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Exploring Chemistry And Applications Of Chalcones: A Comprehensive Review

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Abstract: Chalcones, known as open chain flavonoids, are a unique class of compounds characterized by an α, β-carbonyl configuration. The versatile nature of chalcone hybrids suggests broader pharmacological applications. This review emphasizes the structural variation of chalcones, their biosynthetic pathways and their comprehensive pharmaceutical applications including as anti-carcinogenic, anti-inflammatory, anti-bacterial and anti-oxidant activities. Generally, in the management of microbial infections and oxidative-stress related diseases chalcone derivatives representing a promising revenue for pharmaceutical discovery and development, fostering potential for advanced therapies and improved results.

Keywords: Chalcone, flavonoids, structural variations, pharmaceutical applications.

I INTRODUCTION

Chalcones, also referred to as 1,3-diphenylprop-2-en-1-ones, are organic compounds belongs to open-chain flavonoid family and mainly found in plants [2]. The "Chalcones" was first introduced by Stanislaw Kostecki, a polish chemist in late 19th century. The other names of chalcones are benzyl acetophenone or benzylideneacetophenone [2,5]. These are significant in both synthetic and natural chemistry [4,5]. The chalcone structure consist of a pair of benzene rings joined by three carbon chain in a trans conjugated configuration which make them important intermediates for synthesis of heterocyclic compounds [Fig.1]. Trans isomers are thermodynamically stable [2,3]. They serve as precursor in the synthesis of flavonoids and isoflavonoids [3].

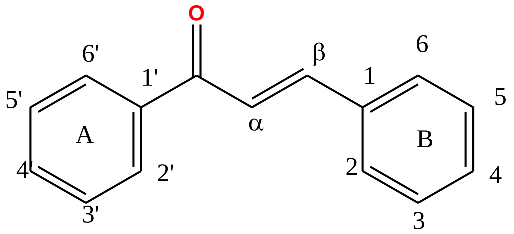


Figure 1. General Structure of Chalcone

Chalcones have wide range of biological activities that is why they have attracted significant attention in pharmaceutical research [fig.2]. As from ages, by using plants and herbs chalcones have been used therapeutically to treat variety of health disorders, includes cancer, inflammation and diabetes [8,12,13,20]. Phloretin and its sugar-bound form (phloretin 2′-0-βglucopyranoside), along with chalconaringenin are the most common chalcones present in food [2,6,10]. The variety of novel heterocyclic compounds with good pharmacological``` profile can be designed from chalcone because it contains a very good synthon.

It has fluorescent activities also due to its delocalised double bonds and a completely conjugated π-electron system on both aromatic rings, which make them potential chemical probes for diagnosis [5,6,10]. It can chemically synthesize by Claisen-Schmidt condensation but other strategies can also be used in their synthesis [4,5].

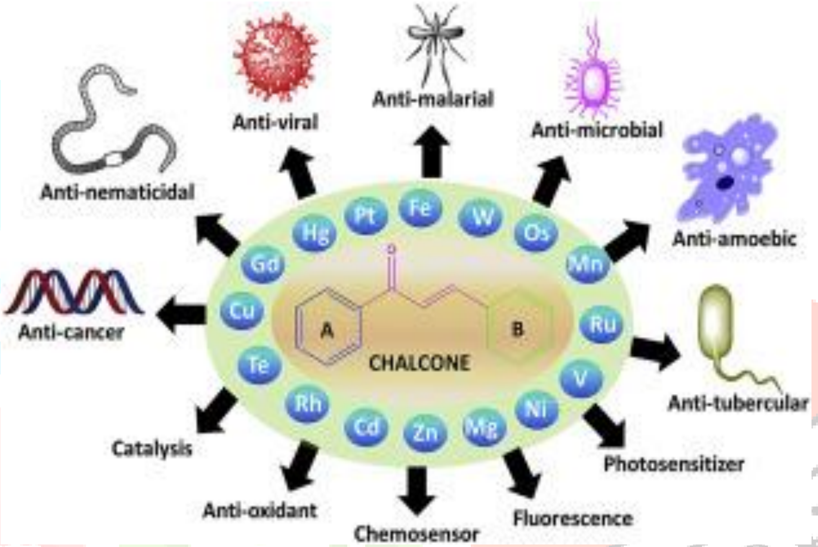


Figure 2. Biological activities of Chalcones

II IMPORTANCE OF CHALCONES

- Chalcones share structural similarity with flavones, aurones, tetralones and aziridines [2,5].
- Chalcones and their derivatives are commonly used as synthetic sweeteners, catalyst for polymerization, fluorescent whitening agent, heat stabilizer, visible light, ultraviolet light [6,10].
- They also contain a ketonic-ethyl group which make them highly reactive to multiple chemical reagents like phenyl hydrazine and ortho-amino thiophenol etc [5].
- 3,2’,4’, 6’-tetrahydroxy-4-propoxydihydrochalcone-4-β'-neohesperdoside, a chalcone derivative has been utilized as artificial sweetener approximately 2200 folds sweeter than glucose [10].
- The chalcones have been found useful in elucidating structure of natural products like hemlock tannin, phloretin, eriodyctiol and naringenin etc [2,6].

III CHEMISTRY OF CHALCONES

The chalcone backbone features a conjugated system of a carbonyl group and double bond, which contributes to its chemical reactivity [5,6]. Substitution on the aromatic rings enable structural variety, enhancing their physiochemical properties and pharmacological activities [2,7].

3.1 Synthesis of Chalcones

3.1.1 Claisen-Schmidt Condensation

The synthesis of chalcones has progressed significantly, originating from the traditional Claisen-Schmidt condensation [2,3,5]. The Claisen Schmidt condensation reaction entails a reaction between aldehyde lacking alpha-hydrogen atoms and a ketone, in the presence of a heterogeneous acid catalyst to produce the desired, α, β-unsaturated ketone. In the laboratory this is considered as one of the easiest and most efficient method of chalcone synthesis (Figure 3) due to the equimolar amount of benzaldehyde and acetophenone [4,5]. The concentration of alkali used in the Claisen-Schmidt reaction, typically varies from 10 and 60%. The reaction is carried out for 14-16 hours at a temperature of approximately 50°C or at 20-25°C for up to a week.

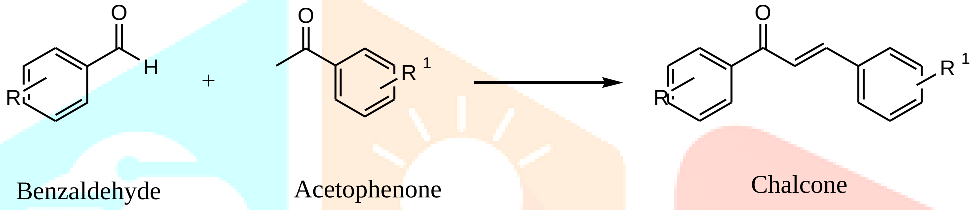
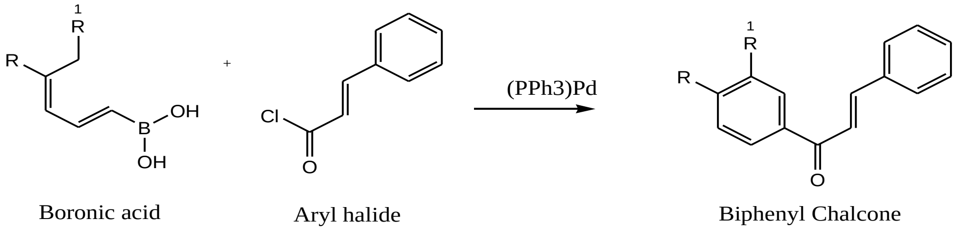


Fig 3. Chalcone Synthesis by Claisen- Schmidt condensation

3.1.2 Green chemistry approaches such as sonochemical reactions, microwave irradiation and solvent free protocols have been developed, enhancing both reaction productivity and environmental responsibility. It emphasizes the use of non-toxic reagents, biodegradable materials and energy-efficient methods to reduce reaction time, waste and environmental pollution [9,10,12]. The implementation of green chemistry approaches leads to the development of eco-friendly chemical processes that benefit both industry and the environment [9,10, 40].

3.1.3 Modern catalytic methods, including ionic liquids, organo-catalysts and transition- metal catalysts, provide site selectivity and allow the integration of diverse functional groups [4,9]. Moreover, coupling reactions like Suzuki and Sonogashira have opened alternative for synthesizing complex chalcone derivatives [24].

3.1.3.1 Suzuki coupling reaction: This approach is commonly used to develop chalcones. The reaction is effective whether the reactant carry electron-attracting or electron-releasing substituents, showing that the electronic properties of the substituent present on the aromatic rings have a little impact on the reaction out.



R,R$_1$= OH, NO2,
Cl, CH3, OCH3

Figure 4. Chalcone synthesis by Suzuki Coupling Reaction

3.1.3.2 Wittig Reaction: The reaction also known as Wittig olefination is considered as alternative efficient method to synthesize unsaturated hydrocarbons. Chalcone derivatives are suitable alkene compound for this methodology. Initially triphenylbenzoylmethylene phosphorane and benzaldehyde are used, followed by heating for 3-4 days by heating with benzene or 28-30 hours in tetrahydrofuran with a minimum production of approximately 68-70%. [41,42] Recent studies have shown that by microwave irradiation the reaction kinetics can be enhanced.

3.2 Characterization of Chalcones

The structural characteristics of produced chalcones can be effectively characterized using UV spectroscopy, Infrared spectroscopy, NMR spectroscopy [5,10,37,40].

3.2.1 UV Spectrum

The chalcones shows two essential absorption band in the UV spectra: Primary band I and a weaker band, band II [5]. Band I generally appears in range of 345–380 nm, though a minor inflection or peak may also be occurred at 305–325 nm. Band II appears in 225–280 nm [5].

3.2.2 IR Spectrum

Asymmetric and symmetric stretching vibrations within the Infrared spectral data of chalcones of the aromatic C–H bonds are observed in the region of 3125–3081 cm^{-1} and 3090–3045 cm^{-1} usually as two low or weak intensity bands [5,10]. The band of C–H stretching of the =C–H group is seen at 3025–3015 cm^{-1}. The bands between 1610–1565 cm^{-1} is associated with the vibrations of the aromatic ring [5,10,37]. The broad weak band at 1459–1425 cm^{-} is appeared due to the in-plane deformation of the =C–H bond. For enones (=C–C=O) the stretching vibrations of carbonyl typically appears between 1645 and 1680 cm^{-1} [5,40].

3.2.3 NMR Spectrum

In the $_{1}$H-NMR spectra of alkene moiety of chalcones were seen at 4.9 and 5.8 ppm. The aromatic regions were observed at 6.8–7.9 ppm [5,10].

In $_{13}$C-NMR spectrum of chalcones, the oxo carbon usually seen in the range of δ 185.8 and 197.1. The carbons adjacent to carbonyl group give characteristic signals between δ 115.9–127.9 and δ 137.0–144.9 respectively [5,10].

IV THERAPEUTIC APPLICATIONS OF CHALCONE DERIVATIVES

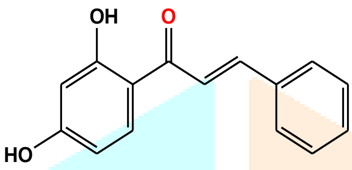
Chalcone serves as a base structure, and chemical substitutions at the aromatic rings (A and B) or modifications of the alpha-beta unsaturated carbonyl compounds have gained significant attention due to their wide range of therapeutical properties [2,3,6]. Recent studies have explored their potential for treating numerous diseases, specifically involving oxidative stress, microbial infections and cancer [1,3,6,8].

4.1 Antioxidant activity

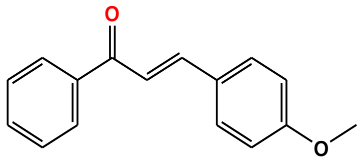
Mechanism: Chalcone derivatives neutralize highly reactive molecules, inhibit lipid degradation and bind metal ions [1,14].

4.1.1 Hydroxychalcones: They contains hydroxyl (-OH) groups on aromatic rings and exhibit antioxidant activities [1]. E.g. 2,4-dihydroxychalcone.

4.1.2 Methoxy chalcones: They contain methoxy (-OCH3) groups. They are potent anticancer and antimalarial agents [14,15]. E.g. 4-Methoxychalcone reduce oxidative stress in cellular models.



2,4-dihydroxychalcone



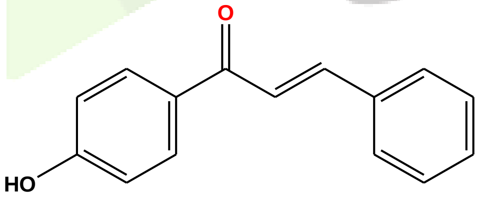
4-Methoxychalcone

4.2 Anti-inflammatory activity

Mechanism: Chalcone derivatives exhibit anti-inflammatory effects by suppressing inflammatory pathways including the inhibition of COX, LOX and NF- kB and also reduce pro-inflammatory cytokine production, such as TNF-alpha [6,13].

4.2.1 Lico chalcone A: A natural chalcone isolated from glycyrrhiza inflate, inhibits the production of pro-inflammatory cytokines like IL-6 and TNF-alpha [13].

4.2.2 4'- Hydroxychalcone: Decreases nitric acid (NO) production by blocking stimulus responsive nitric oxide synthase (iNOS) in macrophages [6,14].



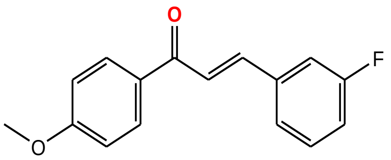
4'- Hydroxychalcone

4.3 Anticancer activity

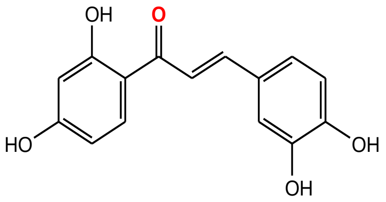
Mechanism: Chalcone derivatives induces apoptosis via activation of caspases and block tumor cells proliferation by targeting PI3K/Akt, MAPK pathways and arrests the cell cycle at various phases [1,8,17].

4.3.1 Fluoro-chalcone: These are fluoro-substituted chalcones. E.g. 3-fluoro-4'-methoxychalcone demonstrate cytotoxicity against breast cancer [1,17].

4.3.2 Butein: A hydroxylated chalcone found in Butea monosperma, induces apoptosis in lung cancer cells by inhibiting NF-kB [8].



3-fluoro-4'-methoxychalcone



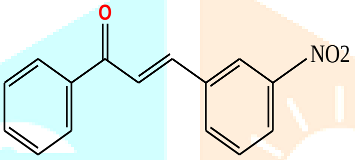
Butein

4.4 Antimicrobial and Antifungal activity

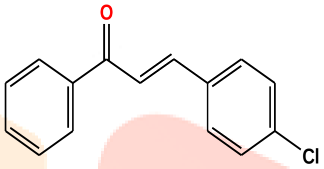
Mechanism: Chalcones have shown significant activity against bacterial and fungal pathogens [3,30]. They disrupt microbial membranes and inhibit key enzymes involved in microbial growth [3,9,30].

4.4.1 Nitro-chalcones: Compounds like 3-nitrochalcones marked antimicrobial potential against Escherichia coli (E. coli) and Staphylococcus aureus (S. aureus) [25].

4.4.2 4’-chlorochalcones: Exhibits antifungal activity against Candida albicans by disrupting fungal cell membranes [30].



3-nitrochalcone



4-chlorochalcones

4.5 Antiviral and Antidiabetic Activity

Chalcones target key enzymes such as proteases and inhibit viral replication [26]. They act as antidiabetic agents by enhancing glucose uptake and modulating signaling of glucose [19,26].

V RECENT STRUCTURAL ADVANCEMENTS IN CHALCONES

Advancements in the core structure of chalcones pave the way to the development of novel derivatives with enhanced pharmacological activities. These derivatives are improved by introducing functional groups at specific positions or by tweaking existing ones on the aromatic rings to improve bioactivity, selectivity and pharmacokinetic characteristics. Substituting heteroatoms like nitrogen, sulfur, halogens and selenium on carbonyl or aromatic moiety further expands their structural diversity.

Chalcones serve as building blocks for heterocyclic synthesis forming flavonoids, pyrazolines, pyrimidines and benzothiazepines, these heterocycles often show notable biological activity making chalcones an indispensable tool in medicinal chemistry.

VI FUTURE PERSPECTIVES

Emerging trends in computational chemistry including molecular docking and QSAR studies, are offering deeper insights into structure-activity relationships, facilitating rational drug design. Future research should focus on enhancing chalcones pharmacokinetics, solubility and bioavailability to transition from laboratory research to clinical application.

Chalcones are versatile scaffold with substantial potential in multiple research areas, their chemical versatility and significant biological relevance continue to encourage exciting innovative applications, establishing them as a key player in modern drug development.

VII CONCLUSION

This review highlights that chalcones shows a wide range of biological activities, such as anti-malarial, anti-cancer, anti-inflammatory, anti-bacterial, anti-fungal, anti-microbial, and anti-oxidant activities with their mechanism of action. Chalcones derivatives are attracting a lot of scientific attention for the research of new potent biological activity due to their diverse range of biological activities. Chalcones ability to interact with various biological targets emphasize their potential in treating a multitude of diseases. Additionally, we have explored various approaches of chalcones synthesis and characterization. Further research addressing bioavailability and toxicity issues will pave the way for chalcone-based therapeutics in clinical practice.

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