Recent Developments on the Synthetic and Biological Applications of Chalcones-A Review

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Abstract: Chalcones are precursors of the biosynthesis of flavonoids present in plants. These motifs serve a wide range of applications, from synthetic to pharmacological to physical spheres. Chalcone derivatives attracted the scientific community all over the world in recent times due to their diversified applications. The presence of reactive α,β-unsaturated carbonyl moiety in chalcones makes them a versatile intermediate in synthesizing various classes of compounds of biological and physical interest. More importantly, the chalcones themselves have been known to possess enormous biological activities and physical properties like semiconductor, non-linear optical, fluorescence, and electronic properties. In this context, the present review summarises the overall developments in the synthetic, pharmacological, and physical applications of chalcones in recent fast. The critical discussion was attempted on the synthetic applications and biological potencies as anti-cancer, antidiabetic, antimicrobial, antioxidant, and anti-inflammatory.

Keywords: antibacterial; annulation; anticancer; antidiabetic; antifungal; anti-inflammatory.

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1. Introduction

Chalcones are 1, 3-diphenyl-2-propen-1-ones consist of a three-carbon α, β-unsaturated carbonyl system, which exhibit a broad spectrum of biological activities. The natural and synthetic chalcones exhibit various pharmacological activities such as anti-inflammatory, antitumor, antibacterial, antifungal, antimalarial, anti-inflammatory, anti-cancer and anti-tuberculosis. The promising activities, ease of synthesis, and simple and reactive chemical structure have significantly attracted chalcones [1]. This review focuses on the developments in the synthetic procedures, their utility as scaffolds in the synthesis of bioactive compounds, biological activity potentials, and their ability to form useful metal complexes, also physical properties associated with chalcone derivatives in the recent past.

2. Synthesis and Synthetic Applications

Of the many methods, the Claisen-Schmidt condensation of aromatic aldehydes and aromatic ketones in acidic or basic conditions (Scheme 1) [2]. The MnO2 nanorods on graphene oxide act as excellent catalysts for chalcones synthesis via Claisen-Schmidt condensation. The catalyst showed recyclability up to six times without significant loss of activity [3]. A simple, expedient, and greener synthetic approach for chalcone derivatives, involving p-toluenesulfonic acid as a solid phase organocatalyst, accelerates Claisen–Schmidt condensation.
under mild and solvent-free reaction conditions was developed (Scheme 1) [4]. The method has advantages with short periods, desired products, simple workup, and easy purification, etc. The fluoro-substituted tris-chalcone derivatives were synthesized from phloroglucinol and benzaldehyde in three steps (Scheme 1) [5]. The tris-chalcones have shown inhibition of hCA I and II isoenzymes, acetylcholinesterase, butyrylcholinesterase. The base-catalyzed Claisen-Schmidt condensation reaction between aromatic aldehydes and ketones in methanol produced corresponding chalcones in good yields [6-11].

Scheme 1. Synthetic route for chalcones.

The bifunctional catalyst derived from a Cinchona alkaloid found it effective to perform the enantio- and diastereoselective Michael addition of α,α-dicyanoolefins chalcones in THF as solvent (Scheme 2) [12] to give the adducts in moderate yields, which exhibit antiparasimal and cytotoxic activity. Chalcones have been efficiently transformed into pyrazoline carbothioamides [13] and pyrazoline carboxamides [14] through (3+2) annulation reactions with thiosemicarbazide and semicarbazide, respectively. The base mediated convenient method for the synthesis of 3-acylpyrazoles and pyrazole-3-carboxylates was developed, which involves diazosulfone as 1,3-dipole and arylidenemalonates and arylidene-1,3-dicarboxyls as dipolarophiles in cycloaddition reaction (Scheme 2) [15]. An environmentally benign method involving citrus extract medium was adopted to transform chalcones by their reaction with hydroxylamine into isoxazoles of antioxidant and antifungal potencies [16-18].

Scheme 2. Cycloaddition and coupling reactions of chalcones.

Indolizines were obtained through the one-pot cascade reaction between chalcone, pyridine, and benzyl bromide via [3 + 2] cycloaddition/oxidative aromatization promoted by Cu(OAc)₂ in the presence of oxygen (Scheme 3) [19]. The method is convenient and does not require the isolation of intermediates.

Scheme 3. Synthesis of fused pyrrolines from chalcones.

Palladium-catalyzed cross-coupling of ethyl acetohydroxamate with 4-bromo chalcones was developed to synthesize functionalized chalcones, wherein the ligand tBuXPhos
found effective towards cross-coupling reaction to produce the product in good yields (Scheme 4) [20]. The hybridization approach followed by tandem cyclization into quinolinone derivatives and then by aldol condensation produces chalcone-sulfonamide compounds. The method controlled the sequential preparation of chalcone-sulfonamide hybrids [21]. Chalcones undergo highly regio- and stereoselective Diels-Alder cycloaddition with dienophiles to give \(N\)-substituted \textit{exo}-4,5,6,7-tetrahydrobenzoxazol-2-ones (Scheme 4) [22]. The \textit{endo}/\textit{exo} stereoselectivity is dependent on the solvent, polarity, and substituents. The chalcones have been efficiently transformed into isoxazolines [23] and pyrrolines [24] in good yields.

The intermolecular \([2 + 2]\) photocycloaddition of chalcones with 2,3-dimethyl-1,3-butadiene under visible-light irradiation forms cyclobutane derivatives (Scheme 4) [25]. Without using any photosensitizer, metal catalyst, and solvent, the reaction proceeded with high regio- and stereoselectivity. Mild reaction conditions and no additives make the reaction easy to operate. Interestingly, chalcones undergo \((2+2)\) cycloaddition themselves under thermal conditions to produce cyclobutane derivatives, whose structures are confirmed by XRD studies [26,27]. The regioselective synthesis of 1-alkyl-2-aryl-3-acyl pyrrolo[2,3-\(b\)]quinoxalines through Heck coupling reaction/heteroannulation was achieved by the \(\text{Pd(OAc)}_2\) catalyzed reaction of \(N\)-alkyl/benzyl-3-chloroquinoxaline-2-amines with chalcones in the presence of \(\text{KO'Bu}\) in DMSO (Scheme 4) [28]. Chalcones efficiently undergo \((3+2)\) annulation reaction with 2-aminothiophenol in the presence of acids to give benzothiazepines [29,30].

![Scheme 4](https://doi.org/10.33263/BRIAC121.180195)

**Scheme 4.** Synthesis of functionalised compounds from chalcones.

A simple and efficient protocol for preparing densely functionalized 3-arylimidazo[1,2-\(a\)]pyridines from 2-aminopyridines and chalcones using \(\text{RuCl}_3\cdot\text{H}_2\text{O}/\text{I}_2\) catalytic system was reported [31]. The method's advantages are low catalyst loading, broad substrate scope, stability of heterocycles, operationally simple procedure, and higher yields, making the approach remarkable. Heteroaryl chalcones found more susceptible to form pyrazole derivatives [32,33] by their reaction with hydrazines

3. Pharmacological Applications

Chalcone, a natural structure, demonstrates many pharmacological activities, including anti-cancer, antidiabetic, antimicrobial, anti-inflammatory, antitumor, anti-Alzheimer, etc., and plays pivotal roles in medicinal chemistry [34]. In cancer chemotherapy, multidrug resistance (MDR) is highly associated with ATP-binding cassette transport proteins' overexpression. The translocation of drugs from the inside to the outside of cancer cells is mediated at the expense of ATP. The chalcone-dithiocarbamate hybrids, of which \((E)\)-2-oxo-
2-((4-(3,4,5-trimethoxyphenyl)acryloylphenyl)amino)ethyl-4-(2-hydroxyethyl)piperazine-1-carbodithioate (Fig. 1A) exhibited antiproliferative activity against MCF7, and PC3 (IC50 = 1.05 μM) cancer cell lines [35]. The cellular mechanism indicated that it could inhibit colony formation, arrest cell cycle at G2/M phase, induce DNA damage against PC3 cells, and mitochondrial apoptosis by caspase activation, and therefore would be a lead for treatment of human prostate cancer. The xanthine/chalcone hybrids, of which chalcone derivative (Fig. 1B) [36] acts as anti-cancer agents with potent inhibition of cancer cell growth (IC50: 1.0 ± 0.1 to 3.5 ± 0.4 μM). Further, its EGFR inhibitory effect shown that IC50 = 0.3 μM on the target enzyme was more potent than staurosporine reference drug (IC50 = 0.4 μM). The 4′-alkoxy chalcones possess antiproliferative activity against PC-3, MCF-7, and HF-6 with IC50 values of 8.08 to 13.75 μM [37].

![Figure 1. A) Chalcone-piperazine-1-carbodithioate that shows antiproliferative activity; B) xanthine/chalcone hybrid that possesses EGFR inhibitory effect.](image)

The chalcone derivative (Fig. 2A) [38] bearing an α,β-unsaturated ketone acts as the most potent inhibitor against NCI-H460, A549, and H1975 cells. It has antiproliferative ability against NCI-H460 cells in a time- and concentration-dependent manner through modulating ROS to induce caspase-3-mediated pyroptosis. The chalcone (Fig. 2B) induced apoptosis of human hepatic and lung cancer cells, which prevented cancer cell migration and invasion. It strongly suppressed tumor growth in a mouse model of xenograft tumors [39]. The pyrazoles derived from chalcones have excellent anti-cancer properties [40]. The enhancement of drug efflux caused by ATP-binding cassette transporters overexpression is an important factor for multidrug resistance (MDR) in cancers. It was found that chalcone and bis-chalcone derivatives displayed the reversal activities of MDR cancer cell lines. The chalcone (Fig. 2C) exhibited the most potent reversal activities against ABCG2- and ABCB1-mediated MDR [41]. The mechanistic studies indicate that it can increase anti-cancer drugs in ABCG2- and ABCB1-overexpressing cancer cell lines.

![Figure 2. The chalcone analogs with: A) antiproliferative activity against NCI-H460 cells; B) induced apoptosis of human hepatic and lung cancer cells; C) reversal activities against ABCG2- and ABCB1-mediated MDR.](image)

Overexpression of P-glycoprotein (P-gp) is one of the major causes of multidrug resistance (MDR), which has become a major obstacle in cancer therapy. The compound (Fig. 3A) [42] displayed the highest activity (RF = 50.19) in reversing DOX resistance in MCF-7/DOX cells, and increase the intracellular accumulation of DOX and inhibit the expression of P-gp at mRNA and protein levels. The α-substituted chalcones (Fig. 3B) [43] possess markable antiproliferative activities with GI50 values of 0.63 μM in the HCC1954 cell line and 0.69 μM in HCT116 cell lines, and it overcomes multidrug resistance. The chalcone pyrido[4,3-
b) pyrazin-5(6H)-one (Fig. 3C) [44] displayed anti-cancer activities against human cancer cell lines such as MCF-7, A-549, Colo-205, A2780, and DU-145 by MTT assay.

1,3,5-Triazinyl chalcone hybrids (Fig. 4A) inhibited A549 cancer cells viability with IC$_{50}$ value of 24.5 µM, about cisplatin (IC$_{50}$ = 21.5 µM). The combined effect of cisplatin with the compound indicated that the combination with cisplatin promoted more cells to enter late apoptosis and necrosis [45]. 1,2,3-Triazole chalcone hybrids (Fig. 4B) [46] possess admirable cytotoxicity against MCF-7, HeLa, and MDA-MB-231 cell lines with lower IC$_{50}$ value compared to cisplatin and were less toxic effect on normal cells. The 1,2,4-triazole/chalcone hybrids of which compound (Fig. 4C) has potent cytotoxicity against A549 cancer cell lines with IC$_{50}$ values of 4.4 µM. It showed an increase in the number of apoptotic cells in a dose-dependent manner and induced apoptosis via an increased level of pro-apoptotic protein g Bax, the release of cytochrome c, and activation of caspase-3/8/9 proteins [47].

Hepatocellular Carcinoma is extremely aggressive and presents low rates of response to chemotherapeutic agents. The quinoline/chalcone/1,2,4-triazole hybrids (Fig. 5A) [48] displayed good activity on different NCI 60 cell lines in a single-dose assay with a growth inhibition rate ranging from 50% to 94% and antiproliferative activities against human cancer cell lines. Thienoquinoline carboxamide-chalcones (Fig. 5B) [49] have an antiproliferative effect and acts as EGFR inhibitors with IC$_{50}$ values of 0.5 - 3.2 µM. The binding mode of the EGFR inhibitor in the EGFR active site revealed that the thienoquinoline ring occupied the ATP-binding site while the chalcone moiety is located in the allosteric site is responsible for enhanced activity.

The compounds 1,3,4-oxadiazole/chalcone hybrids have shown promising anti-cancer activity against leukemia. The compound (Fig. 6A) of the series had strong cytotoxic activities with IC$_{50}$ of 1.95 µM, 2.36 µM and 3.45 µM against K-562, KG-1a, and Jurkat leukemia cell lines, effectively inhibit EGFR (IC$_{50}$ = 0.24 µM), Src (IC$_{50}$ = 0.96 µM), and decreased STAT3
activation [50]. The sulfonamide chalcone derivative (Fig. 6B) [51] possesses anti-cancer properties at 10 μM against sixty human cancer cell lines. It satisfied the pre-determined threshold inhibition criteria. Further, it displayed inhibition against M. tuberculosis H37Rv with MIC values between 14-42 μM.

Diabetes mellitus (DM) is a serious chronic metabolic disorder that occurs due to dysfunction of insulin and poor therapeutic approaches. It necessitates discovering novel drugs to control amplified diabetic populations. The amino and hydroxy chalcones with alloxan-induced diabetic rats (100 mg/kg) indicated their antidiabetic efficacy with decreased blood glucose levels in the diabetic rats compared to control rats [52]. The α-amylase inhibitory effect was shown by chalcones (Fig. 7A) (IC₅₀ = 1.25 ± 1.05 µM), and bis-chalcones (Fig. 7B) (IC₅₀ = 2.40 ± 0.09 µM) as compared acarbose, the thiomethyl and methoxy groups are effective on the activity [53]. The coumarin-triazole hybrids derived from chalcones demonstrated excellent antidiabetic properties [54].

The chalcones were designed to investigate the antibacterial activity, modulatory potential, and efflux pump inhibition against S. aureus multi-resistant strains. Compound (2E)-1-(4'-aminophenyl)-3-(phenyl)-prop-2-en-1-one (Fig. 8A) [55] has reduced the MIC of gentamicin by 70%, and on comparison of the effects of the modified antibiotic activity indicate a loss of synergism with gentamicin due to the addition of chlorine to the substance structure. The chalcone-1,2,3-triazole conjugates (Fig. 8B) [56, 57] have exhibited significant efficacy against bacterial and fungal strains, wherein the synergistic effect associated with chalcone and 1,2,3-triazole moieties. The cationic chalcone analogs (Fig. 8C) [58] displayed good bactericidal activity against tested bacteria, including the drug-resistant species. These membrane-active antibacterial compounds did not allow bacteria to develop resistance and exhibited negligible toxicity toward mammalian cells, reduce the viable cell counts in bacterial biofilms effectively and have low toxicity toward mammalian cells. A series of pyrazole-pyran hybrids [59], pyrazole-oxadiazole conjugates [60] derived from chalcones displayed good antimicrobial activities.
The fungi and mycobacteria are the culprits to cause infectious diseases in human beings. The need of an hour is to develop potent agents that overcome cancer and fungal infections. The synthesized dihydropyrazoles (Fig. 9A) [61] and thienyl-pyrazoles [62] and substituted pyrazoles [63] derived from chalcones showed excellent antifungal and antitubercular activities. Prenyloxylated chalcones display metabolic inhibition against *L. mexicana* and *T. cruzi*. The studies on leishmanicidal and trypanocidal activity of prenyloxy chalcones (Fig. 9B), and (Fig. 9C) [64] exerted metabolic inhibition for *L. mexicana*, and for *T. cruzi*; with selectivity index (SI =IC$_{50}$/CC$_{50}$) values of 80.9, 1.24, and 75.1, 1.43µM, respectively.

![Figure 9](https://biointerfaceresearch.com/)

**Figure 9.** The chalcones exert: A) antitubercular activity; B) metabolic inhibition for *T. cruzi*; C) metabolic inhibition for *L. mexicana*.

Alzheimer's disease (AD) is a common neurodegenerative disease characterized by progressive degeneration and neuronal cell death, resulting in neural network dysfunction. The underlying mechanisms, oxidative damage, and neuroinflammation have contributed to the deterioration of AD. The Nrf2, a transcription factor, regulates the cellular redox balance and is primarily involved in anti-inflammatory responses and is a pivotal cellular defense mechanism against oxidative stress. The lignan conjugates [65], pyrazoles [66], and oxadiazoles/thiadiazoles [67] prepared from various chalcones exhibited markable antioxidant activities comparable to ascorbic acid. The chalcone derivatives (Fig. 10A) [68] found a highly potent Nrf2 activator, which activates Nrf2 and induces expression of the Nrf2-dependent enzymes HO-1 and GCLC at both mRNA and protein levels, and also suppressed the production of nitric oxide and downregulated inflammatory mediators in BV-2 microglial cells. The chalcone-Mannich base analogs of which the compound (Fig. 10B) [69] exerted potent multifunctional properties, viz. inhibits AChE (IC$_{50}$ = 0.44 µM) and MAO-B (IC$_{50}$ = 1.21 µM), self-induced Aβ1–42 aggregation (55.0%, 25 µM), and also antioxidant activity.

![Figure 10](https://biointerfaceresearch.com/)

**Figure 10.** The chalcones exhibit: A) potent Nrf2 activator; B) inhibits AChE and MAO-B.

Amongst the chalcone-O-alkylamine derivatives, compound (Fig. 11A) [70] exhibited a good inhibitory effect on acetylcholinesterase (IC$_{50}$ = 1.3 µM) and butyrylcholinesterase (IC$_{50}$ = 1.2 µM). Selective MAO-B (IC$_{50}$ = 0.57 µM), also showed antioxidant and neuroprotectant activity, indicating that it might be a potential multifunctional agent for AD treatment. The compound (Fig. 11B) [71] has inhibited selective BuChE (IC$_{50}$ = 2.6 µM) and MAO-B (IC$_{50}$ = 5.3 µM). It also showed good antioxidant and neuroprotectant properties. A series of benzothiazepines derived from furanyl chalcones potently inhibited VRV-PL-8a and H$^+$/K$^+$ ATPase [72].
Ferroptosis is associated with the accumulation of lipid hydroperoxides and amyloid cascade hypothesis, the main forms of cell death in Alzheimer's disease. Hydroxylated chalcones (Fig. 12A) [73] inhibited amyloid-β peptide (Aβ) aggregation and ferroptosis simultaneously. In human neuroblastoma SH-SY5Y cells, these chalcones exhibit neuroprotection against Aβ₁₋₄₂ aggregation-induced toxicity and are good inhibitors of ferroptosis induced by the hydroperoxide-detoxifying enzyme Gpx4 using cystine/glutamate antiporter system. The [¹⁸F]4-dimethylamino-4'-fluoro-chalcone (Fig. 12B) [74] showed a higher initial uptake (4.43% ID/g at 2 min) into and more rapid clearance (0.52% ID/g at 30 min) from the brain than FDA-approved drugs, indicating the improvement of the probability of detecting Aβ plaques and the reduction of non-specific binding in the brain. The series of 4'-OH-flurbiprofen-chalcone hybrids (Fig. 12C) [75] exhibited good multifunctional activities, showing the best inhibitory effects on self-induced Aβ₁₋₄₂ aggregation (60.0% and 78.2%), and Cu²⁺-induced Aβ₁₋₄₂ aggregation (52.4% and 95.0%) and therefore these are promising candidate against AD.

The development of novel neuroprotective agents is urgently needed to treat neurodegenerative diseases affecting aging individuals worldwide. The set of chalcone-triazole hybrids (Fig. 13A) [76] displayed neuroprotection in oxidative stress-induced neuronal cell damage, significantly improved neurons’ morphology, and increased the cell survival rate of neuronal cells induced by oxidative stress, and promoted neuroprotection via the SIRT-FOXO3a signaling pathway. The oxygenated chalcones (Fig. 13B) [77] have their abilities to inhibit monoamine oxidases, in particular against MAO-B with an IC₅₀ value of 0.0021-0.0034µM, and against MAO-A with an IC₅₀ value of 0.029-0.072 µM. Oxidative stress-induced degeneration of retinal pigment epithelial cells is known to be a key contributor to the development of age-related macular degeneration (AMD). The pyrazoline derived from chalcones through (3+2) annulation reactions has shown potent affinity anti-inflammatory effect mediated by inhibition of phospholipase A2 [78,79].
4. Physical properties

Conformational differences in the chalcone compounds influence their physical-chemical properties, and the comparative structural analysis is relevant to describe changes in their properties. The analysis of three 1-(4-nitrophenyl)-5-(2,6,6-trimethylcyclohex-2-en-1-yl)penta-1,4-dien-3-ones shown that the polymorphism can affect the properties [80]. The compound 2E-1-(2′-Hydroxy-3′,4′,6′-trimethoxyphenyl)-3-(phenyl)-prop-2-en-1-one (Fig. 14A) [81] has shown s. The azo group tethered chalcone (Fig. 14B) [82] showed good dyeing performance on polyester fibers and excellent fastness properties on PET fiber. The chalcone (2E)-1-(3′-methoxy-4′-hydroxyphenyl)-3-(3-nitrophenyl)prop-2-en-1-one (Fig. 14C) [83] displayed good NLO properties. The compound 2(E)-4-(N,N-dimethylaminobenzylidene)-5-methylcyclohexanone [84], and 3-(benzo[d][1,3]dioxol-5-yl)-1-(3-chlorophenyl)-5-(2,4-dichlorophenyl)-4,5-dihydro-1H-pyrazole [85] derived from chalcone showed good optical properties.

![Figure 14](image1.png)

Figure 14. The chalcones show: A) electrochemical behavior; B) dyeing performance on polyester fibers; C) non-linear optical properties.

The compounds (E)-3-(4-methoxyphenyl)-1-(p-tolyl)prop-2-en-1-one, and (E)-3-(4-diethylamino)phenyl)-1-(p-tolyl)prop-2-en-1-one have shown good corrosion mitigation of mild steel in 0.5 M H₂SO₄ medium [86]. The compounds 4-chloro-N-[3-{(2E)-3-(methoxyphenyl)prop-2-enoyl]phenyl}benzamide [87], and pyrazolines derived from chalcones [88,89] indicated that these exhibit good NLO properties and were good material into fabrication for optoelectronic device applications. An oligo phenylene vinylene was prepared by the anodic oxidation of the 4-dimethylamino-4′-methoxychalcone (Fig. 15A) [90] at a constant potential in nitromethane on a platinum electrode, was thermally stable up to 190°C, and it displayed optical and electrochemical properties. Tetraphenylene-chalcone hybrids (Fig. 15B) [91] exhibit Stokes shifts and solvation effects and significant fluorescence properties in both solution and solid states.

![Figure 15](image2.png)

Figure 15. The chalcones exhibit: A) optical and electrochemical properties; B) Stokes shifts and solvation effects.

The chalcones, [(2E)-3-(3-chlorophenyl)-1-(3-nitrophenyl)prop-2-en-1-one and (2E)-3-(4-fluorophenyl)-1-(4-nitrophenyl)prop-2-en-1-one and [(2E)-1-(9-anthryl)-3-(4-fluorophenyl) prop-2-en-1-one [92] have exhibited third-order nonlinear optical limiting properties, and have some potential sites for electrophilic and nucleophilic attack.
4. Conclusions

The present review summarizes and focuses on the recent developments in the synthesis of chalcones, their versatility as scaffolds in the synthesis of varied classes of compounds of medicinal perspectives, and also describes their structure-activity relationship studies. The discussion on physical properties like semiconductor, optical, and fluorescence properties explores the diverse applications in photosensing and optical switching devices. The structure and structural optimization is promising for potential drug design and discovery, and development. The critical discussion made on anti-cancer, antidiabetic, antimicrobial, anti-inflammatory, antioxidant, anti-Alzheimer activities of chalcones in this review may surely help, particularly the young researchers working in this area.

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Conflicts of Interest

The authors declare no conflict of interest.

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halcone derivatives possessing broad spectrum

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