

Journal of Chemical, Biological and Physical Sciences



An International Peer Review E-3 Journal of Sciences

Available online at www.jcbpsc.org

Section A: Chemical Science

CODEN (USA): JCBPAT

Research article

Studies on Chalcone Derivatives Antioxidant and Stability Constant

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Received: 21 June 2013; **Revised:** 18 August 2013; **Accepted:** 24 August 2013

Abstract: The drug cis-platin development has raised new issues like metal complexes in biochemistry. The modeling of their biochemical properties involves the accurate determination of thermodynamically data, like stability constants. The chalcone 2'-hydroxychalcone and 2'-hydroxy-3,4-dimethoxychalcone have been synthesized and characterized with FT-IR, ^1H -NMR, ^{13}C -NMR spectroscopic techniques. By using UV visible spectroscopy method the mole fraction ratio for Copper, Nickel and Zinc with 2-hydroxychalcone and 2'-hydroxy-3,4-dimethoxychalcone complexes were determined and it was found to be 1:1. The stability constants of this complex have been determined by Job's method. The stability constant (K_f) of Copper, Zinc and Nickel with 2'-hydroxychalcone complexes in acetate buffer pH = 4.4 were determined to be 8.8×10^5 , 1.34×10^5 and 5.6×10^5 respectively. The K_f of Copper, Zinc and Nickel with 2'-hydroxy-3,4-dimethoxychalcone were determined at the same pH and that the values are 5.2×10^5 , 5.4×10^4 and 2.5×10^4 respectively. Antioxidant activity of these chalcones was evaluated by using 1,1'-diphenyl-2-picrylhydrazyl (DPPH) and 2,2'-Azino-bis (3-ethylbenzothiazoline-6-sulfonic acid (ABTS) radicals scavenging methods, which showed that the antioxidant activity of 2'-hydroxychalcone has higher value than the 2'-hydroxy-3,4-dimethoxychalcone. Semi-empirical study results shows that

2'-hydroxychalcone have higher dipole moment than 2'-hydroxy-3,4-dimethoxy-chalcone.

Keyword: chalcone, stability constant, antioxidant, free radicals

INTRODUCTION

Chalcones are open chain flavonoids, valuable intermediates in the synthesis of many active pharmaceutical drugs like biosynthesis of flavonoids. Chalcones represent an essential group of natural as well as synthetic products and some of them possess wide range of pharmacological activity such as antibacterial¹, antitumour², anticancer³, antitubercular⁴, anti-inflammatory⁵, antioxidant⁶, antimalarial⁷, antileishmanial etc. Chalcones and their derivatives are of high interest materials due to their antioxidant properties⁸. Chalcone form an important group of natural compounds which are easy to synthesize. Chalcones are aromatic ketones and key biosynthetic intermediates for combinatorial assembly of different heterocyclic scaffolds⁹. Chalcones display a wide range of pharmacological properties, including cytotoxicity towards cancer cell lines¹⁰, earlier studies have shown that chalcones inhibit cancer cell proliferation and are effective agents *in vivo* against skin carcinogenesis¹¹⁻¹³. The chalcone molecules react with the radicals; they are readily converted to the phenoxyl radicals due to the high reactivity of hydroxyl groups¹⁴. Chalcone molecules have variety of pharmacological activities, attracted medicinal chemists therefore several strategies have been developed to synthesize¹⁵. Chalcones with substituents that increase the electron density of the B ring, such as methoxy, butoxy or dimethylamine groups, did not show significant activity in the inhibition of nitrite production¹⁶. Chalcone is a strong hydroxyl antioxidant, their ability to act as free radical acceptors; the metal complexing properties of these molecules may make some contribution to their total activity. The presence of reactive α , β -unsaturated keto group in chalcones is found to be responsible for their biological activity. Introduction of metal ion in to chalcone compounds can bring about significant changes in biological effects^{17,18}. As metal chelators, the flavonoids play an important role in both the bioavailability and toxicity of a variety of metals. The complexation of Al(III) by quercetin reduces the overload of aluminium in the diet, a metal which has been implicated in neurological and bone disorders^{19,20}. Transition metal ions are found in several bacterial species and are reported to play an important role in different enzymatic and physiological reactions, the interaction of chalcones with metal ions may also change the antioxidant properties and also biological effects of the chalcones²¹. In the present work chalcones have been prepared according to Claisen-Schmidt condensation by condensing ketone with aromatic aldehydes. In this work, we have attempted spectroscopic study on the oxidation and the coordination aspects of 2-hydroxychalcone and 2-hydroxy-3,4-dimethoxychalcone in the presence of Cu(II), Zn(II) and Ni(II) ions.

EXPERIMENTAL

Materials: Benzaldehyde, 2'-Hydroxyacetophenone, 3,4-Dimethoxybenzaldehyde, from Merck and Copper sulphate, Zinc sulphate, Nickel chloride were obtained from S-d-fine-chemical limited Mumbai. 1,1'-diphenyl-2-picrylhydrazyl (DPPH) and 2,2'-Azino-bis(3-ethylbenzothiazoline-6-sulfonic acid (ABTS) obtained from Sigma Aldrich Chemical Co. All the other reagents and solvents were of analytical grade.

Instrumentation: UV-vis Spectra were recorded by Shimadzu-1800 Model UV-Vis spectrophotometer (S.No: A11454806363) using standard 1.0 cm quartz cells. The IR spectra were recorded using KBr pellets in the spectral range 4000–400 cm^{-1} on a Shimadzu – FTIR

spectrophotometer. ^1H and ^{13}C -NMR spectra were recorded at Madurai Kamaraj University, on a Bruker instrument 300 MHz using TMS as internal standard.

Synthesis of the 2'-Hydroxychalcones: Chalcone derivatives were synthesized by Claisen–Schmidt reaction and characterized by spectroscopy techniques. 2'-hydroxyacetophenone (1.36 g, 0.010 M) and benzaldehyde (1.32 g, 0.012 M) were dissolved in 15 ml ethanol and cooled in an ice bath. Then 40% NaOH aq. (5ml) was added in drops wise, and the mixture was stirred at 30°C. Then 6N HCl solution was added slowly with cooling in an ice bath until acidic and stirred for a while. The yellow precipitate obtained was filtered, washed with distilled water carefully until neutral, and then with ethanol. The crude product was recrystallized from ethanol-carbon tetrachloride mixture to obtain yellow flake of crystals ²².

Synthesis of 2'-Hydroxy-3, 4-dimethoxychalcone: 2'-hydroxyacetophenone (1.36 g, 0.010 M) and vanillin (1.90 g, 0.012 M) were dissolved in ethanol (15 ml) in an ice bath, and 45% KOH aq. (5 ml) was added dropwise. The solution was stirred for 96 hour at room temperature. Then 6N HCl solution was slowly added to the mixture kept in an ice bath, and the resulting acidic mixture was stirred for a while. The mixture was extracted with ether, and the extract was washed with saturated NaHCO_3 aqueous, distilled water, and saturated aqueous NaCl and the ether were removed in vacuo after dehydration over anhydrous sodium sulphate. The residue was purified by recrystallisation from ethanol-carbon tetrachloride mixture. Orange powdery crystals were obtained ²².

Determination of Stability constant: Job's method was used to determine the stoichiometric ratio for the reaction between chalcone and metal ion. A method of continuous variations will be employed to determine the binding constant of various metal chalcone complexes. The concentrations of two components are varied inversely to produce a range of ratios between the two, with the total concentration held constant. The solutions were prepared by mixing of two components in equal molar concentration (5×10^{-5} M) in varying ratio from 9:1 to 1:9 and the absorbance was measured at 323 nm and 378 nm for 2'-hydroxychalcone and 2'-hydroxy-3,4-dimethoxychalcone respectively ²³⁻²⁵.

Antioxidant activity of chalcones by DPPH Method: Free radical scavenging capacities of the compound was determined by previously reported procedure using the stable 1,1'-Diphenyl-2-picrylhydrazyl (DPPH) radical²⁶. The antioxidant activity of chalcones was studied at different concentrations in acetate buffer (pH = 4.4). The compound is mixed with (50 μM) DPPH and the reaction with the free radical was monitored spectrophotometrically by observing the decreasing in absorbance at 534 nm ²⁷.

Antioxidant activity of chalcone by ABTS⁺ Method: The antioxidant activity was detected by the method developed by Roberta Re *et al.* A mixture of ABTS (7 μM) and potassium persulphate (2.45 μM) was prepared in water, and incubated at room temperature for 12-16 hrs. The radical produced (ABTS^{•+}) is stable for more than 2 days when stored in dark at room temperature. The product ABTS^{•+} ($\epsilon_{734} = 15000 \text{ M}^{-1} \text{ cm}^{-1}$) was diluted to 50 μM in 10 mM acetate buffer (pH = 4.4) the reduction of ABTS^{•+} by chalcone was monitored spectrophotometrically at 734 nm in accordance with the reduction ABTS^{•+} ion^{28, 29}.

Molecular modeling study: All conformational analysis study was performed on window based arguslab 4.0 software ³⁰. The chalcone structures were generated by arguslab and optimization was performed with semi-empirical PM3 parameterization. Geometry optimizations were carried out, without any symmetry constraints.

RESULTS AND DISCUSSION

Some of the synthetic chalcones which have hydroxy and methoxy substitutions are also found to poses antioxidant activity³¹. Moreover, transition metal complexes of 2'-hydroxychalcones and related ligands have been studied extensively due to their interesting behaviour as weak field or strong field ligands to bivalent metal ions³². The chemical structures of chalcones studied are given in **Fig 1A** and **1B**. UV-Visspectra of 2'-hydroxy chalcone and 2'-hydroxy-3,4-dimethoxychalcone recorded in acetate buffer (pH = 4.4) are shown in **Fig. I**. The electronic spectrum of 2,-hydroxy-3,4 dimethoxychalcone have higher λ_{\max} than the 2'-hydroxychalcone, this may be due to methoxy substituent.

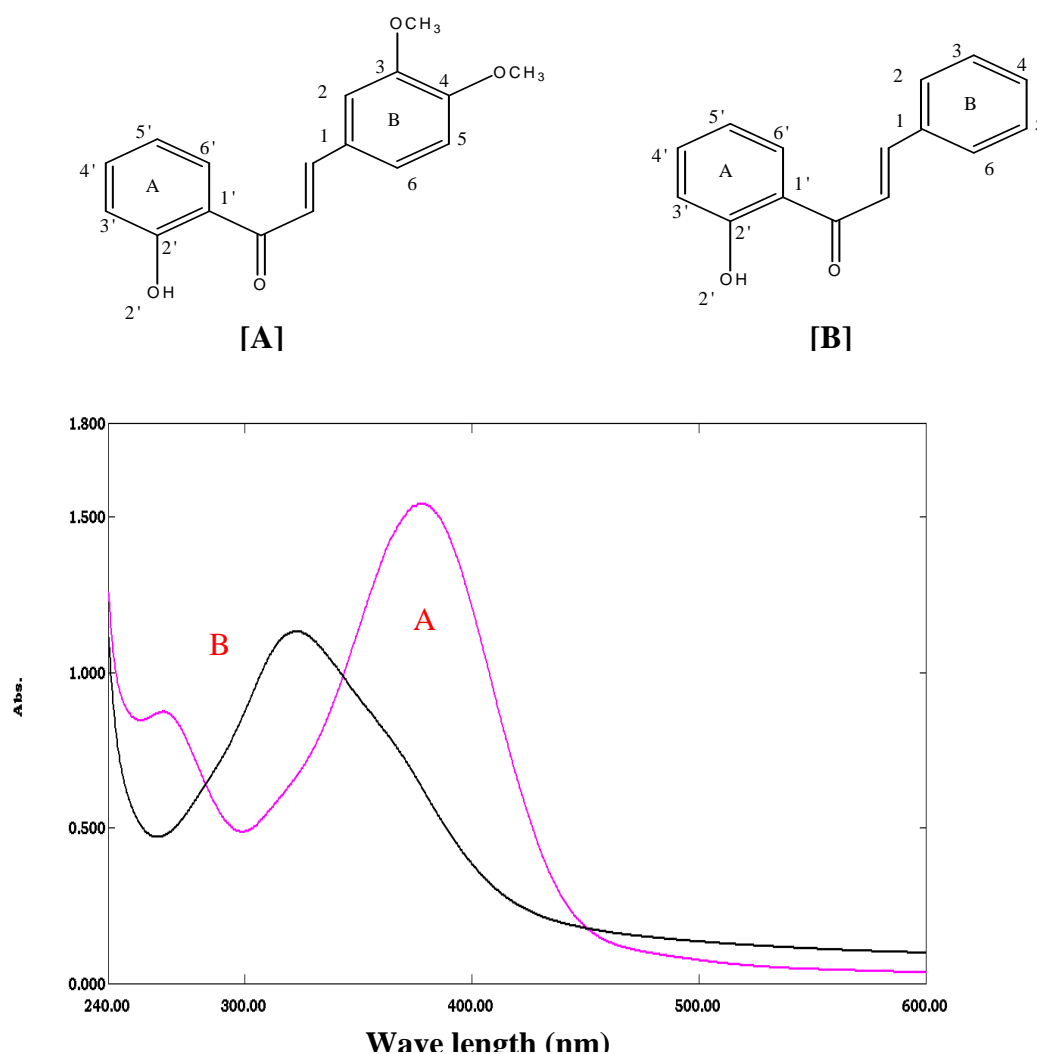


Fig. 1: Chemical structure of 2'-hydroxy-3,4-dimethoxychalcone (A), 2'-hydroxychalcone (B) and their electronic spectrum in acetate buffer pH = 4.4 (A: λ_{\max} 378 nm B: λ_{\max} 321).

Determination of chalcone – metal mole fraction and molar absorptivity: Chalcone are known to participate both antioxidant and chelation reaction³³. The decrease in intensity of absorbance of 2'-hydroxychalcone by the addition of Cu^{2+} metal ion with various concentrations are given in Fig.2.

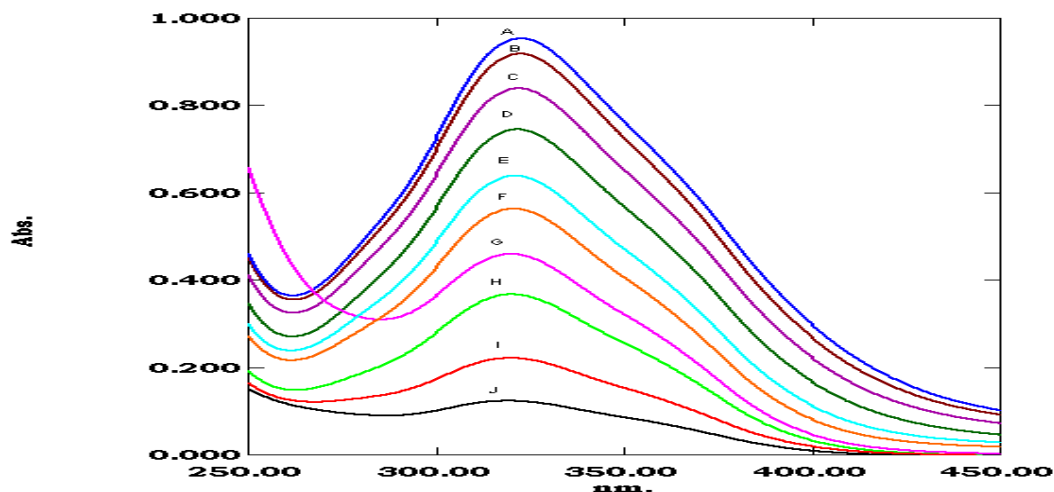


Fig.2: The electronic spectrum of 2'-hydroxychalcone with increasing the metal ion Cu^{2+} concentration (A to J), from A: 5.0×10^{-6} B: 4.5×10^{-5} C: 4.0×10^{-5} to I: 1.5×10^{-5} J: 1.0×10^{-5} M in acetate buffer pH = 4.4.

The decrease in λ_{max} value is the indication of metal chelation by 2'-hydroxychalcone. Similarly 2'-hydroxy-3,4-dimethoxychalcone absorbance peak intensity is decreased by the addition of Cu^{2+} metal ion (figure not shown). The chelation effects of these two chalcones are determined by Job's method. Job's method of continuous variation was used for the determination of stoichiometric composition of metal chalcone complex. After the addition of Cu^{2+} , the intensity of absorbance band of 2'-hydroxychalcone was decreased. The plots of Absorbance at 321 nm, against mole fraction of 2'-hydroxychalcone have maximum absorbance at 0.5. The stoichiometric ratio of the complexation of Cu^{2+} and 2'-hydroxychalcone was identified as 1:1 (**Fig. 3**).

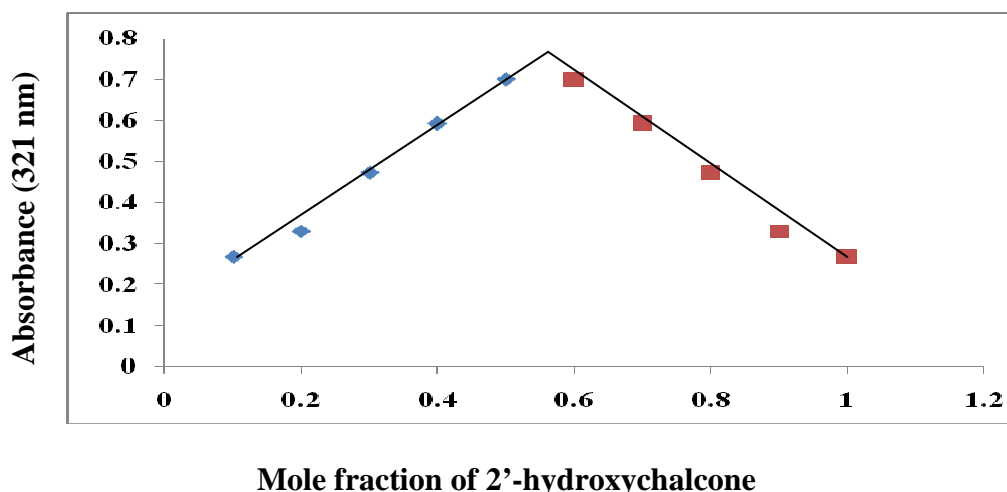


Fig. 3: Absorption versus molar ratios plots 2'-hydroxychalcone at 321 nm.

In order to determine the stability constant of chalcone with metals, the concentration of the complex and their molar absorptivity are must known. The molar absorptivity was calculated by the plotting absorbance at 375 nm against the concentration of complex of 2'-hydroxy-3,4-dimethoxy chalcone with Cu^{2+} , Zn^{2+} and Ni^{2+} ions. The molar absorptivity thus calculated are 29060, 31660 and 31960 $\text{L Mol}^{-1} \text{cm}^{-1}$ for Cu^{2+} , Zn^{2+} and Ni^{2+} respectively (**Fig. 4A**). The molar absorptivity value of 2'-hydroxychalcone thus calculated are 27680, 20980 and 20840 $\text{L Mol}^{-1} \text{cm}^{-1}$ for Cu^{2+} , Zn^{2+} and Ni^{2+} respectively (**Fig. 4B**). The molar absorptivity value of 2'-hydroxy-3,4-dimethoxychalcone with metal ions Cu^{2+} , Zn^{2+} and Ni^{2+} are higher value than the 2'-hydroxychalcone. This is may be due to the higher absorbance of 2'-hydroxy-3,4-dimethoxychalcone.

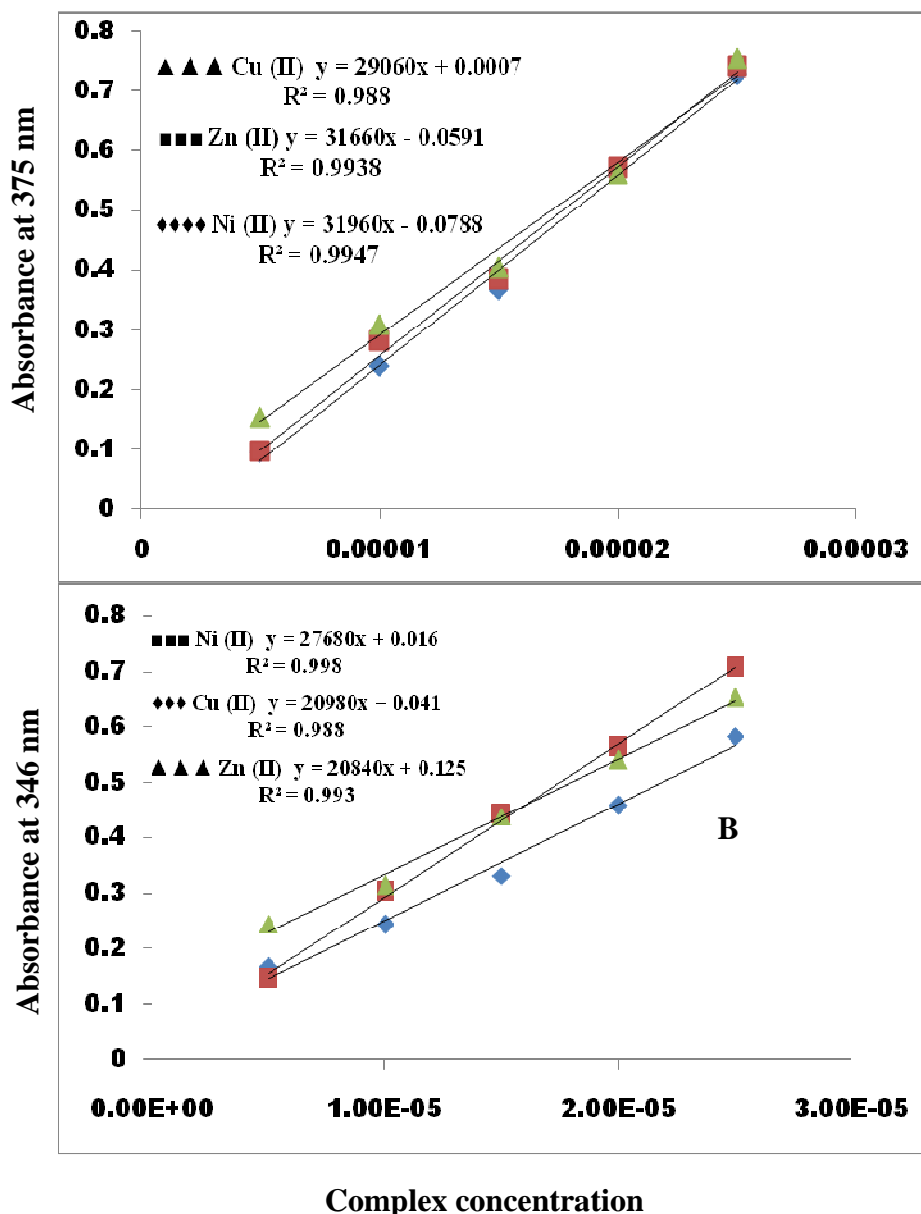


Fig.4: Molar absorptivity determination of 2'-hydroxy-3,4-dimethoxychalcone (A) and 2'-Hydroxychalcone (B) with metal ion Copper, Zinc and Nickel ions, in acetate buffer pH = 4.4.

Determination of binding constant of 2'-hydroxychalcone and 2'-hydroxy-3,4-dimethoxychalcone: Composition of the complex was determined by job's method. Job's method of continuous variation was performed by mixing different proportions of equimolar solution of metal salt and the chalcones^{34, 35}. The final volume in each series was maintained constant. Optical intensity of each mixture was recorded in appropriate metal absorbance and the values are plotted against the volume of variable component Fig. III. The entire job's curve display only one peak as well mole ratio curve, all corresponding to the formation of 1:1 complex between chalcone and metal ion. The value of stability constant at room temperature were found to be 5.6×10^5 , 8.8×10^5 , and 1.3×10^5 L Mol⁻¹ cm⁻¹ for Nickel-2'-hydroxy chalcone, copper-2'-hydroxychalcone and zinc-2'-hydroxychalcone respectively. The stability constant values for nickel-2'-hydroxy-3,4-dimethoxychalcone, copper-2'-hydroxy-3,4-dimethoxychalcone, and Zinc-2'-hydroxy-3,4-dimethoxychalcone were found to be 2.5×10^4 , 5.2×10^5 and 5.4×10^4 L Mol⁻¹cm⁻¹ respectively (Table I). The data given in **Table 1** clearly indicates that the chelating properties of 2'-hydroxychalcone with metal is higher than the 2'-hydroxy-3,4-dimethoxychalcone.

Table -1: The Stability constant of (K_f) of chalcone with metal ion at room temperature (26°C)

| Sl.No | Metals | Stability constant L Mol ⁻¹ | |
|-------|--------|--|----------------------------------|
| | | 2'- Hydroxychalcone | 2'-Hydroxy-3,4-Dimethoxychalcone |
| 1 | Copper | 8.8×10^5 | 5.2×10^5 |
| 2 | Zinc | 1.3×10^5 | 5.4×10^4 |
| 3 | Nickel | 5.6×10^5 | 2.5×10^4 |

Theoretical calculations by Arguslab 4.0 software: To support the experimental results, a theoretical molecular modeling calculation was performed with Arguslab 4.0. The PM3 method of optimization and their energy values are assigned in **Table 2**. 2'-hydroxychalcone has higher dipole moment than the 2'-hydroxy-3,4-dimethoxychalcone, this may be one of the reason for the higher stability constant value obtained for 2'-hydroxychalcone with metals. The Mullikan atomic charge density value of hydroxyl oxygen and ketonyl group oxygen of 2'-hydroxychalcone are -0.2737 and -0.3876 respectively. Similarly the Mullikan atomic charge density value of 2'-hydroxy-3,4-dimethoxychalcone have -0.2729 and -0.3861 for hydroxyl oxygen and keto group oxygen respectively. The atomic charge on hydroxyl oxygen and ketonyl group oxygen of 2'-hydroxychalcone has higher value than the 2'-hydroxy-3,4-dimethoxychalcone. This may be the reason for higher stability constant value of 2'-hydroxychalcone with metals than the 2'-hydroxy-3,4-dimethoxychalcone.

FTIR Study: 2'-Hydroxychalcone was analysed and their characteristic peaks at 1340 cm^{-1} , 1270 cm^{-1} represent C-O stretching and bending vibration, the peak at 3051 cm^{-1} is due to the -OH group and CH=CH moiety is identified by its stretching and bending vibration values at 1641 cm^{-1} and 975 cm^{-1} respectively. The peaks obtained at 3024 cm^{-1} and 1574 cm^{-1} are due to aromatic -C=C- for 2'-Hydroxy-3,4-dimethoxychalcone all the above said functional group peaks are identified along with a new peak at 2833 cm^{-1} which is due to the methoxy group.

Table-2: PM3 Optimized conformational data and molecular properties of chalcones

| Compounds | Heat of formation Kcal/mol | HOMO au | LUMO au | Diff. in MO | Dipole moment (Debye) |
|----------------------------------|-------------------------------|------------|------------|----------------|-----------------------------|
| 2'-hydroxychalcone | -18.1387 | -0.3378 | -0.03799 | 0.2999 | 3.4938 |
| 2'-hydroxy-3,4-dimethoxychalcone | -19.2969 | -0.3382 | -0.04140 | 0.2968 | 2.9197 |

¹H-NMR study

2'-Hydroxychalcone: δ 12.78 (s 1H, 2-OH), 7.91-7.96 (d, 1H and H₆), 7.92-7.96 (1H, H₆), 7.32-7.70 (m, 7H, H_α, H₄', H₂, H₃, H₄, H₅, H₆) and 7.02-7.05 (m, 2H, H₃' and H₅').

2'-Hydroxy-3,4-dimethoxychalcone: δ 12.88 (s, ¹H, 2'-OH), 8.18 - 8.26 (d, ¹H, H₆), 7.91 - 7.95 (d, 1H, H₆'), 7.47 - 7.52 (d, 1H, H_α), 7.46 - 7.54 (m, 1H, H₄'), 7.18 - 7.30 (m, 2H, H₃, H₅'), 6.90 - 7.04 (m, 3H, H₂, H₄, H₅), 3.97 - 3.95 (s, 6H, 2 x -OCH₃).

¹³C-NMR study

2'-hydroxychalcone: δ 192.9 C=O, 162.7 Ar-OH, 144 and 136 -CH=HC-, 117-135.6 aromatic carbon.

2'-hydroxy-3,4-dimethoxychalcone : δ 193.5 C=O, 163.5 Ar-OH, 145.6 and 136.1 CH=CH, 110.2 - 129.5 aromatic carbon and 151.8, 149.22 -OCH₃

Antioxidant Activity: Antioxidants are the agents, which can inhibit or delay the oxidation of an oxidisable substrate in a chain reaction. The antioxidant activity of natural compounds like chalcones is related to a number of different mechanisms such as free radical scavenging, hydrogen donation, singlet oxygen quenching, metal ion chelation and the chalcones are acting as a substrate for free radicals such as superoxide and hydroxide. The antioxidant activity of the two chalcones synthesized was measured with help of standard free radical scavenging assays DPPH and ABTS^{•+} assays as a primary tool.

DPPH method: This is a simple method that has been developed to determine the antioxidant activity of chalcones, which utilizes the stable 1,1'- diphenyl-2-picrylhydrazyl (DPPH) radical. When a solution of DPPH is mixed with a substance that can donate a hydrogen atom, then the DPPH is transformed to the reduced form with the loss of its violet colour. The DPPH absorption peak intensity was suppressed by the 2'-hydroxychalcone, confirming the antioxidant activity of 2'-hydroxychalcone (**Fig. 5**). The suppression of the absorbance of DPPH at 534 nm in a concentration dependent manner is typically shown for 2'-hydroxychalcone (**Fig. 6**). The decrease in absorbance was converted in to percentage of DPPH inhibition by using the following equation

$$\% \text{ DPPH inhibition} = \frac{[\text{Abs}]_0 - [\text{Abs}]_T}{[\text{Abs}]_0} \times 100$$

Where T is the time needed to reach steady state

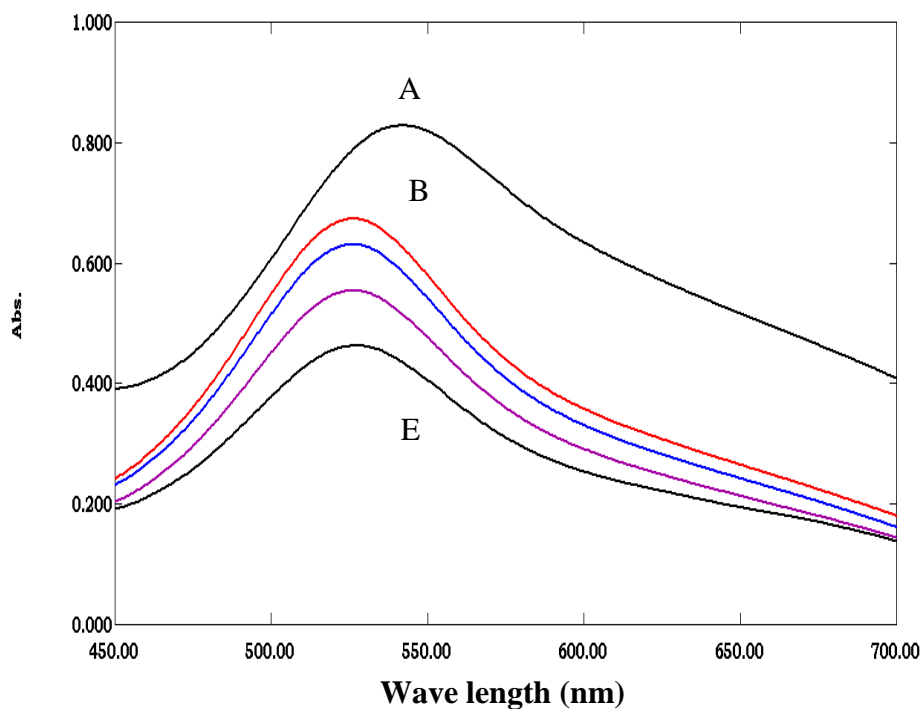


Fig. 5: The concentration dependent decrease of UV-Vis spectra of [A]: DPPH (50 μ M) radical as a function of increasing concentration of 2'-hydroxychalcone [B] to [E] (10 μ M: 15 μ M: 20 μ M: 30 μ M) in ethanol water mixture.

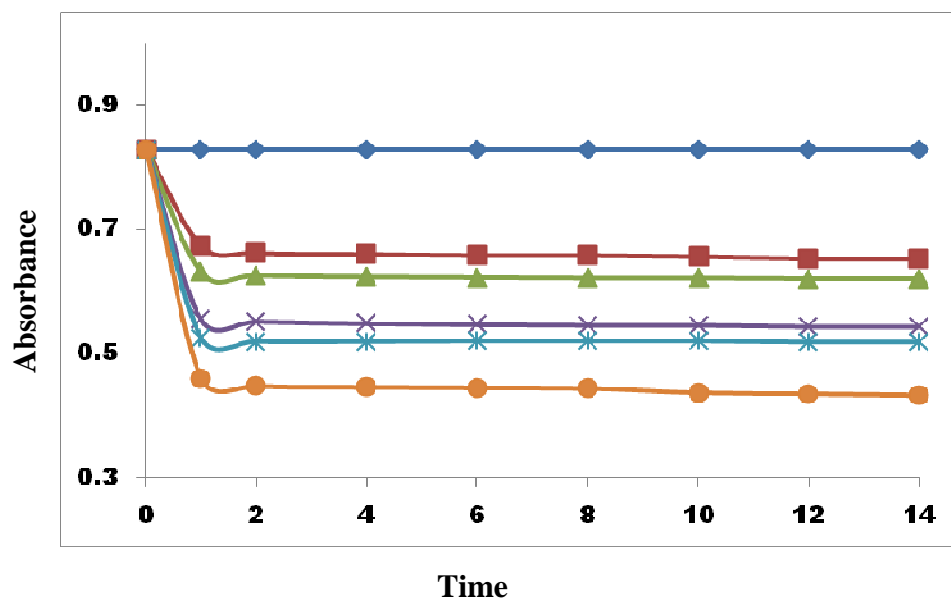


Fig.6: Reaction between DPPH \cdot and 2'-hydroxychalcone in ethanol water mixture (1:1), decrease in absorbance of DPPH \cdot at 534 nm in the presence of different concentration 2'-hydroxychalcone; 10 μ M (■ ■ ■), 15 μ M (▲ ▲ ▲), 20 μ M (xxx) 25 μ M (***) 30 μ M (• • •) and control DPPH \cdot 50 μ M (◆ ◆ ◆).

The experimental results demonstrate that the reaction with DPPH is completed within one minute. The inhibition of DPPH absorbance in a concentration dependent manner of 2'-hydroxychalcone is observed. The inhibition order of 2'-hydroxychalcone and 2'-hydroxy-3,4-dimethoxychalcone in the concentration of 10 μM was 18.5% and 5.8% respectively. **Fig. 7** shows the decrease in DPPH absorbance peak at 534 nm for 2'-hydroxy-3,4-dimethoxychalcone in a concentration dependent manner. The antioxidant activity of 2'-hydroxychalcone has higher than 2'-hydroxy-3,4-dimethoxychalcone, this order of inhibition may be due to 5-OH bond strength and labile nature of the hydroxide hydrogen atom. Arguslab 4.0, PM3 optimized structures of 2'-hydroxychalcone and 2'-hydroxy-2,3-dimethoxychalcone and their bond length values are compared with antioxidant activity. The bond length of $\text{O}_2\text{-H}$ for 2'-hydroxychalcone and 2'-hydroxy-2,3-dimethoxychalcone are found to be 0.964342 \AA and 0.964297 \AA respectively. The increase in $\text{O}_2\text{-H}$ bond length value is agreement with higher antioxidant activity of 2'-hydroxychalcone than 2'-hydroxy-2,3-dimethoxychalcone. The bond length value of $\text{O}_2\text{-H}$ for these two chalcones are well correlated with experimental antioxidant activity.

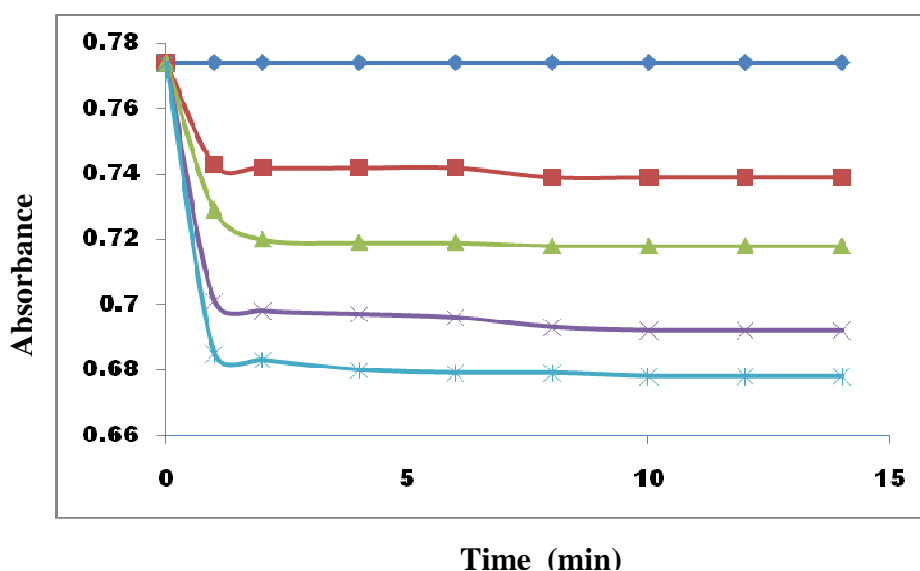


Fig.7: Reaction between DPPH $^{\bullet}$ and 2'-hydroxy-3,4-dimethoxychalcone, decrease in absorbance of DPPH $^{\bullet}$ at 534 nm in the presence of different concentration of 2'-hydroxy-3,4-dimethoxychalcone; 10 μM (■ ■ ■), 15 μM (▲ ▲ ▲), 20 μM (xxx) 25 μM (***) and control DPPH $^{\bullet}$ 50 μM (◆◆◆).

ABTS $^{+\bullet}$ Method: The reduction in the absorbance reading of ABTS $^{+\bullet}$ was measured at 734 nm at exactly 1 minute after mixing with each antioxidant solution. The antioxidant activity of 2'-hydroxychalcone was determined by decolourization (reduction) of ABTS $^{+\bullet}$ radical cation. The suppression of the absorbance of ABTS $^{+\bullet}$ in a concentration-dependent manner is typically shown for 2-Hydroxychalcone (**Fig. 8**). **Fig. 9** shows the decrease in the absorbance of ABTS $^{+\bullet}$ radical cation at 734 nm for various concentrations of 2'-Hydroxychalcone. The experimental results demonstrate that the reaction with ABTS $^{+\bullet}$ is completed within 1 minute³⁶⁻³⁸. In fig. 8 the suppression of ABTS $^{+\bullet}$ in a concentration dependent manner is typically shown for 2-hydroxychalcone. Fig. 9 shows the concentration dependent decrease in absorbance of ABTS $^{+\bullet}$ radical cation at 734 nm for 2'-

hydroxychalcone in a concentration dependent manner is observed. The ABTS^{•+} inhibition order of 2'-hydroxychalcone have higher value than 2'-hydroxy-3,4-dimethoxy chalcone is observed, as similar to DPPH assay results.

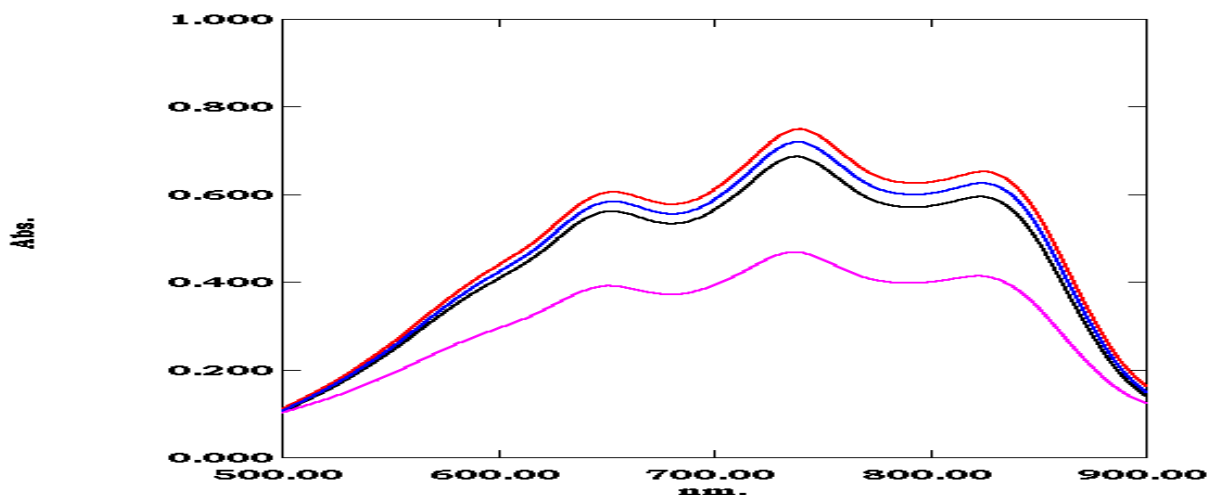


Fig.8: Absorption spectra of ABTS^{•+} (50 μ M) with the addition of 2-hydroxychalcone, lowest spectra relating to the highest concentration of chalcone (30 μ M), in acetate buffer pH =4.4.

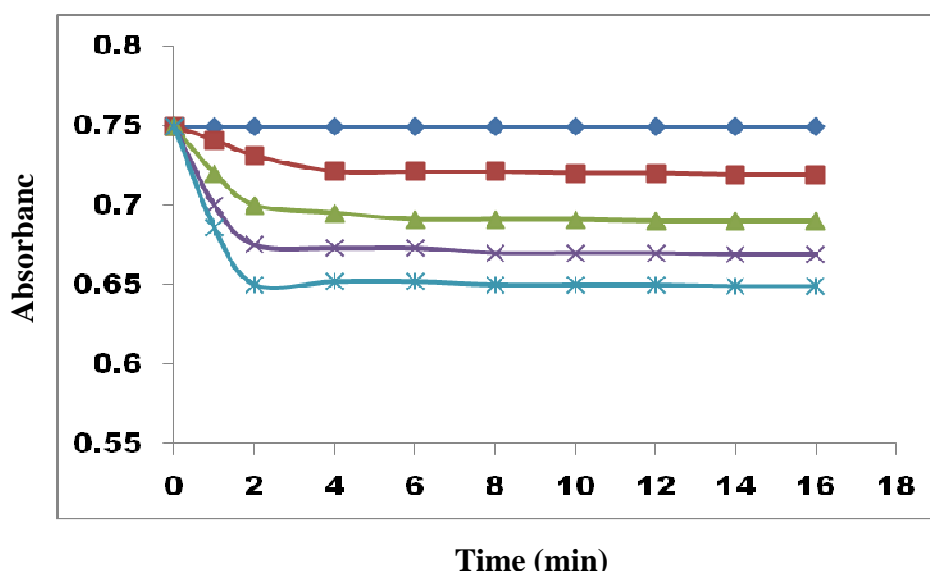


Fig. 9: Reaction between ABTS^{•+} and 2'-hydroxychalcone in ethanol water mixture (1:1), decrease in absorbance (λ_{max} 734 nm) of ABTS^{•+}, in the presence of different concentration of 2'-hydroxychalcone 10 μ M (■), 15 μ M (▲), 20 μ M (×) 25 μ M (**) and control ABTS^{•+} (◆).

CONCLUSION

The two newly synthesized compounds 2'-hydroxychalcone and 2'-hydroxy 3,4-dimethoxychalcone interacts strongly with metal like Copper, Zinc, and Nickel ions. The job's method was applied to

validate the stoichiometric composition of the metal complex and to determine the stability constant. The stability constant for 2'-hydroxychalcone have higher value compared to 2'-hydroxy-3,4-dimethoxychalcone. The antioxidant activities of the compounds under study was examined, the results obtained clearly display the fact that 2'-hydroxychalcone have higher antioxidant activity compared to 2'-hydroxy-3,4-dimethoxychalcone. It is finally concluded that 2'-hydroxychalcone have higher stability as well as higher antioxidant than the 2'-hydroxy-3,4-dimethoxychalcone. These experimental results are also supported by the theoretically evaluated values.

ACKNOWLEDGEMENTS

The authors are grateful to **University Grant Commission New Delhi, (F.No. 39-731/2010)** for their financial support. A special acknowledgement is addressed to The Principal and Management of NMSSVN College for providing research facilities.

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