyanide-based reactions, metal-catalyzed MCRs, organocatalytic MCRs, and domino or tandem processes, allowing chemists to access increasingly complex and functionalized molecules efficiently.

Green and Sustainable Synthesis

Green and sustainable synthesis represents a transformative approach in modern chemistry, aiming to minimize the environmental impact of chemical processes while maximizing efficiency, safety, and resource utilization. As global concerns about pollution, energy consumption, and chemical waste continue to

rise, the development of environmentally benign synthetic methods has become a central focus in both academic research and industrial applications. The principles of green chemistry emphasize atom economy, energy efficiency, use of renewable feedstocks, and reduction of hazardous reagents and solvents. Sustainable synthesis not only addresses environmental challenges but also offers economic advantages by reducing waste, simplifying reaction processes, and enabling safer handling of chemicals.

Recent advances in this field include catalysis using non-toxic metals, organocatalysis, biocatalysis, solvent-free reactions, and multicomponent or tandem reactions, all designed to achieve efficient and selective chemical transformations with minimal environmental burden. The integration of these strategies has allowed chemists to synthesize complex molecules, including pharmaceuticals, natural products, and materials, in a more sustainable and eco-friendly manner.

Photo-redox and Radical Chemistry

Photo-redox and radical chemistry have emerged as a transformative area in modern organic synthesis, enabling the formation of reactive radical intermediates under mild and controlled conditions. By harnessing the energy of light, photo-redox catalysis allows the generation of radicals through single-electron transfer (SET) processes, facilitating reactions that were previously difficult or impossible using conventional thermal or ionic pathways.

Radical reactions are uniquely versatile because radicals are highly reactive yet can be selectively generated and directed using appropriate catalysts, light sources, and reaction design. Photo-redox strategies often employ visible-light-absorbing catalysts, including transition-metal complexes (e.g., Ru and Ir complexes) **or** organic dyes**,** to achieve high efficiency and selectivity while minimising energy consumption and hazardous reagents. The combination of photoredox catalysis and radical chemistry has enabled innovative C–C and C–X bond formations, late-stage functionalizations, and complex molecular constructions**,** including in natural product synthesis, pharmaceuticals, and materials science. Recent advances also integrate asymmetric control, dual catalysis, and sustainable reaction conditions, making photoredox-mediated radical chemistry an essential tool in contemporary organic synthesis.

Conclusion

Modern chemical synthesis has evolved into a highly versatile and interdisciplinary field, integrating innovative strategies and technologies to

construct complex molecules efficiently, selectively, and sustainably. Retrosynthetic analysis provides the foundation for rational synthetic planning, allowing chemists to design efficient routes for target molecules. Building on this framework, transition metal-catalyzed cross-coupling reactions and asymmetric synthesis enable the precise formation of carbon–carbon and carbon–heteroatom bonds with high stereocontrol, while organocatalysis offers metal-free, environmentally benign pathways for enantioselective transformations.

Multicomponent reactions (MCRs) exemplify step- and atom-economical strategies, enabling the rapid assembly of structurally diverse compounds, whereas photoredox and radical chemistry leverage light-driven or radical-mediated processes to access transformations that are otherwise challenging under conventional conditions. Green and sustainable synthesis emphasizes environmentally responsible design, minimizing waste and energy consumption, and ensuring that modern synthetic practices align with ecological and economic priorities.

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Synthesis of Palladium Nanoparticles Using *Cassia absus* Seed Extract

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Abstract

The current study describes a biogenic, environmentally friendly method of producing palladium nanoparticles (PdNPs) utilizing seed extract from *Cassia absus*. The generated PdNPs were analysed using Fourier transform infrared spectroscopy (FTIR) and UV-visible spectroscopy. Using spherical PdNPs and a UV-visible spectrophotometer, the synthesis of PdNPs was verified. The functional groups found in the FT-IR spectrum suggested that the functional groups found in *Cassia absus* might have participated in the bio-reduction reaction for PdNPs synthesis. The produced PdNPs have antioxidant and anticancer qualities. It could be utilized as a non-toxic reducing agent to create PdNPs, which could then be applied in biological Process.

Keywords: *Cassia absus*, Pd Nps,

Introduction

Due to their exceptional optical capabilities, small size, and unique physiochemical features, noble metal nanoparticles have attracted a lot of attention lately. These nanoparticles have applications in energy storage devices, photochemistry, electronics, sensing, and medicines [1]. Various types of metal nanoparticles, such as gold (Au), silver (Ag), titanium, and zirconium, have been reported in the literature. These metal nanoparticles all have a variety of uses, such as catalysis and biomedicine [2, 3].

The prospective uses of palladium nanoparticle (PdNPs) catalysts in biotechnology, biomedical research, and medicine have generated a great deal of attention. Improvements in the production of palladium nanoparticles (PdNPs)

have become extremely important because to their high surface-to-volume ratio and high surface vitality, which make them useful for both homogeneous and heterogeneous catalysis [4]. Common manufacturing methods for delivering PdNPs include chemical [5-7], electrochemical, laser pulse ablation, and sono chemical reduction.

Methods and Materials:

Nanoparticle biosynthesis:

50 millilitres of *Cassia absus* seed aqueous extract and 90 millilitres of palladium acetate solution (1 mM) were combined in an Erlenmeyer flask. The reaction mixture was vigorously stirred at room temperature, and the formation of a brown hue signified the synthesis of PdNPs. The solution was centrifuged for 15 minutes at 2500 rpm to separate the colloidal suspension of metal nanoparticles, and impurities were removed by rinsing twice with deionized water.

Characterization of Nanoparticles

The biosynthesized metal nanoparticles were examined using UV-Visible Spectroscopy (Jasco V670 Spectrophotometer), Fourier Transformed Infrared Spectroscopy (FTIR SHIMADZU), and microscopic methods as scanning electron microscopy (SEM ZEISS EVO18).

Results and Discussion:

Characterization of Metal Nanoparticles

UV-Visible Analysis

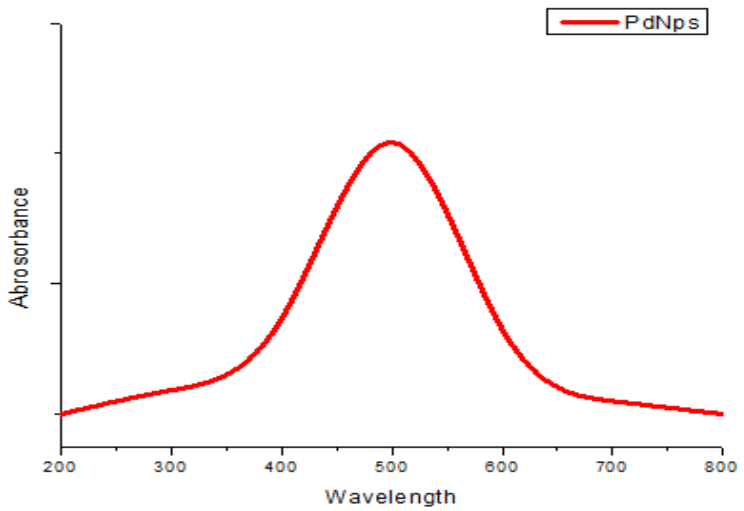

Fig.1. UV-Visible analysis of Cassia absus mediated synthesis PdNPs

The process by which *Cassia absus* aqueous extract promoted PdNP synthesis was examined using UV-visible spectroscopy. The color of the solution changed from brownish yellow to dark brown after a full day of incubation. The color shift in the resultant solution is caused by surface plasmon resonance (SPR), an inherent property of metal nanoparticles. Figure 1 displays the UV-Vis spectra for PdNP synthesis. PdNPs did not exhibit this characteristic peak because of its SPR. Similar findings were observed for the UV vis analysis of PdNPs, and no significant peaks that indicated the production of Pd(2+) of Pd ions appeared in this investigation after 24 hours.

FTIR Analysis

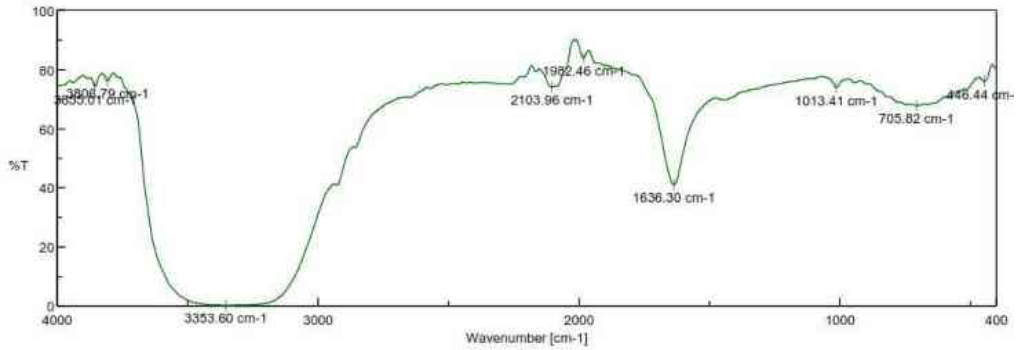

Fig. 2 Fig. 1. FT-IR spectra of PdNPs nanoparticles that were produced

The key compounds involved in the bio reduction process were identified by analysing the infrared spectra of the produced PdNPs and the extract from *Cassia absus*. (Fig. 2). The aqueous extract's spectra revealed strong signals at 1013 cm-1 (polysaccharides), 1636 cm-1 (amide I band), and 3353 cm-1 (hydroxyl group). Alkyl and amide-corresponding minor peaks were also seen at 2103 cm-1. On the other hand, functional moieties such phenolic compounds, which are involved in the reduction, process during PdNPs synthesis, exhibit a decrease in peak intensity in the infrared spectra of *Cassia absus*-assited PdNPs. The variations in peak intensity might be explained by polyphenols adsorption on the surface of metallic nanoparticles through the interaction of electrons in the absence of any potent ligating agents for the conversion of PdNPs.

Sem Analysis

Microscopic analysis of *Cassia absus* assisted PdNPs found by SEM indicated the presence of triangle-shaped particles (Fig. 3). The histogram revealed that the PdNPs' average particle size was 12.14 nm to 20.23 nm.

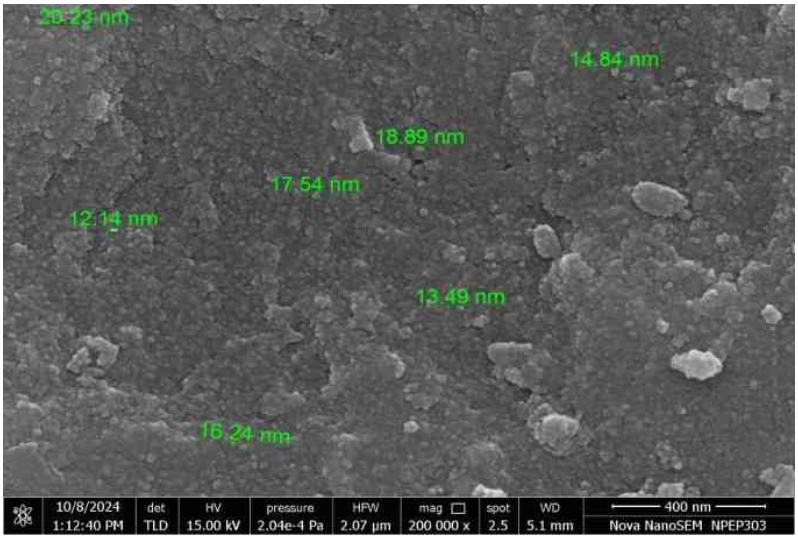

Fig.3. SEM analysis of synthesized pdNPs

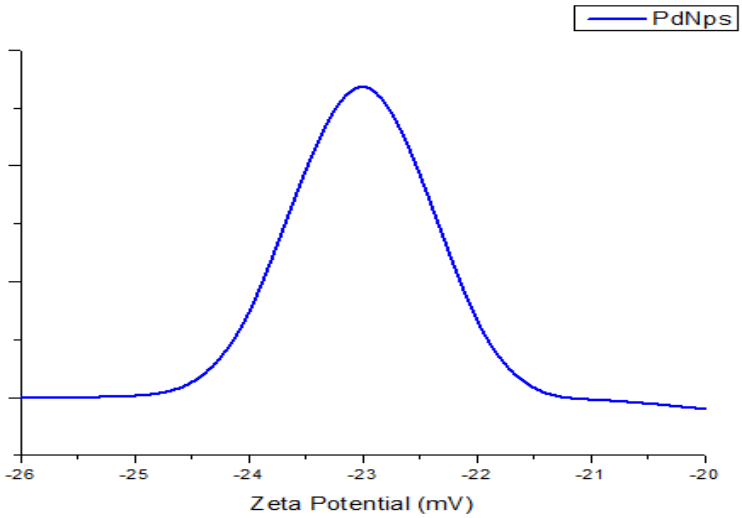

Figure 4: Zeta potential and DLS study of PdNPs mediated by Cassia absus

The zeta potential was used to assess the stability and surface charge of the produced PdNPs. It was discovered that the zeta potential was -23.2 mV (Fig. 4). The discovered zeta potential value, which ranges from -26 to -20 mV, indicates that the nanoparticles are stable and appropriate for biological functions. PdNPs have a particle size of 12 nm, according to DLS (Fig. 6). The particle sizes produced by these various methods are comparable. PdNPs produced by *Cassia absus* were clearly nan scale.

Conclusion

PdNPs were made from *Cassia absus* seed extract. The generation of PdNPs was verified by the color shift and UV-Vis spectrophotometry. The size distribution of spherical-shaped PdNPs was confirmed by SEM examination. The stability and surface charge of the generated PdNPs were examined using the zeta potential. The zeta potential was found to be -23.2 mV. In biological tests, the PdNPs showed significant antioxidant action. The researchers found that a cheap and effective source of PdNPs is *Cassia absus* seed extract.

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Study of Acenaphthylene-1,2'-Pyrrolidine-4',3''-Indoline

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Abstract

This study produced and studied a number of derivatives of acenaphthylene-1,2'-pyrrolidine-4',3''-indoline. Additionally, the best compound's molecular docking studies were examined for antibacterial efficacy. The chemical 5'-(4-methoxyphenyl)-1'-methyl-2H-dispiro [acena phthylene - 1,2'-pyrrolidine-4',3''-indoline]-2,2''-dione shown a strong affinity for the protein. Additionally, all of the produced compounds' antibacterial activity was assessed in vitro and in silico molecular docking, and the results demonstrated good antibacterial activity. The most active analogues were used in the kinetic analysis of enzyme inhibition. In conclusion, oxindole and indoline-2-3-dione-based compounds show high biological activity, which may help create more physiologically active derivative molecules.

Keywords: Synthesis, molecular docking, indoline, acenaphthylene, antibacterial

Introduction

A natural product is any substance produced by a living thing [1, 2]. Any substance produced by life is considered a natural product in the broadest sense [3]. Natural goods can be produced by full synthesis, and the advancement of organic chemistry can benefit greatly from a variety of synthetic goals. Therefore, natural goods simply contrast with those that are not found in nature, not with all products of artificial synthesis. Although natural food has distinct connotations, the term "natural commodity" was generalized for commercial purposes to include cosmetics, dietary supplements, and foods obtained from

natural sources without the addition of chemical additives [4].

In the organic chemical industry, natural products are typically defined as organic distilled chemicals that are separated from natural sources and produced by primary or secondary metabolism [5]. In the field of medicinal chemistry, the idea is also more restricted to secondary metabolites. Although secondary metabolites are not essential for life, they nevertheless help organisms evolve. The mechanism selects and configures different secondary metabolites as chemical warfare agents instead of prey, predators, and rival species [6-8]. Additionally, natural items can aid in the treatment of illnesses due to their pharmacological or biological activity.

Additionally, natural materials are active ingredients in many contemporary medications as well as the more popular ones. Additionally, it is possible to create synthetic versions of natural substances that are stronger and more protective. Additionally, the drug is still located using natural substances. In fact, natural products affect nearly half of the United States. drugs approved for use in food and medicine.

The chemical development of early preclinical drug manufacture has been significantly influenced by the chemistry of natural products, a separate area of chemical science. Research on exploration, understanding of traditional medicines and ethnopharmacology, development of chemical separation technologies, creation of cutting-edge methods for figuring out NMR chemical structures and other methods, and identification of pharmacologically beneficial regions of chemical diversity spaces. Furthermore, natural materials are created by organic synthesis and have a significant impact on the synthesis of organic compounds, creating significant challenges for synthetic methods and tactics [9–11].

The discovery of completely new chemicals (such as Woodward cis-hydroxylation, Sharp lower epoxy, and Suzuki–Miyaura cross-coupling) and the development of contemporary versions of older chemical reactions, such the Evans aldol reaction, are both greatly aided by natural products. In this way, natural products are the main focus of instruction for new synthetic organic chemical scientists.

Kinetic studies of enzyme inhibition (Indole Derivatives)

In order to comprehend the mechanism and types of inhibition of the most active analogues, 6a–e, this work carried out a kinetic investigation of enzyme inhibition (Table 2). Figure 8 shows the calculated kinetic parameters Vmax, Km, Ki, AICc, and R2. The kind of enzyme inhibitions was confirmed using Km and

Vmax values from Michaelis-Menten and Lineweaver-Burk double reciprocal plots, and all of the analogues had decreased Km and Vmax values. On the other hand, all analogues' Ki values were half of the IC50 numerical values, according to the Dixon plot's Ki value. Additionally, the type enzyme inhibitor mechanism was confirmed by the low AICc value and regression coefficient (R2) of curve fitting.

The data shown above (Figure 8) shows that all of the selected drugs have an uncompetitive type of enzyme inhibitor mechanism. The calculated values of Vmax and Km for pure enzyme (without inhibitor) were 965.5 ± 20 µM/min and 420.5 ± 020 µM, respectively.

Note: Mean ± SD (n = 3) is used to express values.

Additionally, a range of kinetics plots, including as the Dixon, Lineweaver-Burk, and Michaelis-Menten models, which showed uncompetitive inhibition, were used to interpret the reaction rate.

Table. Kinetic parameters and types of inhibition of analogues 6a-e.

Molecule	Vmax (µM/min)	Km (µM	Ki (µM)	AICc	R^2	Type of inhibition
6a	652.2 ± 12	315 ± 0.	0.090	230.1	0.910	Uncompetitive type
6b	614.2 ± 41	295 ± 0.	0.110	262.4	0.900	Uncompetitive type
6c	674.5 ± 20	275 ± 0.2	0.115	196.4	0.911	Uncompetitive type
6d	690.1 ± 52	345 ± 0.4	0.105	195.5	0.915	Uncompetitive type
6e	684.5 ± 40	340 ± 0.1	0.095	250.2	0.920	Uncompetitive type

Result and Discussion

Spectral analysis of 1'-methyl-5'-phenyl-2H-dispiro [acenaphthylene-1,2'-pyrrolidine- 4',3"-indoline]-2,2"-dione The reaction of oxindole, benzldehyde, acenaphthenequinone, and sarcosine produced the new hetro 1'-methyl-5'-phenyl-2H-dispiro[acenaphthylene-1,2'-pyrrolidine-4',3"-indoline]-2,2"-dione-compound F. Compound F was obtained with a satisfactory yield of 88%. The chemical melts between 136 and 140 degrees Celsius. The peaks that corresponded to the carbonyl (1719 cm-1) and NH (3245 cm-1) groups as well as other frequencies verified the IR spectra of chemical F. The production of chemical F is further confirmed by the 1H NMR spectra.

Aliphatic (1.91, 2.50, and 4.28 ppm), aromatic (7.23-7.54 ppm), and amine (11.58 ppm) proton signals were detected. The relevant carbon signals of

the spiro compound can be found in the resulting 13C NMR spectra of chemical F. The molecular ion peak is visible in the mass spectrum at 430.1254. According to the electronic spectra, the UV bands are located between 245 and 338 nm.

Conclusion

In conclusion, we used 1, 3-dipolar addition to create a number of spiroheterocycles by combining heterocyclic molecules like oxindole with carbonyl compounds like acetophenone/benzaldehyde and its derivatives with amino acid (sarcosine) and acenaphthenequinone. Spectrochemical techniques were used to characterize the high yield of new heterocyclic compounds produced by the reactions. Studies of the biological activity of the 10 produced compounds revealed that a couple of them were more active. This paper presents the data showing that these ten new compounds are more active than oxindole spiro compounds.

We were able to suggest a potential mechanism of biological action for oxindole and Indoline-2-3-dione derivatives by molecular docking studies. To move the two compounds that made the short list closer to medication creation, more investigation is needed. In conclusion, the compounds based on indoline-2-3-dione and oxindole have good biological activity, which could aid in the development of more physiologically active derivative molecules. In order to comprehend the mechanism and types of inhibition of the active 6a-e analogues, a kinetic analysis of enzyme inhibition is carried out.

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Fly Ash as a Sustainable Resource for Catalysis and Zeolite Synthesis

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Abstract

Fly ash is a residue generated from the combustion of coal in thermal power stations, possesses high thermal stability, metal oxides, porosity, and large surface area. These properties make it a low-cost material for catalytic applications, including catalysts, catalyst supports, and precursors for advanced materials like zeolites and photocatalysts.

Keywords: Fly ash, heterogeneous catalysis, catalyst support, photocatalysis, zeolite.

1.Introduction

The rapid expansion of industrial energy needs has led to a massive production of coal combustion residues, with fly ash being a major component. Fly ash is a grey, alkaline, abrasive, and refractory powder. It contains several essential nutrients beneficial for plant growth, including macronutrients such as P, K, Ca, and Mg, and micronutrients like Zn, Fe, Cu, Mn, B, and Mo. Owing to its favourable geotechnical properties such as specific gravity, internal friction, and permeability, and consolidation behaviour. Fly ash is widely used in construction projects like embankments and roads. Its pozzolanic nature, particularly its ability to react with lime, also makes it valuable in the production of cement, concrete, and other construction materials. Chemically, fly ash is rich in silica (60–65%), alumina (25–30%), magnetite, and Fe_2O_3 (6–15%), which allows it to be utilized in the synthesis of zeolites, alum, and precipitated silica [1-2]. Fly ash is generally divided into Class C (higher lime content, self-cementing) and Class F (higher silica and alumina, lower lime) depending on the coal source [3]. Traditionally disposed of in landfills or ash ponds, fly ash poses environmental risks [4-5]. Therefore, its conversion into value-added materials such as

adsorbents, catalysts, and photocatalysts has gained significant research interest for sustainable and economical applications.

This review objective is to present a systematic summary of fly ash for heterogeneous catalysis, support catalysis, photocatalyst and also including synthesis of zeolites.

2. Fly ash as sustainable catalyst for chemical processes

Fly ash contains metal oxides providing acidic–basic sites, high surface area, and porosity, enabling efficient, low-cost, sustainable catalysis.

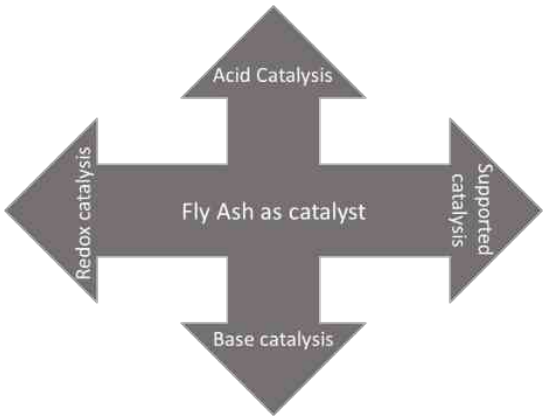

Fig.1. Schematic Representation of Fly Ash as an Acid–Base Supported Catalyst in Chemical Processes

2.1. Fly ash as heterogeneous catalyst

Fly ash, a silico-aluminate by-product of coal-fired thermal power plants, has gained attention as an inexpensive and sustainable catalyst or catalyst support in organic synthesis. A. Rani and her colleagues engineered an original solid-base catalyst by subjecting fly ash sourced from India's Kota Thermal Super Power Station to chemical and heat-based activation processes. The resulting solid base fly ash (SBFA) possessed increased hydroxyl groups on its surface, which enhanced surface basicity and created more active catalytic sites. The catalytic performance was evaluated through the solvent-free liquid-phase condensation of benzaldehyde with cyclohexanone, producing α, α′-dibenzylidenecyclohexanone with conversion above 70% and selectivity greater than 80% [6-7].

Similarly, S. K. Malpani and A. Rani prepared a solid acid catalyst using a microwave-assisted green method by recovering amorphous silica from fly ash and activating it with H_2SO_4, achieving high product yields in esterification and Friedel–Crafts alkylation reactions [8]. Furthermore, S. Fozooni and coworkers

reported hydrogen-peroxide-promoted fly ash as an efficient catalyst for solvent-free synthesis of oxazolone and imidazolone derivatives, offering advantages such as high yields, short reaction times, and good catalyst recyclability [9].

2.2. Fly Ash as a Photocatalyst

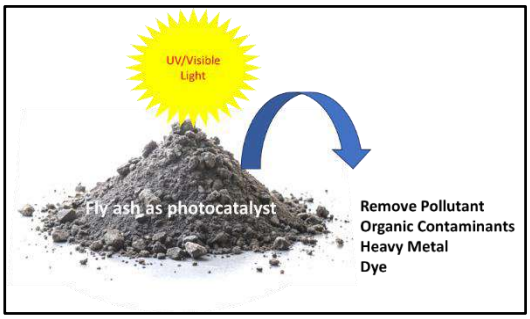

Fig.2. Schematic Representation of Fly Ash as Photocatalyst

The inclusion of semiconductor oxides like Fe_2O_3 and TiO_2 within the porous framework of fly ash positions it as a viable and effective candidate for photocatalysis and ecological restoration.

Li, Q. et al. coated $BiVO_4$ onto fly ash cenospheres (FAC) using a modified metal–organic decomposition method. SEM analysis revealed a dense $BiVO_4$ layer on the FAC surface, while silane coupling facilitated the formation of stable $BiVO_4$ films. XPS results confirmed the presence of lattice oxygen (OI) and adsorbed oxygen (OII) species, which contribute to photocatalytic activity [10]. Kim, H. Y. and co-workers fabricated FA/TiO_2 nanofibers through an electrospinning technique using titanium tetraisopropoxide, poly(vinylpyrrolidone), and fly ash. Once subjected to a thermal treatment at 600 °C, these fly ash-based nanofibers displayed significant adsorption and photocatalytic effectiveness in the degradation of methylene blue. Moreover, these composite materials demonstrated antimicrobial success in inhibiting Escherichia coli [11].

Similarly, Liu, S. et al. synthesized a α-Fe_2O_3-TiO_2/FAC composite using a sol–gel method. The photocatalyst achieved nearly 100% degradation of Rhodamine B within one hour, with hydroxyl radicals (•OH) identified as the dominant active species [12]. Mushtaq, F. et al. prepared $MnFe_2O_4$/CFA magnetic photocatalysts capable of degrading methylene blue under sunlight with ~100% efficiency in 30 minutes and good reusability [13]. Furthermore, Chuaicham, C. et al. developed ZnCr-MMO/FA composites that exhibited significantly enhanced photocatalytic degradation of ciprofloxacin due to improved charge separation and reduced electron–hole recombination. The

effectiveness of these materials in degrading organic pollutants, such as dyes and antibiotics, combined with their ability to remove heavy metals, demonstrates their high value for developing eco-friendly and sustainable water treatment systems [14]. Fly ash-based composites such as Cu/TiO_2, ZnO@FA, and CFA/C HNCPs show enhanced adsorption and photocatalytic efficiency for dye degradation and metal removal [15-17].

2.3 Zeolite Synthesis from fly ash

Several researchers have successfully produced zeolites by using coal-combustion residue using hydrothermal and alkali-based methods. Murayama, N. produced chabazite and zeolite P through alkaline hydrothermal synthesis at 393 K [18]. Inada, M. reported that early microwave irradiation during hydrothermal treatment accelerates the solubilisation of the silica and alumina fractions, promoting zeolite formation [19]. Ojha, K. prepared highly crystalline X-type zeolite with a BET surface area of 383 m^2/g via alkali fusion [20]. Querol, X. studied the effects of temperature, time, and alkali concentration on zeolite synthesis [21]. Other studies showed that microwave heating, mechanochemical methods, and acid pre-treatment enhance crystallization efficiency and adsorption properties of zeolites for heavy-metal removal from industrial wastewater [22-25].

3. Conclusion

Fly ash has gained significant research interest as a sustainable catalytic agent due to its wide availability, low cost, and rich composition of silica, alumina, and metal oxides. Its heterogeneous nature provides both acidic and basic active sites, enabling applications in chemical synthesis, oxidation, esterification, and environmental remediation

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Some Synthetic Methods Used in the Green Synthesis of Coumarin Derivatives

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Abstract

Coumarins possessing a biological activity, which have found applications in pharmaceuticals industry. Their activity and applications are dependent on their chemical structure. Therefore, the synthesis of coumarin derivatives is very important. The demand for these derivatives has increased generation of chemical waste. To minimize the production of toxic organic substances, green synthetic methods have been applied in a sustainable manner. These methods have gained significant attention over the last decade. Green chemistry covers a wide range of techniques. According to the studies discussed in this review, these approaches reduce the utilization and generation of toxic chemicals.

Keywords: Green Chemistry**,** Solvent free**,** one pot Synthesis**,** Microwave assisted**.**

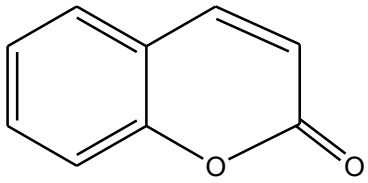
Introduction

Coumarins are heterocyclic compounds widely studied in synthetic organic chemistry. Owing to their diverse pharmacological properties, coumarin derivatives have attracted significant attention in medicinal chemistry, pharmaceutical development, cosmetics, and the food industry. Their biological activity—including anticoagulant, antimicrobial, antioxidant, anti-inflammatory, and anticancer properties—is strongly influenced by structural modifications on the coumarin nucleus.

The growing demand for novel coumarin derivatives has led to an increase in synthetic activity worldwide. However, conventional synthetic approaches often involve hazardous reagents, toxic organic solvents, high energy consumption, and the generation of substantial chemical waste. These drawbacks highlight the urgent need for sustainable and environmentally benign alternatives.

Green chemistry principles offer effective strategies to reduce environmental impact while maintaining or improving synthetic efficiency.

This chapter discusses methods applied to the preparation of coumarin derivatives, emphasizing sustainable technologies & their advantages over traditional methodologies.



Principles of Green Chemistry in Coumarin Synthesis

In the context of coumarin synthesis, green chemistry focuses on: purification Application of these principles has led to the development of innovative synthetic techniques that are both environmentally friendly and economically viable.

Green Synthetic Approaches for Coumarin Derivatives

Ultrasound-Assisted Synthesis

Ultrasound irradiation enhances chemical reactions through acoustic cavitation, which generates localized high temperatures and pressures. In coumarin synthesis, ultrasound:

- Shortens reaction time
- Increases product yield
- Reduces solvent usage
- Improves reaction selectivity

Ultrasound-assisted Pechmann and Knoevenagel condensations have demonstrated significant improvements compared to conventional heating methods.

Microwave-Assisted Synthesis

Microwave-assisted synthesis of coumarin derivatives:

- Reduces reaction time from hours to minutes
- Minimizes energy consumption
- Often eliminates the need for excess solvents
- Enhances product purity

Reactions such as the Pechmann, Perkin, and Knoevenagel condensations have been successfully adapted to microwave conditions.

Ionic Liquids and Deep Eutectic Solvents

Ionic liquids (ILs) and deep eutectic solvents (DES) are green alternatives to volatile organic solvents. Their advantages include chemical properties

These solvents often act as both reaction media and catalysts in coumarin synthesis, improving efficiency while reducing environmental hazards.

Solvent-Free Synthesis

Benefits include:

- Enhanced atom economy
- Simplified purification
- Reduced environmental impact
- Lower operational cost

Many condensation reactions for coumarin synthesis have been effectively performed under solvent-free conditions.

Mechanosynthesis

Mechan synthesis involves mechanical activation, typically using ball milling techniques. This approach:

- Avoids or reduces solvent use
- Enhances reaction rates
- Improves product yields
- Supports scalable and sustainable production

Mechanochemical Pechmann and Knoevenagel reactions have demonstrated promising results in coumarin derivative synthesis.

Multicomponent Reactions (MCRs)

Advantages include:

- High atom economy
- Reduced number of purification steps
- Lower waste generation
- Operational simplicity

MCR strategies have proven highly effective in synthesizing structurally diverse coumarin derivatives.

Green Adaptation of Classical Coumarin Reactions

Several traditional condensation reactions used for coumarin synthesis have been successfully modified using green chemistry approaches:

Knoevenagel Condensation

Widely applied for synthesizing substituted coumarins, this reaction has been adapted to microwave, ultrasound, solvent-free, and ionic liquid conditions.

Perkin Reaction

Green modifications include solvent-free conditions and alternative catalysts to minimize toxic by-products.

Kostanecki–Robinson Reaction

This method has been optimized using greener catalysts and reduced solvent systems.

Pechmann Condensation

One of the most common methods for coumarin synthesis, the Pechmann reaction has been extensively studied under microwave irradiation, ultrasound, ionic liquids, and mechanochemical conditions.

Reformatsky Reaction

Green strategies include the use of recyclable catalysts and environmentally benign solvents.

These adaptations demonstrate that classical synthetic pathways can be successfully transformed into environmentally sustainable processes.

Advantages of Green Synthetic Methods

Compared to conventional methods, green synthetic approaches offer several significant advantages:

- Reduced use and generation of toxic chemicals
- Higher product yields
- Improved purity
- Lower energy consumption
- Shorter reaction times
- Simplified post-synthetic processing
- Enhanced sustainability and economic feasibility

These benefits make green methodologies highly attractive for both academic research and industrial-scale production.

Challenges and Future Perspectives

These include:

- Scalability of laboratory techniques
- Cost and availability of certain green solvents
- Optimization of reaction parameters

- Standardization of green protocols
- Future research should focus on:
- Developing recyclable and biodegradable catalysts
- Expanding mechanochemical and solvent-free methodologies
- Integrating continuous flow systems
- Enhancing life-cycle assessment of coumarin production
- The continued advancement of green chemistry will play a crucial role in ensuring sustainable development in pharmaceutical and chemical industries.

Conclusion

Synthetic methods have revolutionized the synthesis of coumarin derivatives by aligning chemical innovation with environmental responsibility. Techniques such as ultrasound and microwave irradiation, ionic liquids, deep eutectic solvents, solvent-free synthesis, mechanosynthesis, and multicomponent reactions provide efficient and sustainable alternatives to conventional methods.

These approaches minimize toxic chemical usage and waste generation & enhance reaction efficiency, yield, purity, and energy performance. As research progresses, green chemistry will continue to shape the future of coumarin derivative synthesis, supporting environmentally sustainable industrial practices.

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Lithium Hydroxide Catalyzed Knoevenagel Condensation of Various Aldehydes

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Abstract

In this work LiOH used as a green Catalyst in the Knoevenagel condensation process of several aldehydes with ethyl cyanoacetate in DCM. The findings show that in the reaction of benzaldehyde with ethyl cyanoacetate, the sample with a 0.6 molar ratio of Al to Si had the best yield (98%) with 100% selectivity to the arylidene derivative.

Keywords: Lithium Hydroxide, Catalysed, Condensation, Aldehydes

Introduction

The creation of heterogeneous catalysts for unique chemical synthesis has emerged as a significant field of study. These materials' potential advantages over homogeneous systems—simplified recovery and reusability could result in environmentally friendly chemical processes in both academia and industry. An environmentally friendly substitute for chemical processes is the use of solid acidic and basic catalysts in sustainable chemistry and clean technologies. Together with waste reduction, simpler catalyst recovery processes, and safer and simpler operating techniques, the materials offer high yield and selectivity.

The development of polymer-supported catalysts on inorganic surfaces has received a lot of attention lately. It offers reduced environmental risks, ease of workup and product purification, and, for the most part, reusability of the polymer-supported catalysts. These materials combine the qualities of inorganic oxides (hardness, thermal and chemical stability, and transparency) with some of the benefits of organic compounds (simple processing using conventional techniques, elasticity, and organic functionalities). As a result, they have garnered significant interest [1, 2]. Additionally, using these materials provides an impressive and useful way to build innovative chemical libraries in a clean and

effective manner that may find usage in the agrochemical or pharmaceutical industries.

One of the most significant c–c bond-forming processes in organic chemistry is the Knoevenagel condensation reaction. When organic bases are present, this kind of condensation reaction often occurs in a homogenous solution [3]. Catalyst separation and recycling are two of this method's drawbacks. This transformation has been investigated utilising a variety of heterogeneous solid bases [4], such as hydrotalcite [5], hydroxyapatite-encapsulated γ-Fe_2O_3 [6], McM-41 [7], modified silica gel [8], MgO/ZrO_2 [9], and guanidine [10], in attempt to lower effiuents to ecologically acceptable limits.

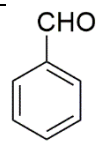
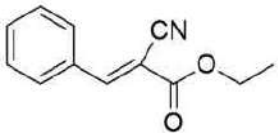
Result and Discussion:

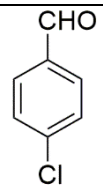
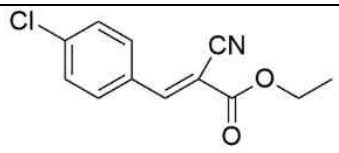
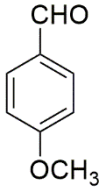
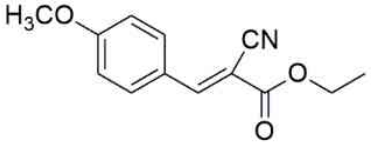
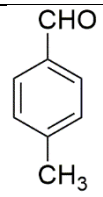
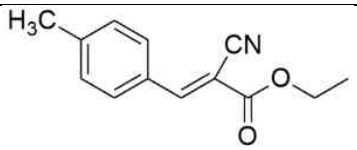
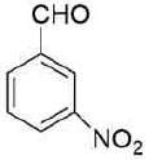
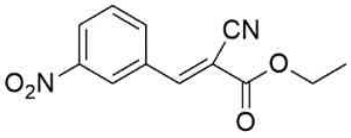
This method was carried out in different solvents and summarize as follow.

Sr. No	Solvent	Time (min)	% Yield
1	Water	120	10
2	DMSO	85	35
3	$CHCl_3$	55	65
4	CCl_4	30	85
5	DCM	10	95

First the reaction was carried out in water the time required is high and less yield was obtained then sane reaction is carried out in DMSO there is slight increase in yield. Finally same reaction was carried out in DCM minimum time is required with more yield.

Table 1: LiOH catalyses the Knoevenagel condensation reaction between ethyl cyanoacetate and aromatic and aliphatic aldehydes.

Sr. No	Aldehydes	Product	Time (min)	Yield %
1			10	97

2			12	92
3			15	90
4			11	89
5			10	87

General Protocol for the Knoevenagel Condensation:

Typically, a round-bottom flask containing 2 mmol of benzaldehyde (0.20 mL), 2 mmol of ethyl cyanoacetate (0.21 mL), and 0.04 g of catalyst lithium hydroxide was refluxed in DCM as a solvent while being continuously stirred. TLC tracked the reaction's development and completion. After cooling the combination and allowing the solvent to evaporate, a solid product was produced. The product was then identified by 1H-NMR, ^{13}C-NMR, and FT-IR spectroscopic techniques after the leftover solid was recrystallised using hot ethanol (5 ml).

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Study of Green Synthesis of Copper Oxide nanoparticles using *Pentalinon latium* Plant Extract

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Abstract

An important environmental issue is the increasing release of untreated textile effluents into aquatic environments. Stable synthetic colors are frequently not neutralized by conventional wastewater treatment. The green manufacturing of copper oxide nanoparticles (CuO NPs) as a sustainable option is examined in this chapter. CuO NPs were created and analyzed using SEM, FTIR, and XRD using *Pentalinon luteum* leaf extract as a reducing and capping agent. The resultant nanoparticles are strong candidates for the photocatalytic breakdown of hazardous industrial dyes because of their notable crystallinity and spherical shape.

1. Introduction

The textile, paper, and tannery industries are the main causes of water pollution in today's industrial environment. By preventing sunlight penetration and photosynthesis, the discharge of dye-laden effluents drastically affects aquatic flora by raising Biological Oxygen Demand. A revolutionary solution to this dilemma is provided by nanotechnology. CuO and other metal oxide nanoparticles have special optical, magnetic, and electrical characteristics. In contrast to conventional chemical synthesis, "Green Synthesis" uses phytochemicals originating from plants, such as tannins, phenols, and sugars, to decrease metal precursors. In keeping with the tenets of green chemistry, this approach is not only economical but also does away with the need for hazardous chemicals.

2. Materials and Experimental Methodology

2.1 Preparing Botanical Precursors and Extracts

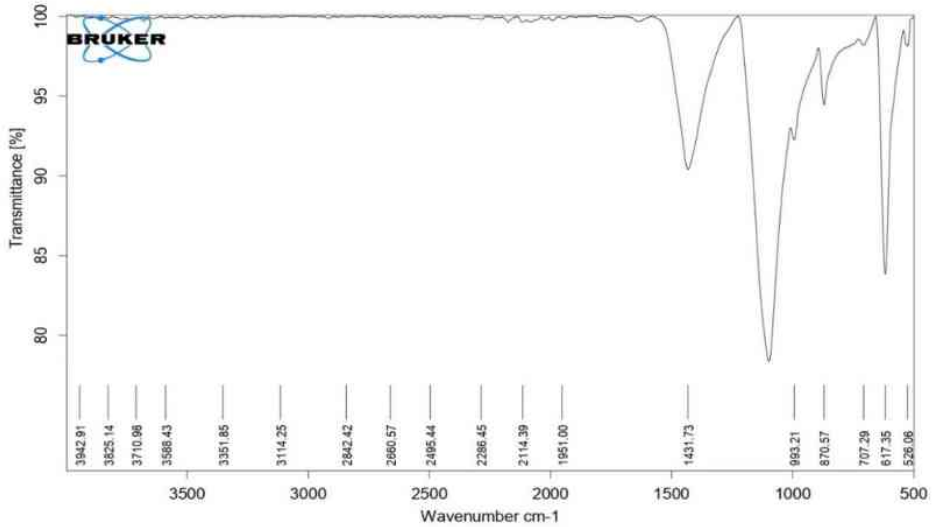
Pentalinon luteum leaves that were gathered from the Karjat district of Maharashtra, India, were used in the synthesis. The preparation entails: After being cleaned with deionized (DI) water, the leaves were left to air dry for six days. The dried biomass was ground into a fine powder. After dispersing 10g of powder in 300 mL of DI water, the mixture was heated to 70°C for 30 minutes. The bioactive substances needed for reduction are present in the resultant filtrate (Whatman No. 41).

2.2 Green Synthesis of CuO-NPs

A wet chemical method was used for the synthesis, which involved adding 2.496 g of copper sulphate to 100 mL of leaf extract. After a 24-hour stirring period, the solution was vigorously magnetically swirled for an hour at 70°C till precipitate formed. To get rid of contaminants, the product was centrifuged at 5000 rpm, dried at 100°C for 12 hours, and then cleaned with ethanol. To guarantee phase purity and crystallinity, the finished powder was calcined for two hours at 400°C.

3. Results and Characterization

3.1 Fourier Transform Infrared (FTIR) Analysis



FT-IR spectra of synthetic copper oxide nanoparticles are shown in Fig. 1

To determine the potential biomolecules in charge of the bio reduction of the produced copper oxide nanoparticles, FT-IR analysis was employed. The FT-IR spectra of copper oxide nanoparticles made from *Pentalinon luteum* leaves is

shown in Fig. 2. The stretching vibration of the Cu-O bond is represented by the absorption bands at 526.06 and 617.35 cm-1.

3.2 Morphological Analysis (SEM)

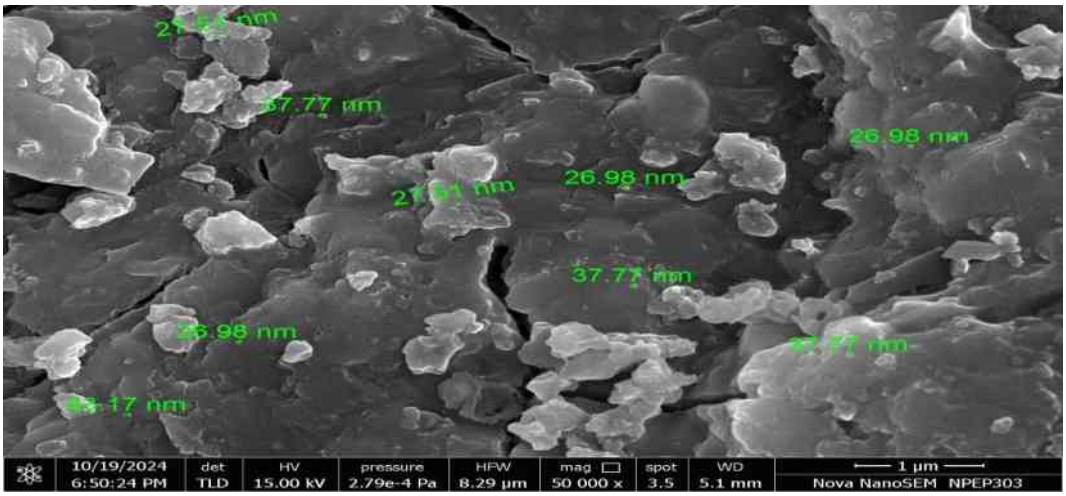


Figure 2: SEM pictures of nanoparticles of copper oxide

Images from Scanning Electron Microscopy (SEM) show that the produced CuO NPs are primarily spherical. The individual crystallite diameters stayed within the Nano scale range of 16.19 nm to 43.17 nm, despite some agglomeration, which is a typical feature of biogenic metal oxides.

3.3 TEM

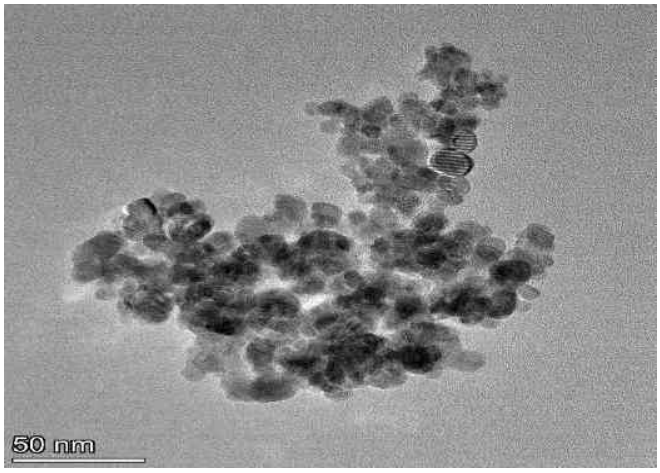


Figure 3: TEM Morphology Pictures

TEM examination was used to determine the size and shape of green produced tin oxide utilizing an aqueous extract from *Pentalinon luteum* leaves. Fig. 3.

Demonstrates how the green produced Copper oxide nanoparticles are spherical in shape and have a cluster-like appearance due to the aggregation of tiny particles. The green produced Copper oxide nanoparticles have a size range of 20–100 nm, according to TEM examination.

4. Discussion and Conclusion

4.1 Synergy of Phytochemicals

The Pentalinon Luteum extract's carbohydrates, flavonoids, and tannins help reduce the ions of Cu (II) to Cu (0), which is then oxidized and stabilized into CuO. High surface-area-to-volume ratios are produced by this environmentally friendly method, which increases the particles' effectiveness as electron carriers in catalytic reactions.

4.2 Conclusion

This work effectively illustrates a low-cost, environmentally acceptable method for producing CuO nanoparticles. The successful creation of crystalline, spherical CuO NPs is confirmed by the characterisation results. 18.17 nm is the average particle size. *Pentalinon luteum's* usefulness as a natural stabilizing agent. The produced nanoparticles have enormous potential for photocatalytic degradation, providing a workable technique to detoxify and decolorize wastewater from the textile sector while safeguarding aquatic biodiversity.

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Synthesis and Biological Evaluation of Pyrazoline Derivatives: Review

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Abstract

Pyrazolines, which are important heterocyclic rings consisting of five carbons and two nitrogens, play an important role in organic and medicinal chemistry as C=C double bonds across the two nitrogen atoms with varying levels of biofriendly properties and versatility. The ability to synthesise many different chemical classes from pyrazolines and have potential to treat first line antibiotics (anti-infectives), second line antibiotics (anti-infectives), third line antibiotics (antiseptic), fourth line antibiotics (analgesisics and antinflammatory agents), fifth line antibiotics (cytotoxics), and sixth line antibodies (antineoplastics) has encouraged research over the last decade on pyrazoline derivatives to synthesise less toxic than their natural counterparts.

Introduction

Medicinal chemists place important emphasis on the utility of heterocyclic compounds because many of them have demonstrated biological activities in numerous pharmacological areas. In addition to that, many researchers have also expressed continued interest in nitrogen-based heterocycles due to versatility and range of biological potentials; however, the pyrazolone class of compounds contains an extensive library of pyrazolone derivatives that exhibit drug candidates. The pyrazolone is one of five-membered heterocycles with two nitrogen atoms adjacent to each other and gives it basicity because of these nitrogen atoms. Additionally, the pyrazoline is a saturated dihydro compound of

the pyrazole and contains one endocyclic double bond (the double bond must also be counted as part of the overall charge). For instance, the three forms of the pyrazoline include the 1-pyrazoline, the 2-pyrazoline, and the 3-pyrazoline. The said forms depend on the location of the double bond within the chemical structure. Among the three pyrazoline isomers, the 2- pyrazoline is the most studied of the three isomers. Chalcones are compounds from the class of chemicals that have an abundance of applications in multiple industrial sectors due to their versatility [1-8].

Chalcones serve as key intermediates for synthesizing pyrazolines and other heterocycles. This article reviews advanced, efficient, and eco-friendly methods to produce pyrazoline derivatives from chalcones, accelerating their development. Natural pyrazoles are rare due to organisms' challenges in forming N-N bonds, with few reported in literature. Examples include piperidine alkaloids from Piperaceae plants like Piper nigrum (used for flavouring and remedies), sesquiterpene pyrazolines from Artemisia (with antibacterial, antifungal, and anticancer effects), and pyrazoline alkaloids from marine sponges/corals (cytotoxic and anti-inflammatory). Pyrazolines are prominent heterocycles prized in medicinal chemistry for diverse bioactivities [9-17].

Pyrazoline derivatives exhibit diverse pharmacological effects, serving as non-nucleoside HIV reverse transcriptase inhibitors, neurotensin receptor modulators for analgesia, non-steroidal mineralocorticoids, and agents for anticancer, antimicrobial, antitubercular, antimalarial, antifungal, antidiabetic, anti-inflammatory, antiviral, and cytotoxic applications. Medicinal chemists leverage the pyrazoline ring to design drug-like molecules, many of which appear in commercial therapeutics like sulfinpyrazone (uricosuric), oxyphenbutazone (anti-inflammatory), and methampyrone (analgesic/antipyretic). These compounds also show promise against neurodegenerative diseases such as Alzheimer's and Parkinson's. Structural modifications enhance efficacy, safety, and broad therapeutic potential [18-22].

Clinically Available Drugs Containing Pyrazoline Scaffolds

Pyrazoline rings have become critical frameworks for the design of new medications, due to their many potential uses. Some examples include ramifenazone/anti-inflammatory; antipyrine/anti-inflammatory; morazone/anti-inflammatory; famrofazone/ anti-inflammatory; muzolimine/diuretic; metamizole/antipyretic; edaravone/amyotrophic lateral sclerosis; ibipinabant/CB1 receptor inverse agonist; and axitinib/VEGFR-2 inhibitor (a second-generation

VEGFR inhibitor for treating metastatic renal carcinoma) [23-24].

Conclusion

Benefits of pyrazoline derived anticancer agents utilizing the low toxicity, high potency and many therapeutic mechanism properties the pyrazoline derivatives have proven to be useful in the development of anticancer agents various studies on the anticancer properties of different pyrazoline structures have been conducted to determine if there is any antibacterial or antifungal activity in the substance. The review summarises some key research efforts on pyrazoline based drugs. The key discussion points include the advantages that chalcone-derived pyrazolines show when used in combination with other therapies to enhance their efficacy. Further studies of the structure activity relationships (SAR) of various substituents of the pyrazoline scaffold have been conducted to show how certain substituents inhibit biological targets. The review also focuses on one of the main aspects of designing derivatives with improved selectivity and bioavailability. In addition to other considerations, the review highlights some of the main factors of the toxicity profile and mechanisms of action (Biological Mechanism) of pyrazoline's. Thus, allowing for a comparison between molecular design and the metabolic results. Overall, the review provides an overview of recent progress in the development of synthetic routes for pyrazolines to produce pyrazolines with highly active biological properties, to aid researchers looking to develop new agents for the treatment of oncology and infectious disease.

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An Efficient Synthesis of 1, 3-Oxazine Derivatives Catalyzed Under Humic Acid as a Green Catalyst

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Abstract

We found that humic acid promoted the green synthesis of 1, 3-oxazine compounds. The process requires just 15 mg of catalysts for complete transformation. The condensation reaction of formaldehyde with primary amines, and β-naphthol/α-naphthol containing electron-withdrawing and electron-donating substituents, via mild reaction conditions at room temperature catalysed under humic acid to produce as an effective and green precursor in multicomponent reaction. This technique offers various advantages over new synthetic approach, including mild, low cost, catalyst recyclable, and slower time for reaction.

Keywords: β-naphthol, Amines, Formaldehyde, Humic acid, Solvent-free reaction.

1. Introduction

Over the last decade, corporations and research scientists have created and accepted the one-pot multicomponent reaction as a viable tool for synthesizing innovation in the development of drug procedures. [1-3] Multicomponent reactions (MCRs) are a pure efficient technology with major properties such as a high rate of conversion, a few by-products, quick production of chemicals with complex structures, and a diverse selection of molecules for biomedical design factors. [4] An excellent method used mild or aqueous condition is widely used in combination or gaining importance to traditional biological usage as an outcome of the above intractable challenges. [5-8]

Altered 1, 3-oxazine molecules have drawn a great deal of attention because of their distinct biologically active elements and their

antimicrobial, anti-cancer, anti-malarial, and anti-HIV properties as show in Figure 1. [9, 10] *Burke and co-workers investigated* in 1953 the synthesis of different derivatives undergo Mannich-type reaction with β-naphthol, aryl amine, and formaldehyde. [11, 12] In part because of their diverse biological properties, 1, 3-oxazine analogs which include anticonvulsants, [13] analgesic, [14] antibacterial, [15] anti-cancer, [16] anti-tubular,[17] other actions garnered a lot of interest. Previously, the oxazine synthesis variety of methods has been reported. [18-21] The synthesis of various derivatives has been developed via multi-component reactions. [22] Many efforts are taking place to promote ecologically suitable and affordable biosynthetic methods for biochemical modifications that use water, mild, or catalyst-free conditions instead of poisonous chemicals, which are incombustible and benign.[23-31]

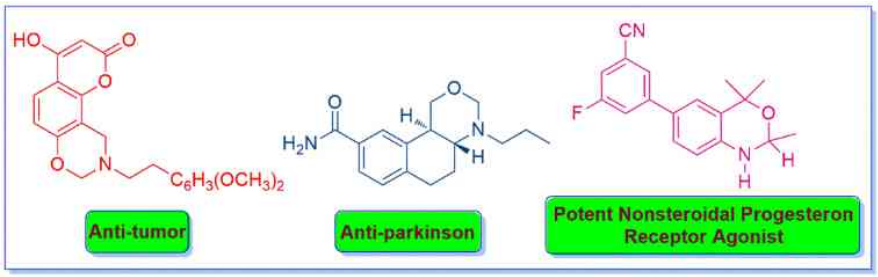
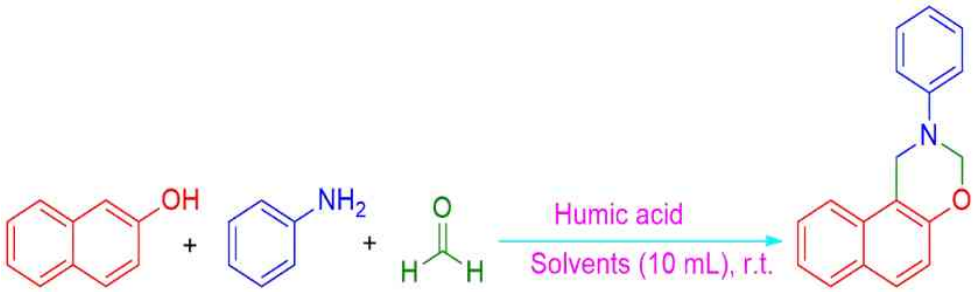


Figure 1. Biologically active molecules for industrial development

2. Results and discussion

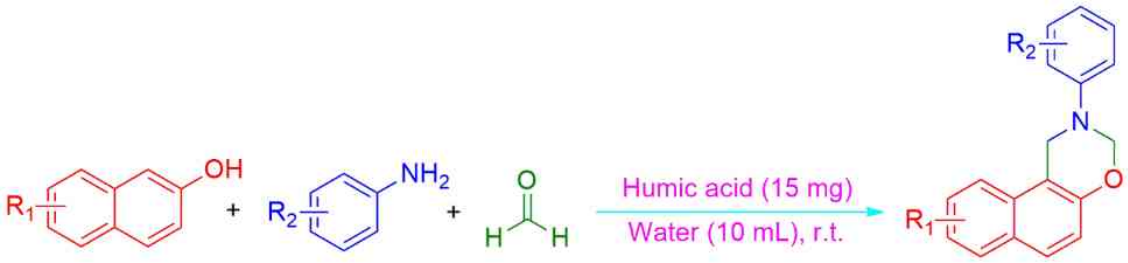
The 1, 3-Oxazine compounds were synthesized under aqueous medium at r.t. using the humic acid. The 98% yield have been observed under 15 mg catalyst added in the reaction. **(Scheme 1)**



Scheme 1: Oxazine derivatives prepared undergo humic acid

A wide area of scientific methodology of aromatic amine substrate with electron-donating and electron-withdrawing substrate react with formaldehyde and β-naphthol to prepare the 1, 3-oxazine substrate to form excellent results. **(Table 2)**

Table 2 Various derivatives study of 1, 3-oxazine [a]



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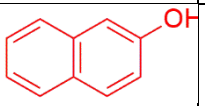
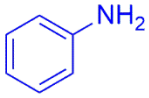
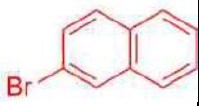
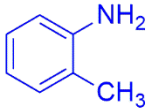
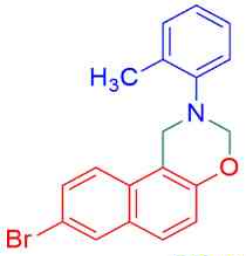
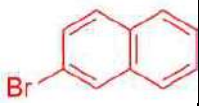
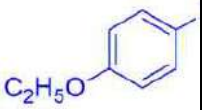
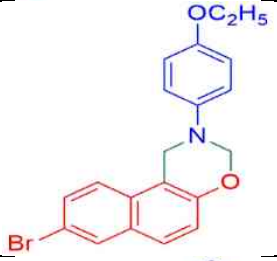
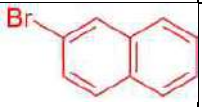
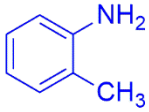
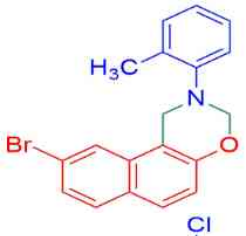
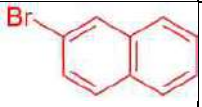
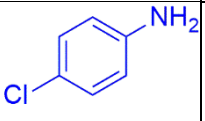
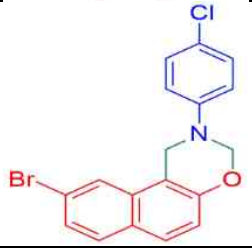
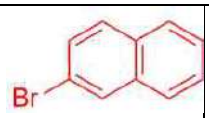
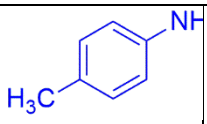
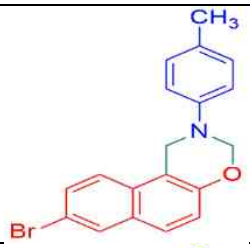
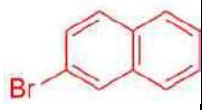
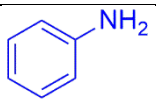
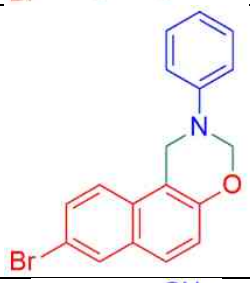
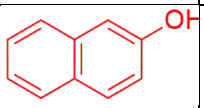
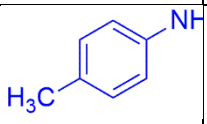
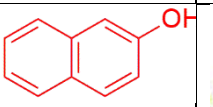
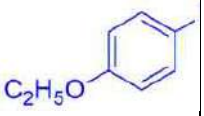
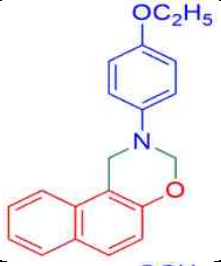
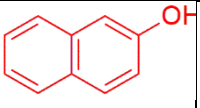
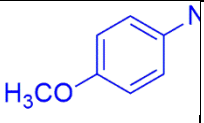
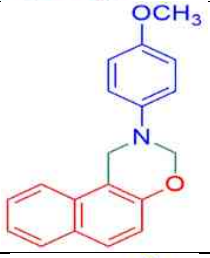
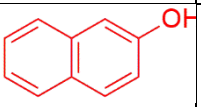
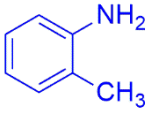
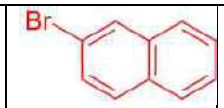
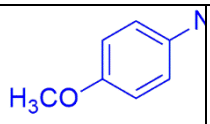
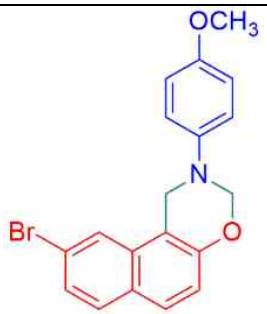
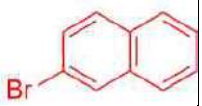
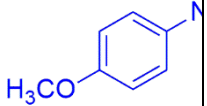
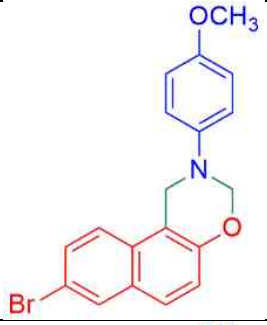
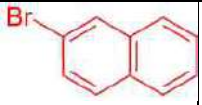
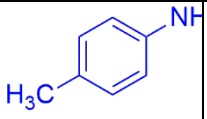
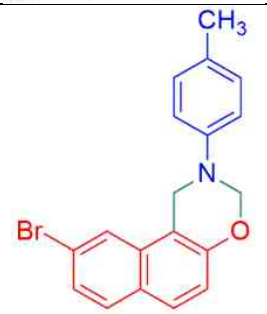
1				20	98
2				30	91
3				30	94
4				35	92
5				30	95

6				30	93
7				30	96
8				30	96
9				30	94
10				20	96
11				30	98

12				20	98
13				20	98
14				20	94

[a] Parameter: Aniline (10 mmol), *β*-naphthol (10 mmol), Humic acid (15 mg), and formaldehyde (20 mmol) in water (10 mL), [b] Product in %

3. Conclusion

Humic acid is a biodegradable, recoverable, inexpensive, and readily accessible organic acid to preparation of the product by using β-naphthol, amine, and formaldehyde aaded in water under at 30°C temperature. This approach is highly effective and eco-friendly, and it exemplifies the minimum requirements for biological activity.

4. Experimental Section

The reaction carried out in between formaldehyde (0.06 g), aniline (0.93 g), β-naphthol (1.44 g), and humic acid (15 mg) in water (10 mL) with continue stirring at room temperature. The reaction conversion is identifying by using aluminium TLC plate. When complete conversion of reaction has been made then mixture was added in (5 mL) water and filter it. The aqueous layer of humic acid

was recycled and reused for the next 4 cycles without losing acidic properties. Spectral data:

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Nanomaterial Synthesis Methods of Niobium Dioxide: Review

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Abstract

This review explores various contemporary synthesis methodologies for niobium dioxide nanomaterials, emphasizing their structural, optical, and electrical properties. The excerpt highlights the difficulty in synthesizing pure niobium dioxide (NbO_2) nanostructures due to the stability of niobium pentoxide (Nb_2O_5) and NbO_2's narrow stoichiometric range. It then introduces various synthesis methods and emphasizes the importance of understanding how synthesis parameters influence the material's properties for advanced electronic applications. In this review we have identifies three primary fabrication routes: physical vapor deposition, wet chemical synthesis, and thermal reduction.and also wet chemical methods, including hydrothermal and solvothermal processes, offer scalable routes for producing diverse morphologies such as nanorods and nanospheres.

Keywords*:* Niobium dioxide, Nanoparticles, synthesis methods

Introduction

Niobium dioxide (Nb_2O_5) is a narrow-gap n-type semiconductor with a bandgap typically ranging from 0.5 eV to 1.2 eV [1]. It has attracted considerable academic and industrial interest due to its second-order Peierls-type metal-insulator transition at ~1081 K, a relatively high temperature. [2,3]. This transition is accompanied by a structural shift from a distorted body-centered tetragonal phase (I41/α) to a symmetric rutile phase (P42/mnm), driven by the

pairing and unpairing of Nb-Nb dimers [3,4]. The ability to trigger this transition via thermal or electrical stimuli results in current-controlled negative differential resistance, making NbO2 a prime candidate for threshold selectors in 3D stackable resistive random-access memory and neuristors for neuromorphic computing [5–7].

its promising characteristics, the synthesis of pure-phase (Nb_2O_5) nanomaterials remains a technical challenge [7]. Niobium pentoxide (Nb_2O_5) is the most thermodynamically stable state in the niobium-oxygen system, and (NbO2) itself exists within a very narrow stoichiometric range, often leading to the formation of mixed-phase NbOX or over-stoichiometric nanoparticles [1,8,9]. Furthermore, while bulk NbO2 properties are well-documented, the performance of (Nb_2O_5) in nanostructured forms—such as nanorods, nanosheets, and thin films is highly sensitive to the precise control of morphology, crystallinity, and oxygen vacancy concentration during processing [8,10].

To address these challenges, several nanomaterial synthesis strategies have been developed. Hydrothermal and solvothermal methods are widely utilized for their efficiency in producing controlled morphologies like nanorods and nanospheres at relatively low temperatures [10,11]. Other prominent techniques include the thermal reduction of Nb2O5 precursors using carbon-based reducing agents at high temperatures, and physical vapor deposition methods such as RF magnetron sputtering followed by vacuum annealing to induce crystallization [7–9]. This section reviews the methodologies for synthesizing NbO2nanostructures, emphasizing the relationship between synthesis parameters and the resulting structural and electronic properties.

Synthesis Methods

Physical Vapor Deposition: PVD techniques, particularly magnetron sputtering, are widely used for the fabrication of polycrystalline (Nb_2O_5) thin films [12].

Magnetron Sputtering: High-quality films can be produced using a metallic Nb target in an optimized argon–oxygen atmosphere [12]. Optimal deposition conditions identified for homogeneity and crystallinity include a DC power density of 9.87 W Cm-1 a substrate temperature of 720^0C, and low gas pressures of 8 m torr [12]. Alternatively, films can be sputtered from stoichiometric ceramic (Nb_2O_5) targets, though these often result in amorphous phases that require post-deposition vacuum annealing to become polycrystalline [7,8].

Molecular-Beam Epitaxy: For achieving single-phase rutile NbO2 films, MBE is employed at growth temperatures between 660^0 C and 770^0 C [13]. Precise

control of oxygen partial pressure is necessary to avoid the formation of undesired NbO or (Nb_2O_5) phases [13].

Wet Chemical Synthesis: Wet chemical routes, such as hydrothermal and solvothermal processes, are valued for their scalability and ability to produce various morphologies like nanorods and nanospheres [10].

Hydrothermal Reduction: This involves heating niobium precursors, such as niobium oxalate or NbCl5, in an autoclave at temperatures typically ranging from 1600 C to 2000 C [14]. Oxalic acid often acts as a reducing agent in these reactions, facilitating the formation of lower oxidation state oxides like tetragonal (Nb_2O_5) and cubic NbO [14].

Surface-Mediated Growth: Specialized nanostructures can also be grown by placing substrates (like metallic niobium films) in an alkaline solution, such as 0.01MKOH, and heating them to 1750 for 6 hours in a high-pressure reactor [15].

Thermal Reduction:

This solid-state methodology involves the reduction of pre-synthesized Niobium Pentoxide (Nb_2O_5) precursors.

Process: The synthesis is accomplished by heating (Nb_2O_5) at elevated temperatures in the presence of reducing agents [9].

Reducing Agents: Carbon is frequently used as a reducing agent for this purpose [9]. Additionally, (Nb_2O_5) can be reduced to (Nb_2O_5) or NbO when heat-treated in a hydrogen (H2) atmosphere [16].

Conclusion:

Niobium dioxide (Nb2O5) is a vital material for future electronics because it can switch between an insulator and a conductor when triggered by heat or electricity. This unique property makes it a top choice for building advanced computer memory and high-speed electronic switches. The review of synthesis methods shows that while vacuum-based techniques like sputtering create very high-quality films, they often require extremely high temperatures. On the other hand, chemical methods like hydrothermal synthesis are more flexible and can grow tiny rods and particles at much lower temperatures, making them easier to produce on a larger scale. Another common method involves heating existing niobium oxides with carbon to transform them into (Nb_2O_5) though this requires very careful control to avoid creating the wrong type of oxide. The biggest challenge moving forward is finding ways to create pure (Nb_2O_5) more reliably. To use this material in everyday gadgets, future research

must focus on making these high-performance structures at lower temperatures that won't damage other parts of a computer chip.

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Innovation in Science and Technology

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Abstract

Scientific and technological innovation is essential to expanding knowledge, raising living standards, and fostering long-term economic prosperity. It entails the creation and use of novel concepts, techniques, and technologies that turn scientific discoveries into workable answers to societal problems. Modern research and industrial development have been greatly impacted by the rapid advancements in disciplines like information technology, biotechnology, nanotechnology, and renewable energy. These developments have reinforced communication networks, increased productivity, improved healthcare systems, and promoted environmental sustainability. Research and development initiatives, industry-academia cooperation, and successful government policies that promote scientific inquiry and technical development all contribute to the process of innovation. Innovation has many advantages, but it also has drawbacks, including a lack of money, moral dilemmas, and national differences in technology. To maintain innovation and guarantee long-term scientific and technological advancement, ongoing investments in education, research facilities, and interdisciplinary cooperation are crucial. This chapter emphasises the idea, importance, major forces, and new developments in scientific and technological innovation, highlighting its influence on how society will develop in the future.

Introduction

Global competitiveness, social advancement, and economic growth are now all fuelled by scientific and technological innovation. Technological breakthroughs and scientific discoveries constantly transform businesses, enhance people's quality of life, and address difficult global issues, including energy scarcity, healthcare crises, and climate change [1,2]. Innovation is the process of turning novel concepts, information, and scientific discoveries into useful applications, goods, procedures, or services that benefit society [3,4]. Rapid advancements in

sectors including biotechnology, nanotechnology, renewable energy, artificial intelligence, and information technology have transformed scientific research and economic development during the past few decades [5].

Scientists and engineers are now able to solve complicated problems more successfully thanks to the integration of interdisciplinary techniques, which has further accelerated innovation [6]. Governments, academic institutions, and business sectors all play vital roles in fostering innovation through research funding, policy support, and cooperation networks.

This chapter discusses the concept of innovation in science and technology, including its importance, important technological fields, challenges, and prospects [7,8].

Concept of Innovation

The process of introducing novel concepts, techniques, goods, or technologies that enhance current systems or produce completely original solutions is referred to as innovation. Research and development (R&D), experimentation, and the application of scientific knowledge are frequently the sources of innovation in scientific and technological contexts.

Innovation can be categorised into several types:

- **Product Innovation:** Product innovation involves the development of new or significantly improved goods and services. Examples include smartphones, electric vehicles, and advanced medical devices.
- **Process Innovation:** Process innovation refers to improvements in production or operational methods that increase efficiency and reduce costs. Automation in manufacturing and digital technologies in supply chain management are examples.
- **Technological Innovation:** Technological innovation involves the application of scientific discoveries to develop new technologies that transform industries and everyday life.
- **Social Innovation:** Social innovation focuses on developing solutions that address societal challenges such as poverty, healthcare access, and education.

Importance of Innovation in Science and Technology

Innovation plays a vital role in shaping modern societies. Its significance can be understood through several key aspects:

- **Economic Growth**

Technological innovation enhances productivity, creates new industries, and

generates employment opportunities. Countries investing heavily in research and development often achieve higher economic growth.

- **Improvement in Quality of Life**

Innovations in healthcare, communication, transportation, and energy improve living standards and provide solutions to everyday problems.

- **Advancement of Scientific Knowledge**

Innovation drives scientific exploration and discovery, expanding our understanding of the natural world.

- **Global Competitiveness**

Nations that promote innovation are better positioned to compete in the global economy.

- **Drivers of Innovation**

Several factors contribute to the development and promotion of innovation in science and technology.

- **Research and Development (R&D)**

Investment in R&D is a fundamental driver of innovation. Universities, research institutions, and industries conduct research to generate new knowledge and technological solutions.

- **Education and Skilled Workforce**

A well-educated workforce with strong scientific and technical skills is essential for fostering innovation.

- **Government Policies and Funding**

Governments support innovation through research grants, tax incentives, intellectual property protection, and infrastructure development.

- **Collaboration and Networking**

Collaboration between academic institutions, industries, and government agencies facilitates knowledge exchange and technological progress.

Major Areas of Technological Innovation

- **Information and Communication Technology (ICT)**

Advances in computing, cloud technology, and digital communication have transformed global connectivity, data management, and business operations.

- **Artificial Intelligence and Machine Learning**

Artificial intelligence enables machines to perform tasks that require human intelligence, such as data analysis, pattern recognition, and decision-making.

- **Biotechnology**

Biotechnology has revolutionised medicine, agriculture, and environmental management through genetic engineering, vaccine development, and biopharmaceuticals.

- **Nanotechnology**

Nanotechnology involves the manipulation of materials at the nanoscale, leading to innovations in electronics, medicine, and materials science.

- **Renewable Energy Technologies**

Renewable energy sources such as solar, wind, and bioenergy are critical for sustainable development and reducing dependence on fossil fuels.

Role of Universities and Research Institutions

Innovations in science and technology are largely produced by universities and research centres. These institutes support the creation of new technologies and scientific discoveries through interdisciplinary cooperation, laboratory testing, and academic study.

Universities' technology transfer offices, incubator centres, and startup ecosystems make it easier to commercialise research discoveries and bring ideas to market.

Challenges in Innovation

Despite its importance, innovation faces several challenges:

- **Limited Funding**

Insufficient financial support for research and development can hinder technological progress.

- **Intellectual Property Issues**

Balancing the protection of intellectual property rights with the open sharing of scientific knowledge can be challenging.

- **Ethical and Social Concerns**

Technologies such as artificial intelligence, genetic engineering, and surveillance systems raise ethical and societal questions.

- **Technology Gap**

Developing countries often face barriers in accessing advanced technologies due to limited infrastructure and resources.

Future Prospects

It is anticipated that multidisciplinary research, digital transformation, and

sustainable development objectives would propel scientific and technological innovation in the future. Future developments will be greatly influenced by emerging technology including smart cities, improved materials, quantum computing, and space exploration technologies.

International collaboration and open innovation platforms will further accelerate scientific progress and technological development. Governments and institutions must continue to invest in education, research, and infrastructure to support innovation.

Conclusion

The technological innovation is a major driver of economic growth and societal advancement. Innovation solves global issues and enhances human well-being by turning scientific discoveries into useful applications. To maintain innovation and guarantee a sustainable and successful future, ongoing investments in research, education, and cooperation are crucial.

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