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Chalcones

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Abstract –*α, β-unsaturated carbonyl compounds are known as chalconesthey are formed by reacting benzaldehyde and acetophenone in presence of catalyst and ethanol by claisen Schmidt reaction. It is aromatic ketoneand biologically it is very important.*

Key Words: *Chalcones; pharmacological activities; radical scavenging; fluorescent probe, pyrazole*

1. INTRODUCTION

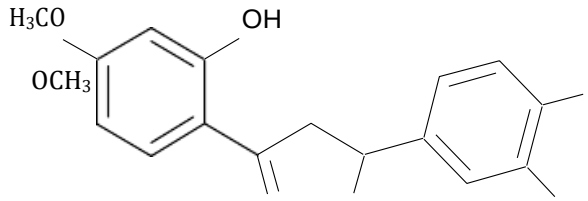
It attracted interest due to its pharmacological activities. It showed activity as antioxidant, antibacterial, antifungal, anticancer and antidepressant.They are open chain compound. Two aromatic rings are present in chalcones which are joined byα, β unsaturated carbonyl group through three carbon. One ring have electron deficient group while second ring have hydrophobic group. Para position of second ring is very important for its pharmacological activity. Naturally chalcones occur as flower pigment and also in heartwood, leaves bark and roots of many plants.If halogen is introduced inbenzoid part of unsaturated ketone then biological activity of chalcones is enhanced. Few changes in their structure yield a significant diversity which is also useful to use them as new medicinal agent with less toxicity. These methods used aremicrowave assisted [1], ultrasonicradiations [2] by grinding [3] etc. have been developed. They become center of attraction for scientist crucial interest of scientists in as it becomes an important intermediate in synthesis of different pharmaceuticals. They behave as pharmacological agent showing activities like antibacterial [4-5], antioxidant [6-8], anticancer [9-11], antifungal [12-14], anticancer and anti-inflammatory [15-17], antidepressant[18-20]. They are also behave a non-azo dyes [21].

2. PHARMACOLOGICAL ACTIVITIES

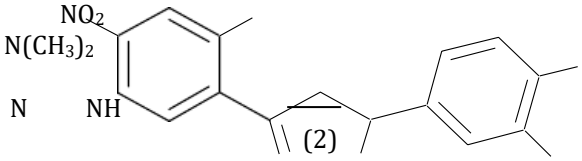
2.1Antioxidant activity

Oxidative damage which are induced by free radicals and reactive oxygen species, are prevent by antioxidant. This is liable for several issues such cancer and ageing etc.Chalcones, facilitatesin plant defense mechanisms to scale back the destruction at molecular level by counteracting reactive oxygen and therefore harm caused by microorganisms, insects and herbivores [6].The inhibitory activity of those unit area are associated to its (i) lapton donation capacity, (ii) its ability to stabilize and delocalize the odd lapton and (iii) chelation of transition metal ions (iv) oxygen extinctionbehaveas substrate for radicals [7].

Synthetic chalcones are used for free radical scavenging..Conjointly Tan Nhut Doan et al. [8] also synthesized a group of allylic chalcones and pyrazolicchalcones by free radical scavenging.They examined these chalcones and connected compounds for their antioxidant properties by victimization of 1, 1-biphenyl-2- picrylhydrazyl (DPPH) radical scavenging technique. Vitamin C was chosen as 4,5- dihydro-1H-pyrazol-3-yl)-5-methoxyphenol (**1**) and N,N-Dimethyl-4-(3-(4-nitrophenyl)- 4,5-dihydro-1H-pyrazol-5-yl)-benzamine (**2**) exhibited the best DPPH scavenging activity(89.64% and 89.27%, respectively) whereas the chalcones which were the precursor for these compounds failed to show any activity. Results of this proves that the pyrazole ring is liable to thisactivity.



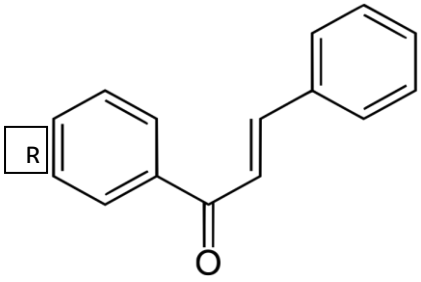
(1)



(2)

Three simple methoxychalcones are studied by NurettinYayli et al. [8] for their superoxide radical scavenging activities. Theydid it by employing a quite common technique in which the substrate taken by them was xanthine of xanthine oxidase was utilized to provide the superoxide radicals which were then consumed with in the presence of antioxidants. Determination of other radicals were then done spectrophotometrically by the reaction with Nitro blue tetrazolium salt (NBT).The results expressed because concentration of check sample giving fifty percent reduction with in the absorbance of management at 560 nm clearly mirrored the result of methoxy group on their potential to scavenge superoxide

radicals. One of these chalcones having methoxy group at ortho-position was found to be most active antioxidant (IC_{50} 0.598 mg/mL) even more active than the reference compound (Butylated hydroxyl toluene IC_{50} 1.02 mg/mL). The order of the superoxide radical scavenging activity of these three chalcones followed the order *o*-methoxychalcone (IC_{50} 0.598 mg/mL) >*m*-methoxy (IC_{50} 2.708 mg/mL) >*p*-methoxy (IC_{50} 4.343 mg/mL).With these results many artificialchalcones have been made which are having antioxidant property.



R =o OCH_3

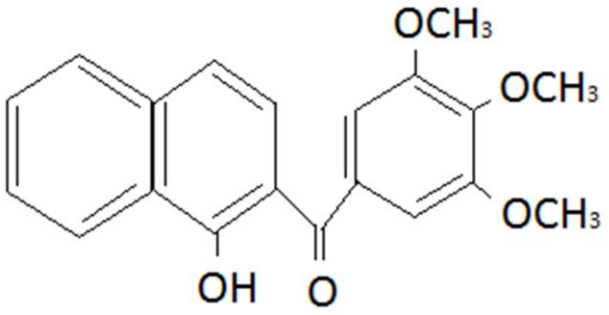
m= OCH_3

p= OCH_3

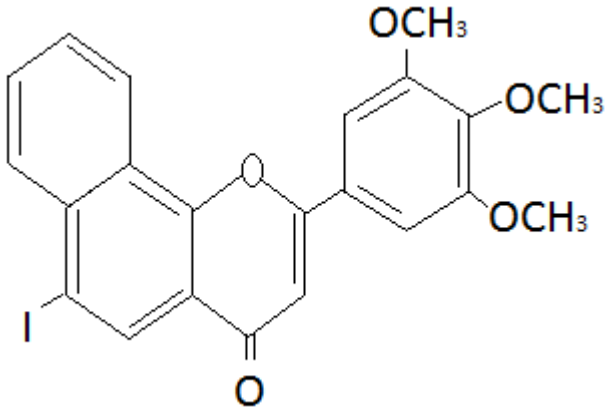
Thirty three chalcones and its derivatives are being studied by Ruby John Anto et al. [9] to grasp result of variedsubstituent connected to each aromatic ring of chalcone. They tested these compounds for superoxide radical scavenging activity and lipid molecule peroxidation inhibition. Results showed most of the chalcones was found to superoxide expect chlorine substituted chalcones. Theforemost active superoxide radical scavenger noticed was compound 1-(2'-Hydroxy-5'-methylphenyl)-3-phenylprop-2-en- 1-one (IC_{50} 10.5 µg/mL) the dihydroxyl chalcones (1-(2'-hydroxyphenyl)-3-(-2- hydroxyl phenyl) prop-2-en-1-one, IC_{50}4.0 µg/mL) exhibited the very best lipid peroxidation inhibiting activity. One another chalcone substituted with 2'-OH and4'-OCH_3 (IC_{50} 8.8 µg/mL) tried to be very terribly economical in inhibition of lipid peroxidation. Compounds having methyl group were active superoxide scavengers which are solely unsubstituted compounds and their dimethyl derivatives were found active for lipid peroxidation. From the study, it reveals that the *o*- and *p*-substitution by laptone donating groups might increase the inhibitor activities of chalcones which can openup a way to the more active and efficient synthetic antioxidants.

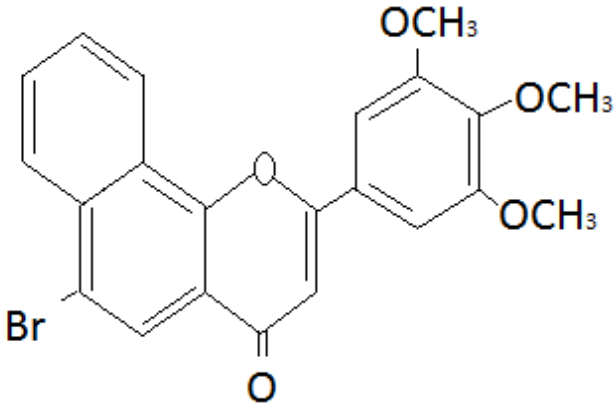
2.2 Antibacterial activity

Sainath B. Zangade et al. [10]. Synthesized numerousnovelchalcones and their corresponding flavones containing naphthyl moiety. The chalcones were synthesized by victimization the traditionalClaisen-Schmidt condensation technique. All the compounds were subjected to antibacterial activity test against *Pseudomonas auriginosa*(Pa) and *Staphylococcus aureus* (SA) using cup-plate agar diffusion technique. To perform diffusion technique antibiotic streptomycin (zone of inhibition Pa= 30 and Sa= 28 mm) is employedas standard antibiotic and solvent used was five percent DMF solvent. Most of the tested compounds showed important germicidal behavior however the compounds 1-(1'-hydroxy-4'-iodonapthyl)-3-(3,4,5- trimethoxyphenyl) prop-2-en-1-one (**c**), (zone of inhibition Pa=27 and Sa=30 mm), its corresponding flavone (**d**), (zone of inhibition Pa=28 and Sa=26 mm) and



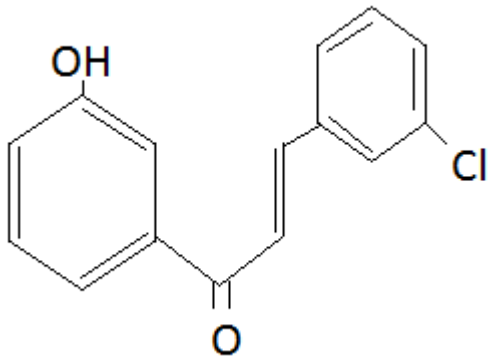
bromine substituted flavone instead of iodine group, (**e**), (zone of inhibition Pa=29 and Sa=26 mm) were reported most active antibacterial agents at concentration of 100 µg/ml. This study showed that inhibition of microorganism growth will increases with the rise of halo substitution.(c,d,e)

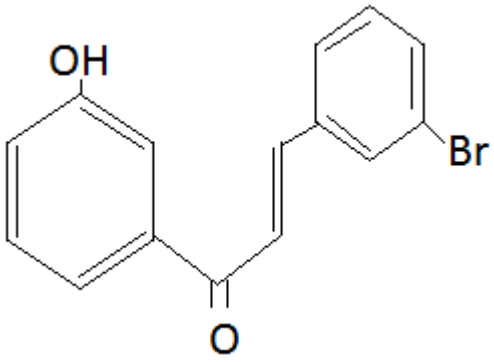




Farzana Latif Ansari et al. [11] synthesized two sets of chalcones tounderstand a lot ofabout the antibacterial activity of substitutedchalcones, by conventional and microwave assisted synthesis methods. In the set-I each phenyl rings were substituted by halogens, nitro, methoxy, hydroxyl etc at different positions. In set-IIchalcones were containing one heterocyclic ring such as pyridine, pyrrol, furan, thienyl and indolyl. For in vitro bactericidal action these compounds were tested against sic bacterial strains named*B. bronchiseptica*, *M. leuteus*, *P. picketti*, *E. coli*, *E. aerogenes*and *S. setubal*by using agar well-diffusion method. Standard drug (zone of inhibition 31and 34 mm respectively) used for for this method is Ceficimethe compounds that were used for testing were active against*B. bronchiseptica*with a zone of inhibition ranging from 9.5-18.5 mm in diameter. The study proved that chalcones containing electron withdrawing halogen groups like bromo- and chloro- groups {3-(3-bromophenyl)-1-(3'-hydroxyl phenyl)prop-2-en-1-one,(**f**) and 3-(3-chlorophenyl)-1-(3'-hydroxyphenyl)prop-2-en-1-one} (**g**), showed the greatest antibacterial activity (zone of inhibition 18.5 and MIC values 0.2 and 0.3 mg/mL respectively) while least active compounds were that which was more polar and electron withdrawing nitro-groups. Moderate activity were shown by chalcones containinghydroxyl and methoxy substituent. This showed the order of bactericidal activity for various chalcones had been found X > OH > OCH_3>NO_2.

High value of hydrophobicity constant, octanol- water partition coefficient andmolarvolumes were also reported in most bactericidal chalconeswithexceptionof–OCH_3substitutedchalcones.For set II chalcones, the antibacterial activity was reflected due to heterocyclic ring present in it. Most active bactericidal were those chalcones which contain thiophene moiety found except nitro substituted chalcones. These results supported earlier hypothesis that nitro group decreases the bactericidal effect. On the basis of these experiments various chalcones possessing high antibacterial activity were synthesized. (f) and (g)



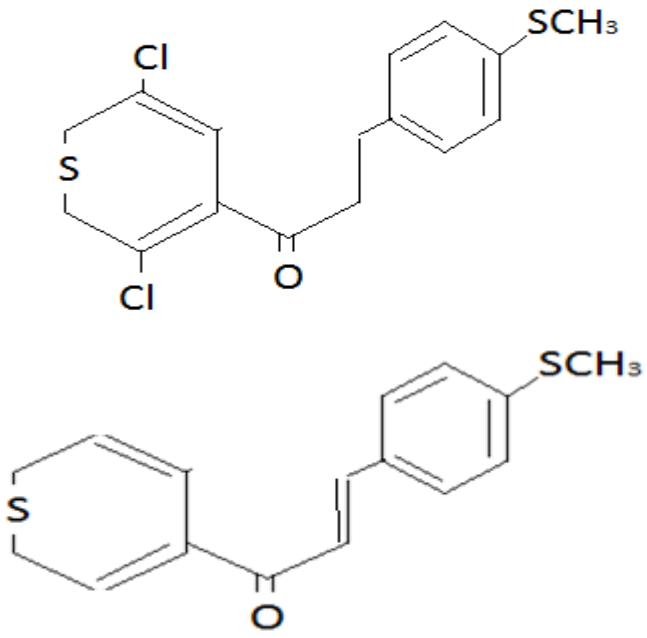


Y. Rajendra Prasad et al. [15] performed QSAR analysis on a set of thirty three synthesized chalcones tested for their antibacterial activity against human pathogenic gram +ve bacteria, *Bacillus pumilis*]. Amplicillin is used as standard antibacterial agent and DMSO as solvent. ADME weight, HOMO energy and Kappa 2 index were used to generate QSAR model. Activity of substituted chalcones reduces with high value of HOMO energy. Energy of HOMO increases by electron donating group which delocalized electrons in π-space of benzene. Bactericidal potential will increases by electron withdrawing group like halogens. Bacterial growth is inhibited with high value of ADME weight and Kappa 2 index. Antibacterial activity against Bacillus pumilis will increases if chalcones derivatives having electron withdrawing substituents on ring having high degree of binding linearity with high molecular weight will be synthesized.

2.3 Antifungal activity

Novel chalcones having group piperazine or 2,5 dichlorothiopene synthesized by Tomar et al. [14] and tested for their microbial activities. Antibacterial and antifungal activities were tested against different bacterial strain of all synthesized compounds. They did this on specific fungi *Candilaglabrata, CandilaKursei and Candilaalbicans*. Comparing the results as zone of inhibition and MIC values of tested chalcones with the standard drug fluconazole (29 mm and 50 µg/mL for each), most of the compounds were showing significant activity against all the three chosen fungi. One chalcone carrying 2,5-dichlorothiophene moiety and un substituted phenyl ring (h) was found to be most potent antifungal agent with zone of inhibition of 26 mm for each strain and MIC values 2.22, 3.17 and 4.65 µg/mL, respectively. It was even more active than the standard one. Other two compounds with piperazine moiety were highly active agents possessing zone of inhibition and MIC values comparable with that of the most active chalcone in this study. From this analysis, it was also found that compounds substituted with electron negative nitro group were less active towards the inhibition of fungal growth.

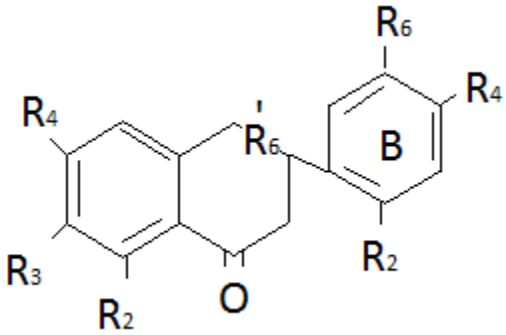
(h and i)



Anti-fungalactivities ofSulphur substituted chalcones either as thiophene moiety or thiomethyl group wasanalyzed by Seema Bag group [13]. They synthesized two series of α,β-unsaturated compounds, one with thiophene moiety and other with phenyl ring substituted with thiomethyl group. Compounds was having a phenyl ring that have various substitutions. All synthesized compounds were tested against both fluconazole resistant as well as fluconazole sensitive strains of *Candida albicans*(NCIM 3446 and ATCC 10231 respectively). The results of two series samples confirmed the perception as the chalcone having both unsubstituted thiophene moiety and *p*-thiomethyl substituted phenyl ring in the same molecule. Molecule (**i**) was found to be the most active fungal growth inhibitor (IC_{50} 05 µg/mL for both strains) fluconazole was chosen as reference. (IC_{50} 100 and 20 µg/mL respectively).If Bromo group is attached to thiophene moiety then it retarded its activity. If fluorine is substituted at p position then maximum activity was reported. As more halogen was incorporated then antifungal activity decreased. Also the presence of heavier phenyl group or nitro reduced the activity of chalcones. On the other hand, introducing methoxy group on *p*-position or hydroxyl on any position proved helpful in enhancing the antifungal activity. P.M.GurubasavarazaSwamy et al. [16] synthesized and a group of chalcones and their derivatives bearing hydroxyl benzo furan moiety and compare their fo antifungal activity against *Candida albicans*and *Asperagillusflavus*using cup plate method. They used DMF as solvent control and standard drug was taken griseofulvinfor comparison. They studied eleven compounds, two substituted chalcones 1-(3-hydroxybenzofuran-2-yl)-3-(4- methoxyphenyl)prop-2-en-1-one was reported highest activity almost equal to standard chosen {zone of inhibition at 100 µg/mL 22 mm (tested chalcone) and 24 mm (griseofulvin) for the two strains each}. Results proved that antifungal activities of chalcones may be enhanced by introducing electron releasing group or hydrogen at proper position in aromatic rings. Nitro group substitution should be avoided.

2.4 Anticancer and anti-inflammatory activities

Methoxylated and hydroxylated derivatives are prepared by Ahcene Boumendjel et al. [16] by using simple condensation of substituted aldehydes with required acetophenone called Claisen Schmidt condensation. They tested prepared chalconein vitro antimitotic activities against K562 leukemia cells stained with propidium iodide at a concentration of 10 µM for 24 h. Flow cytometry was used to determine distribution of total population in phases. Vincristine was chosen as standard compound for this study. Amongst the tested chalcones, four compounds, (**j-k**) were found showing even higher cell cycle arrest in G2/M phase than the reference compound whereas the other two, (**n**and **o**) were showing equal potential than reference chosen. Substituted chalconesj,k and l were exposed to a set of eleven different human and murine cell lines (like MCF7, N2A, NIH3T3, SW48, HNO150, HCT116, Messa, CEM, K562, RL, L1210) representing various solid tumors and hematological malignancies by using MTT assay for analyzing their cell growth inhibition property.. Substituted chalcones**l** was reported as most effective against almost all types of cells by observing the IC_{50} concentration values in µM (drug concentration required to induce 50% loss of cell viability with reference to untreated cell after 24 h incubation)



10, $R_2' = R_4' = OCH_3$, $R_2 = R_4 = R_6 = OCH_3$

11, $R_2' = R_6' = OCH_3$, $R_2 = R_6 = OCH_3$

12, $R_2' = R_6' = OCH_3$, $R_2 = R_4 = R_6 = OCH_3$

13, $R_2' = R_4' = R_6' = OCH_3$, $R_2 = R_4 = R_6 = OCH_3$

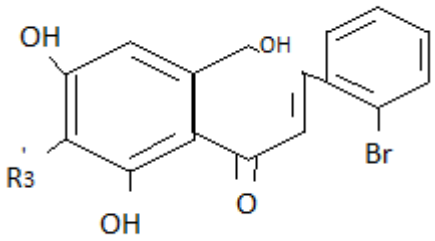
14, $R_3' = R_4' = OCH_3$, $R_2 = R_4 = R_6 = OCH_3$

15,$R_2' = OCH_3$, $R_4' = NH_2$, $R_2 = R_4 = R_6 = OCH_3$

The above data for in vitro antimitotic activities showed that significant inhibition of cell growth was found to be 4 for most effective chalcones by reporting optimum value of lipophillic character (C log P). Activity is reduced by replacing methoxy group on ring A by ethoxy or methyl groups as lipophillic character changed. Also the Dimethoxylation and trimethoxylation of the two phenyl rings showed enhanced antimitotic behavior of various chalcones. If substitution is on ring B then it influenced the activity less than ring A. To check toxicity level of highly active chalcones, (**12**), was further subjected to in vivo studiesinhealthy animals and was reported nontoxic up to the maximum tested dose level (1mg/Kg) thus they can be used as very good anticancer agents. VijayKotra et al. [17] synthesized a new series of quinolinyl and chloroquinoliny lchalcones. They studied the effect of quinoline moiety present in chalcones on their anticancer and anti-inflammatory activities (as evident from the literature, both quinoline and chalcone alone exhibits anticancer activities). They screened selected chalcones for their in vitro anticancer potential on RAW cell lines using MTT assay which was based on the appearance of highly colored blue formazan product by mitochondrial reduction of yellow MTT tetrazolium dye and noted the results as % inhibition of cell growth. Among the eight tested compounds, 3-(4-chlorophenyl)-1-(3- methyl-1-phenyl-2-naphthyl) prop-2-en-1-one exhibited the highest 103 % inhibition. Three more compounds named 1-(3-methyl-1-phenyl-2-naphthyl)-3-(2-thienyl)prop-2- en-1-one, 1-(7-chloro-3-methyl-1-phenyl-2-naphthyl)-3-(2-furyl)prop-2-en-1-one and 1- (7-chloro-3-methyl-1-phenyl-2-naphthyl)-3-(2-thienyl)prop-2-en-1-one were found to show significant anticancer activity (101.59, 100.20 and 100.14% inhibition, respectively). Anti-inflammatory activity of ten chalcones were also evaluated in albino rats of either sex weighing between 200-250 g using carrageenan induced acute paw edema method. Indomethacin was taken as standard for comparison. Mostly the chalcones possessing high anticancer activity were found to exhibit appreciable reduction in paw edema (which is beneficial for cancer treatment) up to 81.78 % at a concentration level of 20 mg/Kg as compared to the standard (82 %, 10mg/Kg). Babasaheb P. Bandgar et al. [18] synthesized a large number of chalcones by doing condensation of substituted acetophenones with 2, 4-dimethoxybenzaldehyde and 3, 4, 5-trimethoxybenzaldehydes using and analyzed their anticancer and anti-inflammatory activities. Substituted chalcones can be used as anticancer agent against five human cancer cell lines responsible for renal cell carcinoma, pancreatic carcinoma, non-small cell lung carcinoma and colon carcinoma. Flavopiridol (700 nM) and Gemcitabine (500 nM) were chosen as reference. Results proved that nitro substitution at *p*-position of ring A increased the cell inhibition tendency of chalcone up to 100% as compared to the references chosen. Result was quite surprising some compounds containing nitro group exhibit carcinogenic and mutagenic behavior. If the substitution in 3,4,5-trimethoxychalcones on ring A was done than it affected their anticancer activity (ranging from 50-95 %) in the order of OCH_3> OH > Cl > Br. Results also proved that with increase in number of methoxy group, anticancer activity will also increases.

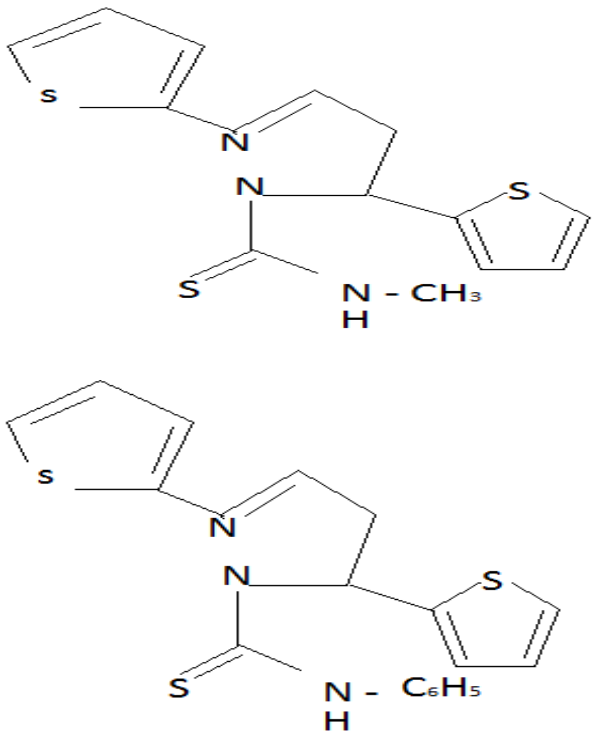
2.5 Antidepressant Activities

Drugs that were given to person for curing depression, which is a very serious brain which sometime induce suicidal characteristics, are associated with several undesirable side effects. So there is an urgent unavoidable need for more efficient antidepressants with minimum intolerable side effects. Inspired from the fact that a hydroxyl chalcone obtained by central ring opening of naturally existing flavonoid, Apigenin [17] (bearing antidepressant activity) was found to possess antidepressant activity, Xin Sui [18] et al. synthesized a series of 2', 4', 6'-trihydroxy chalcones and evaluated them for their antidepressant activity in male Kunming mice (20-24 g, local breed) by using forced swimming test (FST) and tail suspension test (TST). Fluoxetine was taken as reference for comparing the results. One of the tested compound, 3-(2- bromophenyl)-1-(2', 4', 6'-trihydroxyphenyl) prop-2-en-1-one (**p**) (10mg/Kg) was found to be most active antidepressant with a significant decrease in duration of immobility (period of immobility = 69.4 s and for reference it was 57.4 s at same dose level). Results revealed the effect of nature of various substituents and their position in ring B on antidepressant activity of differentchalcones. (p)



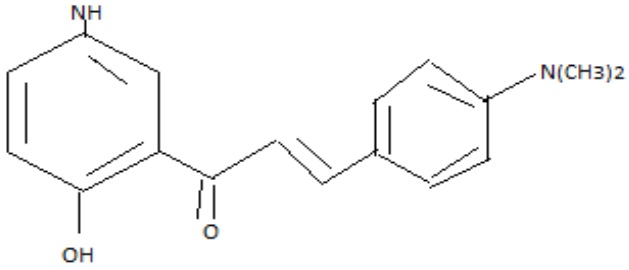
Various chalcones {1-(2-Thienyl)-3-phenyl/(2-thienyl)prop-2- en-1-ones} were used by ZuhalOzdemir et al. [18] to prepare a set of 3-(2-thienyl) pyrazoline derivatives in order to study their antidepressant effects on local breed albino mice using Porsolt's behavioral despair test i.e. forced swimming test (FST). They compared the results with tranylcypromine sulfate, an antidepressant drug. Among the analyzed, compounds with 2- thienyl moiety at 5-position of pyrazoline ring except one were found to decrease the duration of immobility up to appreciable extent. Two substituted chalcones,1-*N* methylthiocarbamoyl-3,5-di-(2 thienyl)- 2-pyrazoline (19) and1-*N*- phenylthiocarbamoyl- 3,5-di-(2-thienyl)-2-pyrazoline (20) showed highest as antidepressant activity with duration of immobility 43 sec and 48 sec (observed immobility period was of 57 sec at same dose level of 10 mg/Kg for standard drug).

Antidepressant activity will be enhanced by introducing thienyl moiety at fifth position ofpyrazoline ring.



2.6 AS FLUORESCENT PROBE

Fluorescent probe is a substances which shows variation in thefluorescence characteristics under influence of external environment at molecular level and nontoxic to human body. Chalcones are biologically active compounds. If molecule contains both electron donating and electron withdrawing substituent the absorbance and fluorescence behavior in UV visible region will be enhanced. And due to this effective intramolecular charge transfer process took place (ICT). Zhicheng Xu et al. [21] studied the effect of polarity of solvent on absorbance and emission characteristics of a substituted chalcone4'-dimethyl-2, 5-dihydroxychalcone (**s**). They used steady-state absorption and fluorescent spectrum in various non-polar and polar solvents like diethyl ether, carbon tetrachloride, tetrahydrofuran, dimethyl formamide, acetone dimethyl sulfoxide, methanol and ethanol. By plotting a curve of stokes shifts versus orientation polarizabilitythey analyzed the fluorescence quantum yields and also the difference in dipole moment values of the molecule in ground and excited state. Atomic charges were redistributed in higher energy state due to ICT from an electron donating group i.e. dimethyl amino group to an electron withdrawing group i.e. carbonyl moiety due to larger difference in dipole moment values. A significant bathochromic shift was observed for fluorescence and minor changes in the absorbance pattern of the molecule under observationswere observed in different solvent environment. That was attributed to large extent of solvation of molecule in excited state than in ground state. As the polarity of the solvent was increased, the emission maximum shifted to higher wavelength (solvents from CCl_4 to DMSO, values from 488 nm to 533 nm). But in protic solvents although with higher polarity, smaller λ_f values (529 nm & 530 nm for ethanol and methanol respectively) were noted due to intermolecular H-bonding between the solvent and - $N(CH_3)_2$ that decreased the availability of lone pair of electrons for charge transfer process.



3 CONCLUSION

From this research, it is proved that chalcones and various substituted chalcones and the compounds having structure similar to chalconesshows variety of pharmacological activities and experiments and research can be done for their efficient use as an active biological agent.

ACKNOWLEGEMENT

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