Chapter

Biological Role of Chalcones in Medicinal Chemistry

Sunil Tekale, Samson Mashele, Ofentse Pooe, Shivaji Thore, Pravin Kendrekar and Rajandra Pawar

Abstract

Chalcones are promising synthons and bioactive scaffolds of great medicinal interest due to their numerous pharmacological and biological activities. They are well recognized to possess antimicrobial, anticancer, antitubercular, antioxidant, anti-inflammatory, antileishmanial, and other significant biological activities. This chapter highlights recent updates and applications of chalcones as biologically, pharmacologically, and medicinally important entities.

Keywords: synthesis, characterization, PK/PD study

1. Introduction

Chalcones (trans-1,3-diaryl-2-propen-1-ones) (1) are \( \alpha,\beta \)-unsaturated ketones consisting of two aromatic rings (ring A and B) having diverse array of substituents (Figure 1). Chalcone skeleton contains two aromatic rings linked by an aliphatic three-carbon chain. The two rings of chalcone are interconnected by a highly electrophilic three-carbon \( \alpha,\beta \)-unsaturated carbonyl system that assumes linear or nearly planar structure. They possess conjugated double bonds and a completely delocalized \( \pi \)-electron system on both the aromatic rings.

Chalcones, named so by Kostanecki and Tambor, are commonly known by different names such as benzyldieneacetophenone, phenyl styryl ketone, \( \beta \)-phenylacrylophenone \( \alpha \)-phenyl-\( \beta \)-benzylethylene, etc. and constitute the central core of biologically active heterocyclic compounds. Chalcones constitute good synthons for a variety of novel heterocycles of high therapeutic potential and good pharmaceutical profile [1, 2]. Chalcones themselves are identified as interesting entities associated with several biological activities [3].

The structural modifications of the chalcone rings have led to a high degree of diversity that has proven useful for the development of new medicinal agents, and thus chalcones have become an object of continued interest in both academia and industry. The chalcones are well documented for a broad spectrum of biological activities including antimicrobial, anticancer, cytotoxic, antioxidative, anti-inflammatory, antiviral, and others [4]. Currently, chalcone derivatives have been widely used for the treatment of viral disorders, cardiovascular diseases, stomach cancer, food additives, and cosmetic formulation ingredients [5]. However, much of the pharmacological potential of chalcones and their recent updates need to be understood. The purpose of this chapter is to cover and describe the recent developments, preferably after 2015 to date, the utility of chalcones as medicinally...
significant scaffolds, and their biological activities. It covers and highlights the recent advances in the use of chalcones as antimicrobial, anticancer, antitubercular, antioxidant, anti-inflammatory, and miscellaneous applications in biological and medicinal fields.

2. Biological activities of chalcones

2.1 Antimicrobial chalcones

Antimicrobial agents are the drugs used to treat infectious diseases caused by different types of bacteria and fungi. The use of these drugs is now common, and continuous efforts are put by the scientific community to search for newer antimicrobial agents due to antimicrobial resistance (AMR) shown by the microbes. Mutation, gene transfer, phenotypic change, and selective pressure are some of the causes behind AMR [6]. Antimicrobial or drug resistance is commonly developed by bacteria, fungi, parasites, and viruses when the microbe no longer responds to a drug that previously treated them effectively. This AMR can lead to several issues including difficulty in controlling the disease, a longer stay of the microbes in the host, higher risks of spreading, and increase in mortality rates. Infectious diseases are one of the common problems encountered globally. Although several commercially marketed drugs are available, the search for new drug molecules becomes essential for the treatment of infectious diseases [7]. Consequently, the search for new antimicrobial agents becomes essential. Herein we discuss the recent updates in the search of chalcones as an attempt to develop antimicrobial agents:

Methoxy-4′-amino chalcones (2) showed good in vitro antimicrobial activities against *Escherichia coli*, *Staphylococcus aureus*, and *Candida albicans*. A molecular docking study also supported the observed results showing good interactions with the active sites of dihydropteroate synthase enzyme of *E. coli* and *S. aureus* [8].

The quinoxalinyln chalcones (3) synthesized by the Claisen-Schmidt condensation were found to be good antimicrobial agents. The antimicrobial studies were carried out against *Staphylococcus aureus*, *Escherichia coli*, and *Candida albicans* using the disk diffusion method. The selected chalcones were evaluated for anticancer and cytotoxicity activity against MCF-7 cancer cell lines using the MTT assay method showing good anticancer activity [9].

Some fluorinated chalcone-triazole hybrids (4) were studied for antimicrobial activities against *S. epidermidis*, *B. subtilis*, *E. coli*, and *P. aeruginosa* bacterial and two fungal strains, namely, *A. niger* and *C. albicans*, by standard serial dilution method [10]. The results of the in vitro antimicrobial activity were compared with ciprofloxacin and fluconazole standard drugs.
Dehydroacetic acid chalcone-1,2,3-triazole hybrids (5) were shown to possess good in vitro antimicrobial activities against *Staphylococcus epidermidis*, *Bacillus subtilis*, *Escherichia coli*, and *Pseudomonas aeruginosa* bacteria and two fungal strains, viz., *Aspergillus niger* and *Candida albicans* [11].

Thiazole-based chalcones including thiazolo[2,3-b]quinazoline and pyrido[4,3-d]thiazolo[3,2-a]pyrimidine analogs (6 and 7) screened against both gram-positive and gram-negative bacteria revealed that the tilted compounds had minimum inhibitory concentration (MIC) values in the ranges of 1–4.0 μg/ml against *S. aureus*, *B. subtilis*, *M. luteus*, *E. coli*, and *P. aeruginosa* [12]. The results were found to be comparable with the ampicillin and ciprofloxacin standards.

Burmaoglu et al. reported antimicrobial activity of fluoro-substituted chalcones (8) and (9) against *S. aureus*, *S. pyogenes*, *E. faecalis*, *E. coli*, and *P. aeruginosa* bacteria and *C. albicans*, *C. glabrata*, and *C. parapsilosis* fungal strains. Some of the tested compounds also exhibited antitubercular activity against *Mycobacterium tuberculosis* [13].

Chalcones incorporated with a piperazine ring (10) exhibited promising antimicrobial activity against *Escherichia coli*, *Aspergillus niger*, *Salmonella typhi*, *Penicillium chrysogenum*, and *Staphylococcus aureus* bacterial strains as well as *Aspergillus flavus*, *Bacillus subtilis*, and *Candida albicans* fungi [14].

Talniya and Sood documented the synthesis and antibacterial activity of chalcones (11) against *Bacillus subtilis* bacteria and *Aspergillus niger* fungi by disk diffusion method [15]. The chalcones possessing o-chloro, p-chloro, and p-hydroxyl substituents showed remarkable antimicrobial activity against the screened microbes.

Oxazolidinones incorporated with chalcone hybrids (12) were evaluated for in vitro antibacterial and antifungal activities by using the serial dilution method [16]. Results showed moderate antimicrobial activities as compared with the standard drugs ciprofloxacin and linezolid.

Novel diarylsulfonylurea-chalcone hybrids (13) were evaluated by agar well diffusion method against various strains of bacteria and fungi including *Bacillus subtilis*, *Escherichia coli*, *Bacillus pumilus*, *Staphylococcus aureus*, *Micrococcus luteus*, *Candida albicans*, and *Penicillium chrysogenum*. Most of the compounds showed promising antibacterial and antifungal activity suggesting that the diarylsulfonylurea-chalcone hybrids can be used for the treatment of diseases caused by these microbial organisms [17].

Vanillin moiety containing chalcones (14), (15), and (16) were synthesized by the Claisen-Schmidt condensation of vanillin with different acetophenone derivatives and were studied for antimicrobial activities by using agar disk diffusion and microdilution methods [18]. The researchers found *S. aureus* and *C. albicans* to be the most sensitive strains and *E. faecalis* to be the least sensitive against these chalcones. The presence of halogens in chalcones increased their microbial susceptibility. The structures of some antimicrobial chalcones are shown in Figure 2.

### 2.2 Anticancer chalcones

Cancer is a widely spreading disease all over the world, necessitating the need to develop new anticancer agents [19]. Anticancer or antineoplastic drugs are those that are effective in the treatment of malignant or cancerous disease. Increasing recurrence of mammalian tumors and severe side effects of chemotherapeutic agents reduce the clinical efficiency of a large variety of commonly used anticancer agents, and thus, there is always a constant need to develop alternative or synergistic anticancer drugs with minimal side effects [20].
The treatment of cancer is a complicated process as the drugs used target human cells and albeit cells that have undergone genetic changes and are dividing at a fast and uncontrolled rate. However, only a few anticancer drugs can differentiate between normal tissue cells and cancer cells to a large extent. Thus, there is always a constant need to develop alternative or synergistic anticancer drugs with minimal side effects. This part of the present chapter highlights significant and recent developments in chalcones used as anticancer agents:

Sulfonylpiperazines linked with [1,3]dioxolo[4,5-g]chromenones (17) were synthesized by the aldol condensation and evaluated as antioxidants against DPPH, ABTS, as well as antiproliferative agents against non-cancer MDCK cell lines [21].

The design, synthesis, and antitumor potential of chalcones (18) were studied against human breast adenocarcinoma MCF-7 cells in a concentration-dependent manner [22]. They triggered significant changes in cell morphology and biochemical/molecular parameters and revealed the apoptosis inductor nature of the titled compounds and their application as promising alternatives for the treatment of neoplasia, especially in terms of drug resistance development.

Novel anthraquinone-chalcone hybrids (19) possessing amide functionality were synthesized, then characterized, and reported for good cytotoxic potential against K562, Jurkat, and HL-60 leukemia cell lines [23].

![Structures of antimicrobial chalcones.](image)
An apoptosis is an important phenomenon, which affects many diseases, such as cancer and Alzheimer’s disease. Chalcones (20) induced apoptosis of human hepatic and lung cancer cells and inhibited cancer cell migration and invasion [24].

The bis-chalcone derivatives (21) were studied for their ability to inhibit xanthine oxidase and growth inhibitory activity against MCF-7 and caco-2 human cancer cell lines in vitro. The bis-chalcone with fluoro group at the 2nd or 2, 5th position of B-ring was found to be a potent inhibitor of the enzyme possessing IC_{50} values in the low micromolar range. The activities of the compounds were found to be around seven times higher than the standard allopurinol [25].

Chalcones (22) were synthesized and evaluated for anticancer activities on human colorectal carcinoma cell line HCT116 by Dias et al. [26]. Halogens at the third position of the chalcones were found to enhance the anticancer activity of the titled compounds.

Leao et al. reported the chalcone derivatives (23) and (24) for cytotoxicity against human tumor cells [27]. Some novel xanthine-chalcone hybrids (25) and (26) were reported as promising anticancer agents [28].

A series of novel dithiocarbamate-chalcone derivatives (27) and (28) was designed, synthesized, and evaluated for antiproliferative activity against three selected cancer cell lines (EC-109, SK-N-SH, and MGC-803). Almost all the synthesized compounds exhibited moderate to potent activity against all the tested cancer cell lines [29].

Pd(II) and Pt(II) complexes of chalcones (29) were studied for in vitro antimicrobial and antitumor activities against different microorganisms and the human hepatocellular carcinoma cells indicating their use as promising antimicrobial agents and anticancer drug candidates [30].

Some novel Pt(IV) complexes of chalcone analogs (30) were synthesized and evaluated for antiproliferative activity by using MTT assay. The in vitro evaluation revealed that all Pt(IV) complexes showed good activity against the three human cancer cells [31].
The overexpression of the CYP1 class of enzymes is associated with the development of human carcinomas. The pyridine-4-yl series of chalcones (31) were synthesized and screened for the inhibition of CYP1 isoforms in Sacchrosomes TM and live human HEK293 cells. The chalcones bearing tri-alkoxy groups on non-heterocyclic ring displayed selective inhibition of the CYP1A1 enzyme with IC$_{50}$ values less than 70 nM [32].

The pyrazolic chalcone analogous compounds (32) were synthesized and evaluated as potential chemotherapeutic agents for the treatment of hepatocellular carcinoma [33]. Some of the screened compounds exhibited potent cytotoxic activity against all the cancer cell lines tested and had good cytotoxic activities.

DNA ligases play a crucial role in causing cancer. Gupta et al. reported the inhibition DNA ligases resulting in DNA nick-sealing activity followed by the antiproliferative activity of the indole-chalcone based benzopyran chalcones (33) on cancer cells [34].

Indolizine-chalcone hybrids (34) were synthesized and studied for apoptosis and anticancer effect on human lymphoma cells by S. Park and coworkers [35].

Prenyl and geranyl group-bearing chalcones (35) were synthesized by using regioselective iodination followed by the Suzuki coupling reaction and studied for in vitro anticancer activity against human tumor cell line K562 by MTT assay. Morphology changes revealed that the chalcone derivatives inhibited the proliferation of K562 cells by inducing apoptosis [36].

![Figure 4. Structures of anticancer chalcones (29-39).](image-url)
Leukemia is a hematologic malignancy with poor prognosis in humans. Diprenylated chalcone (36) was studied as a new potential antileukemia agent [37].

Chalcones (37) were studied for antiproliferative activities against the human TRAIL-resistant breast (MCF-7, MDA-MB-231), cervical (HeLa), ovarian (Caov-3), lung (A549), liver (HepG2), colorectal (HT-29), nasopharyngeal (CNE-1), erythromyeloblastoid (K-562), and T-lymphoblastoid (CEM-SS) cancer cells by Mai [38]. Triazole incorporated with chalcones (38) and (39) was synthesized and evaluated for 3-(4,5-dimethylthiazole-2-yl)-2,5-diphenyltetrazolium bromide (MTT) cytotoxicity assay against a series of four human cancer cell lines (MCF-7, MIA-PaCa-2, A549, HepG2) [39]. The structures of anticancer chalcones are depicted in Figures 3 and 4.

2.3 Antitubercular chalcones

Tuberculosis (TB), caused by the acid-fast gram-positive bacillus, *Mycobacterium tuberculosis*, remains the leading source of bacterial infectious disease [40]. *M. tuberculosis* establishes an infection through an invasion of alveolar macrophages. The *Mycobacterium tuberculosis* encodes for more than 60 adenylating enzymes, mainly tRNA synthetases, acyl-AMP ligases, etc. [41]. Currently, the treatment of TB employs four first-line drugs, isoniazid, rifampin, pyrazinamide, and ethambutol, which must be administered in the body daily for a 2-month intensive phase. However, for susceptible TB strains, this therapy is 95% effective. The emergence of multidrug-resistant (MDR) strains, defined as resistant to isoniazid and rifampin, requires the use of less effective and more toxic second-line TB drugs. Herein we discuss some recent updates in the application of chalcones against tuberculosis:

New sulfonamide-bearing chalcones (40) were synthesized by the Claisen-Schmidt condensation and were reported as excellent antituberculosis hits showing low selectivity, being equally inhibitory to *M. tuberculosis* and mammalian T3T cells [42].

Gomes et al. studied antitubercular activities of chalcones (41) and (42). The chalcones showed good selectivity towards *M. tuberculosis* with low cytotoxicity against Vero cells and thus possess promising antitubercular potential [43].

Spirochromone annulated chalcone conjugates (43) were documented for antitubercular activity against *Mycobacterium tuberculosis* H37Rv strain. Molecular docking studies performed against the receptors revealed MTB phosphotyrosine phosphatase B protein as the most probable target based on the high binding-affinity scores [44].

Babu et al. studied chalcones containing nitrophenyl moieties (44) for antitubercular activity using MABA assay and antibacterial and antifungal activities by cup plate method. Molecular docking study predicted the inhibition of thymidine kinase of the *Mycobacterium tuberculosis* [45]. Anti-tubercular chalcones are depicted in Figure 5.

![Figure 5. Structures of anti-tubercular chalcones.](image-url)
2.4 Antioxidant chalcones

Antioxidants are the compounds that inhibit the oxidation process. These substances can prevent or slow damage to cells caused by free radicals. Oxidation is a chemical reaction that generates free radicals, thereby leading to chain reactions which may damage the cells of organisms and hence responsible for oxidative stress resulting in chronic diseases such as heart diseases, stroke, cancer, arthritis, respiratory diseases, Parkinson’s disease, and other inflammatory conditions [46].

Cao et al. documented a series of 4’-OH-flurbiprofen-chalcone hybrids (45) and evaluated them as potential multifunctional agents for the treatment of Alzheimer’s disease. Besides, the compounds were reported for good antioxidant activities, MAO inhibitions, biometal chelating abilities, and in vitro anti-neuroinflammatory activities [47].

Selenoenzymes and nuclear factor erythroid 2-related factor 2 (Nrf2)-regulated phase II enzymes constitute the main components of cellular redox and antioxidant systems giving information about multiple interrelations involved in the oxidation processes. Chalcones (46) were proved to interfere with the biosynthesis of Nrf2-regulated selenoenzymes [48].

El-Sayed et al. documented the antioxidant activity of chalcones (47) [49].

The chalcone derivatives (48) were synthesized by the Claisen-Schmidt condensation with KOH in ethanol at room temperature under sonication conditions and screened for antioxidant potential by Polo et al. [50].

The chalcones (49) were studied as potent antioxidants by Tajammal and coworkers. These compounds have lower IC₅₀ values than the Trolox and ascorbic acid standards [51].

A series of chalcone (50) analogs were designed, synthesized, and screened for antioxidant activities. The chalcone was found as a promising anti-ischemic stroke drug candidate, providing novel dual-antioxidant mechanism strategies and concepts for oxidative stress-related disease treatment [52]. The prenylated chalcones (51) were reported for good antioxidant activity [53]. Figure 6 represents the structures of antioxidant chalcones.

2.5 Anti-inflammatory chalcones

Anti-inflammatory drugs are the drugs which are used to reduce pain and inflammation. In other words, these are pain-relieving drugs. These drugs work mainly by inhibiting the cyclooxygenase enzymes, COX-1 and COX-2, that produce
prostaglandins [54]. Herein we discuss some of the efforts for the development of chalcone-based heterocycles as effective anti-inflammatory compounds:

Indole-based chalcones (52) were synthesized and evaluated for in vitro COX-1 and COX-2 inhibitory activity [55].

α-Substituted 2’,3,4,4’-tetramethoxychalcones (53) and (54) were evaluated for their ability to modulate inflammatory responses to influence on heme oxygenase-1, nitric oxide synthase, and cytokine expression levels. Anti-inflammatory activity was correlated with thiol-alkylating activity, i.e., stronger electrophiles substituted with CF₃, Br, and Cl were found to be more potent than the remaining derivatives [56].

Zhang et al. identified methoxy chalcones (55) as a potential candidate for treating acute inflammatory diseases [57].

Pyrazole- and morpholine-containing chalcones (56) were reported for anti-inflammatory activity by Gadhave and Uphade. The anti-inflammatory activity performed by carrageenan-induced rat paw edema method showed good potency of some of the tested compounds as compared with the standard diclofenac drug [58].

Nurkenov et al. studied the in vitro anti-inflammatory effect of chalcones (57) to inhibit the lipopolysaccharide-induced production of anti-inflammatory cytokine interleukin-6 and tumor necrosis factor [59].

The imidazole containing chalcone molecule (58) demonstrated noteworthy anti-inflammatory activity as compared with the standard drug, indomethacin [60].

1-[3-Methoxy-4-(5-nitro-furan-2-ylmethoxy)-phenyl]-3-(substituted phenyl)propenones (59) synthesized by the condensation of furfural and apocynin were evaluated for anti-inflammatory activity [61]. The structures of anti-inflammatory chalcones are shown in Figure 7.

2.6 Miscellaneous applications of chalcones

Besides the above-discussed applications, chalcones are useful for miscellaneous applications. Some of them are mentioned as follows:
**Leishmania** is a genus of trypanosomes responsible for the disease leishmaniasis. Leishmaniasis is spread through sand flies of the genus *Phlebotomus*, primary hosts being the vertebrates. The chalcone (60) was evaluated against 29 promastigotes of *Leishmania donovani* exhibiting low toxicity against mammalian cells [62].

A series of new chalcone-rivastigmine hybrids (61) was designed, synthesized, and evaluated in vitro for the ability to inhibit human acetylcholinesterase and butyrylcholinesterase. Results showed that these compounds exhibited selective activity in micro- and submicromolar ranges as compared with the standard rivastigmine and thus the compounds can serve as the lead ones for the treatment of Alzheimer’s disease [63].

Sang et al. reported AChE/BChE inhibitory, MAO-A/MAO-B inhibitory, and antioxidant activities of chalcone-O-carbamate derivatives (62). Results revealed that the compounds show highly selective BChE inhibitory activity with IC50 values of 1–3 mM range [64].

Some 1,3,4-oxadiazole/thiadiazole-chalcone conjugates (63) were synthesized and evaluated for in vitro and in vivo antiviral activities against TMV. These conjugates have low binding constant values which were comparable to the standard ningnanmycin [65].

Amide tethered 7-chloroquinoline-chalcone bifunctional hybrids (64) were synthesized and employed as antimalarial agents against the resistant strain of *Plasmodium falciparum*. Methoxy substituent at the para position of ring B on chalcones and longer alkyl chain lengths significantly improved the antiplasmodial profiles of the chalcone derivatives [66].

The halogenated 1-tetralone or 6-amino-1-tetralone chalcone derivatives (65) were synthesized and evaluated for inhibitory effects against ROS production in LPS-stimulated RAW 264.7 macrophages. The structure-activity relationship revealed that amino moiety at the sixth position of 1-tetralone chalcones plays an important role for greater ROS inhibitory potency [67].

Chalcone derivatives (66) were studied for hepatoprotective ability, and the results were compared with the standard hepatoprotective drug silymarin. The experimental results were supported by a molecular docking study [68].

Triazole-linked 4-aminoquinoline-chalcone/N-acetylpyrazoline conjugates (67) were synthesized and evaluated for antiplasmodial activities against cultured chloroquine-resistant strain. The activities were found to be dependent on the length of the alkyl chain as well as on the presence of methoxy substituents on the chalcone rings [69].

Chalcone analogs (68) were synthesized and evaluated for cytotoxic effects in human hepatoma HepG2 cells. The percentage of apoptotic cells was significantly higher in the compounds than that in the control cells [70].

The oxygenated chalcones (69) were found to inhibit monoamine oxidases, and the lead compounds were found to be nontoxic at 200 μg/mL in normal rat spleen cells [71].

Hameed et al. studied the quinoline-based chalcone compounds (70) as reverse transcriptase inhibitors. Bromo- and chloro-substituted chalcones exhibited a high degree of inhibition against the reverse transcriptase [72].

Histoplasmosis is a fungal infection caused by the dimorphic fungus *Histoplasma capsulatum*. Hydroxyl group-bearing chalcones (71) and (72) were studied for histoplasmosis by Wanessa et al. [73].

Sashidhara et al. documented the antiulcer activity of some novel quinoline-chalcone hybrids (73) in various ulcer models in Sprague Dawley rats. Additional studies including in vitro metabolic stability and in vivo pharmacokinetics showed their potential to act as an orally active and safe candidate for the development of an antiulcer agent [74].
Pyrene ring-bearing chalcone (74) was studied as a sensitive and highly selective sensor for the detection of aluminum (Al\(^{3+}\)) ions by fluorimetric studies by Suresh et al. The chalcone was found to be useful for the electrosorptive removal of Al\(^{3+}\) ion and several other biological applications including the bio-imaging of bacterial cells [75].

Chalcones (75) were reported for potent antimalarial activities against *Plasmodium falciparum* using Rieckmann’s method. Allyloxy, hydroxy, and alkoxy functional groups increased the antimalarial activity of the chalcone derivatives [76].

Human African trypanosomiasis is an infectious disease that affects the lives of people living in rural areas of Africa. Beteck et al. studied the antitrypanosomal activities of indanone-based chalcone analogs (76) by screening against *T. b. brucei* [77]. The structures of chalcones having miscellaneous activities are depicted in Figure 8.

![Figure 8. Structures of chalcones having miscellaneous activities.](image)

3. Conclusion

Chalcones and their analogs possess significant biological activities including antimicrobial, anticancer, antitubercular, antioxidant, anti-inflammatory, antileishmanial, enzyme inhibitory, and miscellaneous applications and hence acquire a unique place in medicinal chemistry. The growing interest of synthetic organic, pharmacological, and medicinal chemists towards chalcones and their
derivatives will be continued in the future also. This chapter is expected to provide a stimulus for researchers to design, synthesize, and carry out further investigation on the pharmacological effects of new chalcone derivatives for different biological activities.

Conflict of interest

The authors declare no conflict of interest.

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