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RECENT PROGRESS IN CHALCONE DERIVATIVES: SYNTHETIC STRATEGIES, PHARMACOLOGICAL ACTIVITIES AND MOLECULAR INSIGHTS

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ABSTRACT

Chalcones represent an important class of flavonoid-related compounds that occur in both natural and synthetic forms. They are structurally characterized by an α, β- unsaturated carbonyl framework, which plays a crucial role in their chemical reactivity and pharmacological potential.[6,7] These compounds are widely distributed in plants and are involved in various physiological processes, including defense mechanisms and metabolic functions.[13] Owing to their simple structure and ease of modification, chalcones have gained significant attention as promising scaffolds in medicinal chemistry and drug discovery.[17,21] Conventional synthetic approaches such as Claisen-Schmidt condensation remain widely used; however, recent advancements have introduced modern techniques including micro- assisted synthesis and green chemistry approaches that improve reaction efficiency, reduce time, and minimize environmental impact.[1,2,14] Chalcone derivatives exhibit a wide range of biological activities, including antimicrobial, anti-inflammatory, antioxidant, anticancer, and antitubercular effects. These properties are primarily attributed to the presence of an electrophilic α,β- unsaturated carbonyl group, which facilitates interaction with biomolecular targets such as enzymes and proteins.[6,12] Furthermore, computational approaches such as molecular docking and in silico studies have enhanced the understanding of ligand-target interactions, thereby supporting rational drug design.[60-62] This review provides a comprehensive overview of recent developments in chalcone chemistry, including synthesis, characterization, biological activities, and mechanisms of action. Special emphasis is placed on structure-activity relationship (SAR) and the influence of substituents on biological properties. The future potential of chalcone derivatives in pharmaceutical research is also highlighted.

KEYWORDS: Chalcone; Claisen –Schmidt condensation; Microwave synthesis; Green chemistry; Antimicrobial; Molecular docking; SAR.

1. INTRODUCTION

Chalcone are an important class of bioactive compounds belonging to the flavonoid family, chemically defined as 1,3-diary-2-propen-1-one derivatives.[6,7] their structure consists of two aromatic rings linked by a three-carbon α,β-unsaturated carbonyl system, which is responsible for their unique physicochemical and biological properties. Due to their structural simplicity and high reactivity, chalcones serve as valuable intermediates in organic synthesis and are widely explored as pharmacologically active scaffolds.[17,21]

Naturally occurring chalcones are found in a variety of plant sources such as liquorice and hops, where they act as key intermediates in the biosynthesis of flavonoids and related compounds.[13,17] These molecules contribute to plant defense mechanisms by exhibiting antimicrobial and antioxidant activities. Their diverse pharmacological potential has attracted considerable attention in recent years, particularly due to their ability to interact with multiple biological targets.[13]

Numerous studies have reported that chalcone derivatives possess a broad spectrum of biological activities, including antimicrobial, anti-inflammatory, anticancer, and antiviral properties.[6,16] These activities are largely associated with the α,β-unsaturated carbonyl moiety , which acts as an electrophilic centre capable of reacting with nuleophilic sites in proteins and enzymes, thereby modulating various cellular pathways.[12]

Recent developments in chalcone research have focused on improving synthetic strategies and expanding their pharmacological applications. Traditional methods are increasingly being complemented by modern approaches such as microwave-assisted synthesis and environmentally friendly techniques, which offer advantages such as reduced reaction time, improved yields, and sustainability.[1,2] In addition, computational tools such as molecular docking and quantitative structure – activity relationship (QSAR) studies have provided deeper insights into chalcone-target interactions, facilitating the design of more potent derivatives.[30,60]

This review aims to present a detailed overview of chalcone chemistry, including synthesis, characterization, biological activities, mechanism of action, and structure-activity relationships, with a focus on their potential applications in drug discovery.

2. CHEMISTRY OF CHALCONES

Chalcones are characterized by the presence of an **α, β-unsaturated carbonyl system,** which plays a crucial role in their reactivity and biological activity, The general structure can be represented as.

Ar– CO– CH=CH– Ar´

where Ar and Ar´ are aromatic rings.[7]

2.1 Structural Features

The conjugated system present in chalcones allows electron delocalization the molecule, enhancing stability and reactivity. This conjugation is responsible for their UV-visible absorption and characteristic coloration was explain.[7]

2.2 Functional Groups and Reactivity

- **Carbonyl group (C=O):** participates in nucleophilic addition
- **Double bond(C=C):**acts as electrophilic centre
- **Aromatic rings:** allow substitution and structural modification

The α,β-unsaturated system enables chalcones to act as Michael acceptors, which essential for their biological activity.[6,12]

2.3 Chemical Reactions

Chalcones undergo several reactions

- Michael addition
- Cyclization to flavonoids
- Oxidation and reduction
- Substitution reactions

These reactions make chalcones versatile intermediates in organic synthesis.[45]

2.4 Stereochemistry

Chalcones predominantly exist in the **trans (E)-form,** which is more stable and biologically active due to reduced hindrance.[27]

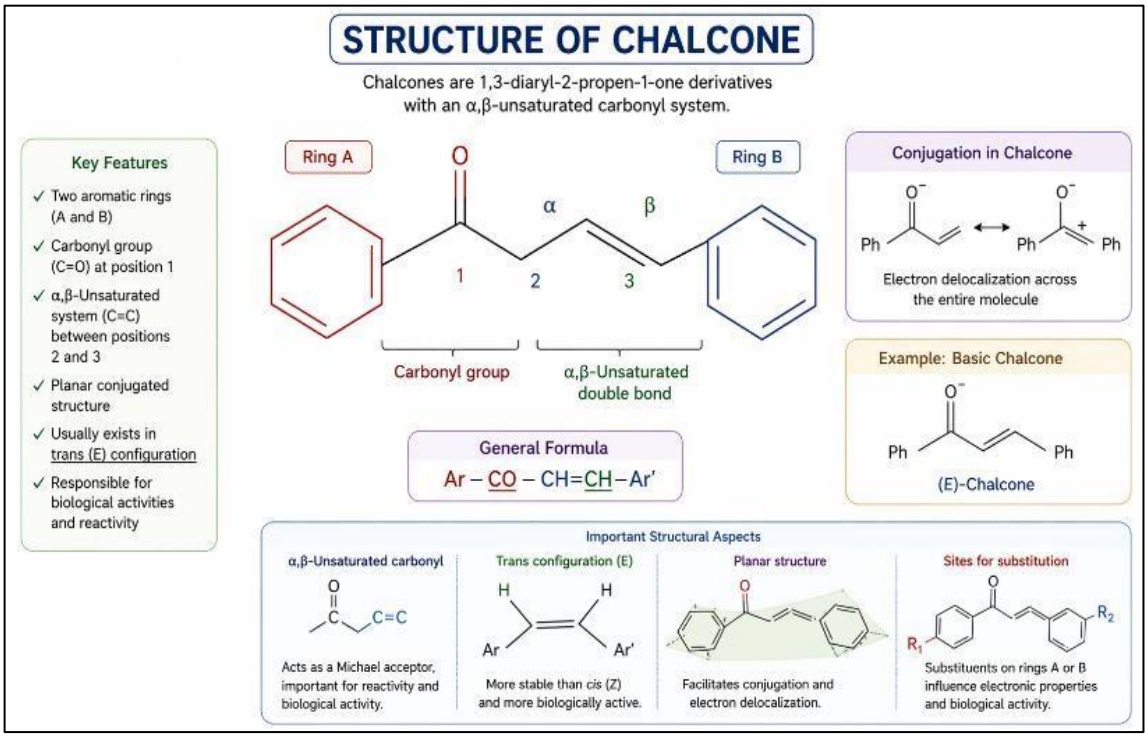

Fig.1: General structure of chalcone showing α, β -unsaturated carbonyl system.

3. METHODS OF SYNTHESIS

3.1 Claisen–Schmidt Condensation

The Claisen–Schmidt condensation is the most widely used method for chalcones synthesis.[45,46]

Reaction

Aromatic aldehyde + Aromatic ketone → Chalcone. (Fig.no. 2)

This method is simple and provides high yields.

Mechanism

1. Formation of enolate ion
2. Nucleophilic attack aldehyde
3. Formation of β -hydroxy ketone
4. Dehydration

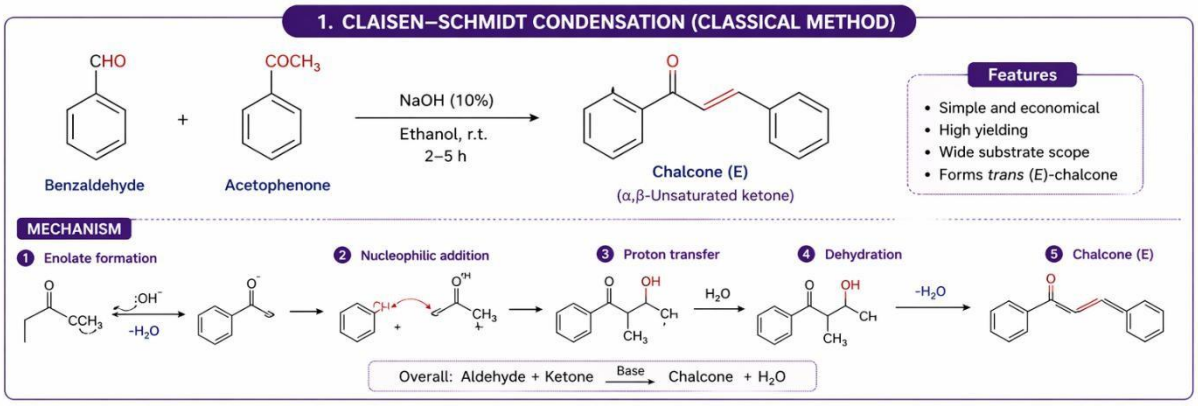

Fig. 2: Claisen – Schmitt condensation mechanism for chalcone synthesis.

3.2 Microwave-Assisted synthesis

Microwave irradiation significantly reduces reaction time and improves yield.[1,9] It enhances molecular collisions and reaction efficiency.

Studies have shown.

- Faster reactions (minutes vs hours)
- Higher purity products • Reduced solvent use.[3,32,34]

3.3 Green Synthesis

Green chemistry approaches focus on eco-friendly synthesis using.

- Non-toxic solvents
- Reusable catalysts
- Energy-efficient methods.[14,33]

MicellRESUar media and ionic liquids have been successfully used for chalcones synthesis.[14]

3.4 Solvent-Free Synthesis

Solvent-free methods reduce environmental impact and improve reaction efficiency. These methods are widely used in microwave-assisted synthesis.[35]

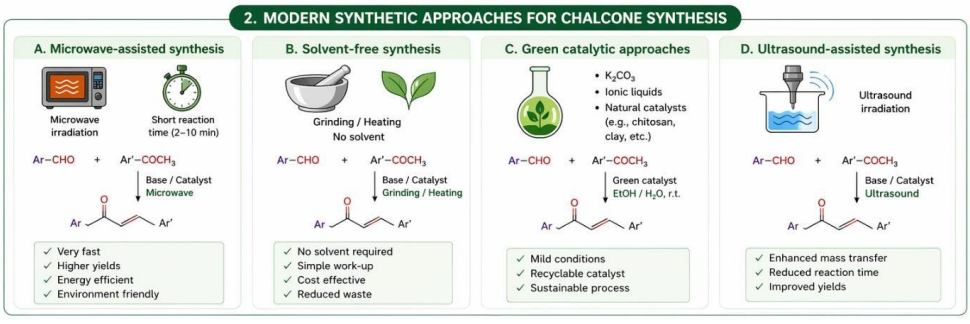

Fig.3: Modern synthetic approaches for chalcone derivatives.

4. CHARACTERIZATION OF CHALCONES

Characterization of chalcone derivatives is essential to confirm their chemical structure, purity, and functional group composition. Various spectroscopic techniques such as IR, NMR, and Mass spectroscopy are commonly employed to establish the identity of synthesized chalcones.[51,54]

4.1 Infrared (IR) Spectroscopy

IR spectroscopy is a powerful technique used to identify functional groups present in chalcone based on their characteristic vibrational frequencies.

IR confirms

- Presence of carbonyl group

- Conjugated system
- Functional group substitutions

Key Functional Groups peaks in Chalcones

1. Carbonyl Groups (C=O Stretching)

Range :1650-1680 cm^{-1}

- This is the most important peak for chalcone.
- Appears slightly lower than normal ketone (~1715 cm^{-1}) due to conjugation with C=C double bond.
- Confirms presence of α,β- unsaturated ketone system.

Interpretation

Lower frequency = strong conjugation→ confirms chalcone structure.[51,52]

2. Olefinic Double Bond (C=C Stretching)

Range: ~1600 cm^{-1}

- Represents α, β-unsaturated double bond.
- Confirms formation of enone system.

If peak is strong → good conjugation.[51-54]

3. Aromatic C-H Stretching

Range: ~3000– 3100 cm^{-1}

- Indicates presence of benzene rings
- Usually appears as multiple peaks

4. Additional Peaks

- -OH group: ~3200 3500 cm^{-1} (broad peak)
- - OCH_3 group:~ 2830– 2850 cm^{-1}
- - NO_2 group**:** 1500– 1550 cm^{-1}

These peaks help identify substituted chalcone derivatives.

4.2 NMR Spectroscopy

NMR spectroscopy provides detailed structural information about chalcones, including proton environment and carbon skeleton.

- Confirms double bond formation
- Confirms trans configuration
- Identifies substituents.[52]

4.2.1 ^{1}H NMR (Proton NMR)

Typical Range: δ6–8 ppm

1. Olefinic Protons (– CH =CH–)

- Appear at δ 6.5 – 7.5 ppm
- Show doublet signals due to coupling
- Large coupling constant (J ≈ 15– 16 Hz). Confirms trans (E)- configuration**.**

2. Aromatic Protons

- Appear at δ 7 – 8 ppm
- Multiplet pattern
- Confirms presence of benzene rings

3. Substituent Peaks

- – OH proton**:** δ 9– 12 ppm (broad)
- – OCH_3 proton: δ ~3.5–4 ppm

4.2.2 ^{13}C NMR (Carbon NMR)

- Confirms carbon framework
- Identifies functional groups
- Supports IR findings

Key Range: δ190– 200 ppm

1. Carbonyl Carbon (C = O)

- Appears at δ 120– 150 ppm

2. Olefinic Carbons

- Appear at δ 120– 150 ppm

3. Aromatic Carbons

Appear at δ 110– 140 ppm

4. Substituent Carbons

- –OCH_3: δ ~55– 60 ppm

4.3 Mass Spectrometry

Mass spectrometry is used to determine.

- Molecular weight
- Molecular formula
- Fragmentation pattern

1. Molecular Ion Peak (M^{+})

- Represents exact molecular weight of chalcone
- Confirms successful synthesis

2. Fragmentation Pattern

Chalcones show characteristic fragmentation.

Common Fragmentations

- Loss of CO group
- Cleavage at α,β- double bond
- Formation of benzoyl fragments

Example Fragmentation Flow

Chalcone →Break at C=C→

Aromatic fragment + carbonyl fragment

3. Base Peak

- Most intense peak
- Represents most stable fragment.

Importance of MS

- Confirms molecular structure
- Detect impurities
- Supports IR and NMR data.[51-54]

o **Overall summary of characterization.**

Sr.no	Technique	Information Obtained
1	IR	Functional groups
2	^{1}HNMR	Proton environment
3	^{13}CNMR	Carbon structure
4	MS	Molecular weight & fragmentation

5. BIOLOGICAL ACTIVITIES OF CHALCONES

Chalcones exhibit **broad-spectrum pharmacological activities** due to their reactive α, βunsaturated carbonyl system and structural flexibility.[6,16,21] Their biological effects arise from interaction with enzymes, proteins, and cellular pathways.

5.1 Antimicrobial Activity

Chalcones exhibit antimicrobial activity by.

- Disrupting cell membranes
- Inhibiting enzymes
- Interfering DNA replication

Explanation

- Chalcones increase membrane permeability, leading to leakage of ions and proteins.
- Inhibit bacterial enzymes such as DNA gyrase→ prevents replication.
- Interfere with protein synthesis.

Studies confirm activity against Gram-positive and Gram-negative bacteria.[25,41,66]

5.2 Anti-Inflammatory Activity

Chalcones inhibit inflammatory mediators such as COX and LOX enzymes, reducing prostaglandin synthesis.

Explanation

- Chalcones inhibit cyclooxygenase (COX) and lipoxygenase (LOX) pathway.
- Reduce cytokine production
- Block TNF – α signalling pathway.[47]

5.3 Antioxidant Activity

Chalcones act as a free radical scavenger, neutralizing ROS and preventing stress.

Explanation

- Phenolic groups donate electrons /hydrogen
- Stabilize free radicals • Prevent lipid peroxidation.[20]

5.4 Anticancer Activity

Chalcones are multi-target anticancer agents.
Mechanisms include.

- Induction of apoptosis
- Cell cycle arrest
- Inhibition of angiogenesis
- Proteasome inhibition by chalcones in cancer cells.[12]

Explanation

- Induce apoptosis via mitochondrial pathway
- Arrest cell cycle at G2/M phase
- Inhibit angiogenesis and tumour proliferation.[23]

5.5 Antitubercular Activity

Chalcones inhibit Mycobacterium tuberculosis by interfering with essential enzymes.
Chalcone → inhibits mycobacterial enzymes → disrupts cell wall synthesis → inhibits bacterial growth.[27]

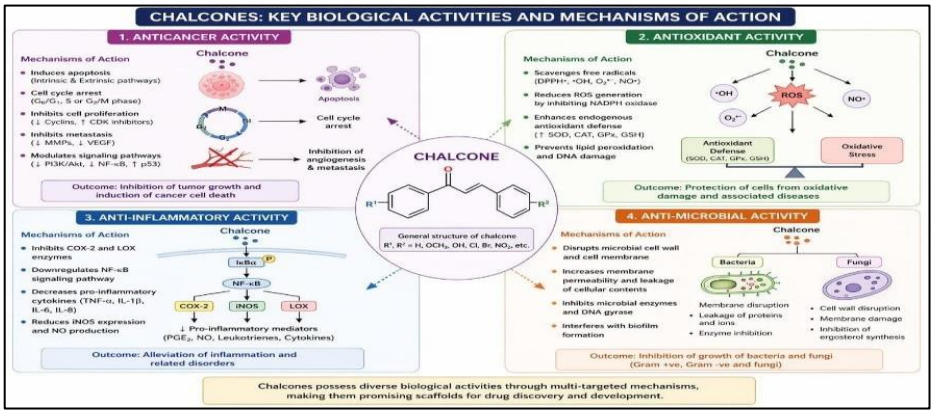

Fig.4: Biological activities and mechanisms of action.

6. MECHANISM OF ACTION

The biological activity of chalcones is primarily due to the α, β-unsaturated carbonyl group, which acts as a Michael acceptor.[12]

Mechanisms include.

- Enzyme inhibition
- Protein interaction

- DNA binding
- ROS modulation

7. STRUCTURE-ACTIVITY RELATIONSHIP (SAR)

SAR studies show that biological activity depends on substituents.

7.1 Effect of substituents

i. Electron Donating Groups (EDG)

Examples: –OH, $–OCH_3$

- Increase antioxidant activity
- Enhance hydrogen bonding
- Improve radical scavenging

ii. Electron Withdrawing Groups (EWG)

Examples: $–NO_2$, –Cl, –F

- Increase antimicrobial and anticancer activity
- Enhance electrophilicity.[30]

7.2 Position of substitution

Position	Effect
Para	Highest activity
Meta	Moderate
Ortho	Steric hindrance

7.3 Conjugation Effect

- More conjugation → higher activity
- Stabilizes molecule
- Enhances binding with proteins

7.4 Lipophilicity

- Increased lipophilicity → better membrane penetration
- Improves drug absorption

7.5 Heterocyclic substitution

- Enhances biological activity
- Improves selectivity.[18]

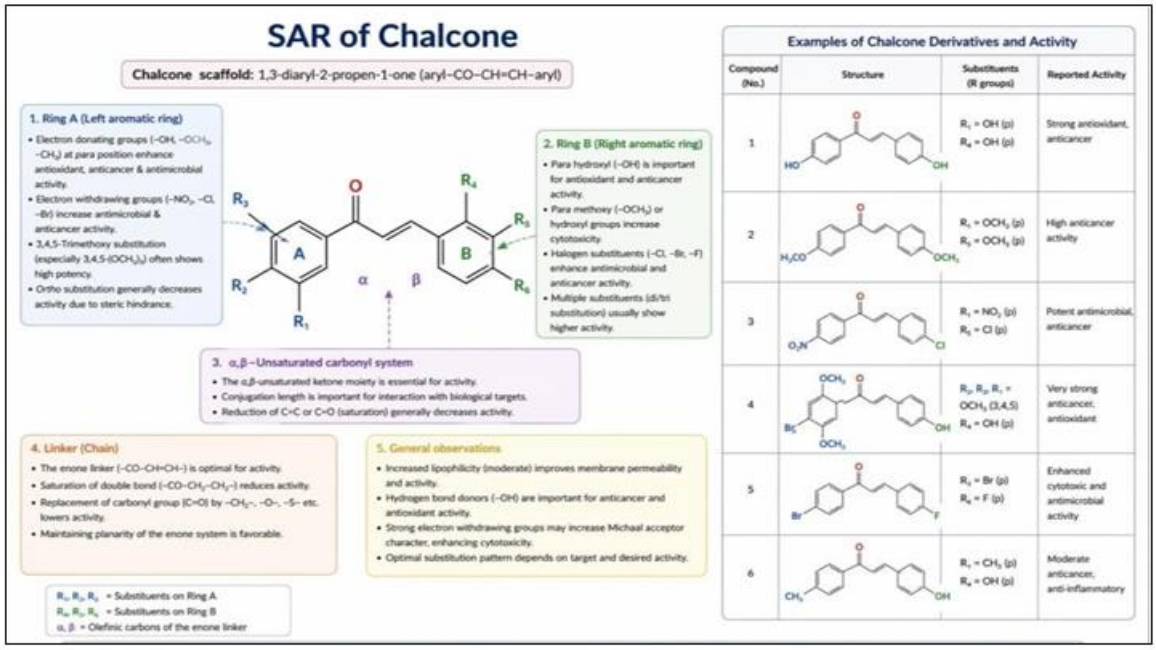

Fig. 5: SAR of Chalcone.

8. MOLECULAR DOCKING STUDIES

Docking studies is essential for drug design and target identification.

Docking predicts how chalcones bind to proteins.

Importance

- Predicts biological activity
- Save time and cost
- Helps in drug optimization.[60]

8.1 Software used

- Chem Sketch[60]
- PyRx[61]
- SwissADME[62]

These studies predict binding affinity and pharmacokinetics.

8.2 Docking process

Ligand (chalcone) + Protein (1KZN, 4WMZ)

↓

Binding interaction

↓

Calculation of binding energy

9. APPLICATIONS OF CHALCONES

Chalcones have wide applications.

9.1 Pharmaceutical Applications
- Antimicrobial drugs
- Anticancer agents
- Anti-inflammatory drugs

9.2 Cosmetics
- Antioxidant creams
- Anti-aging formulations

9.3 Agriculture
- Pesticides
- Plant growth regulators

9.4 Chemical Industry
- Intermediate in synthesis
- Dye production.[15]

10. FUTURE PERSPECTIVES
Future research directions include.

10.1 Drug Development
- New derivatives with better activity
- Target- specific drugs

10.2 Green Chemistry
- Eco-friendly synthesis
- Sustainable production

10.3 Clinical Studies
- Human trials
- Safety evaluation

10.4 Computational Approaches
- AI – based drug design
- Advanced docking studies

11. CONCLUSION
Chalcones represent a highly versatile and promising class of compounds in medicinal chemistry. Their simple structure, ease of synthesis, and diverse biological activities make them valuable scaffolds for drug development. Advances in synthesis techniques, particularly microwave-assisted and green chemistry approaches, have improved efficiency and sustainability. The presence of the α,β-unsaturated carbonyl system plays a crucial role in their biological activity through mechanisms such as enzyme inhibition and protein interaction. Structure– activity relationship studies have further enhanced understanding of how substituents influence activity. Additionally, molecular docking studies have provided insights into target interactions, facilitating rational drug design. Future research focusing on clinical studies, green synthesis, and computational approaches will further expand the therapeutic potential of chalcone derivatives.

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