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The study of Chemical Structure (NMR and FTIR) of Chalcones Obtained from New Heterocyclic Synthesis Based on 5-Chloroisatin

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Abstract

Nowadays, cyclic compounds in chemistry are among a large group of cases studied and researched. These compounds have become very important and crucial in medicine and treatment, such as their use from chemical medicine to sedatives and depression treatments. It should be noted that many of these compounds have been naturally and readily identified in nature. Our aim in this study is to synthesize new derivatives of 5-chloroisatin that are the basis for the synthesis of various heterocyclic compounds such as Pyrazolines, Tryptanthrin, Acridine derivatives and Pyran derivatives. One of the advantages of this method is the synthesis of a single container, which have been synthesized solvent freely. The results of the study were completed by examining the chemical structure (NMR and FTIR).

The results showed that in the FTIR spectrum of this compound 3a, the tensile vibrations of alkene and aromatic C-H bonds at the absorption frequency of 3100 cm-1, the tensile vibration of the NH bond at 3194 cm-1, the carbonyl group C = O amide at 1722 cm -1 and the conjugated ketones at 1662 cm-1 Tensile vibrations of the C = C groups have appeared in 1600, 1620 and 1450 cm-1. Investigation of the H NMR1 spectrum for δ shows aromatic Hydrogen in the range of 6.83 to 8.40 ppm with a total of 8 integrals. Also, the study of C NMR13 spectrum shows the aromatic and alkene group carbons in the range of 111.11 to 141.68 ppm.

The carbon uptake of the carbonyl amide group into the Indoline ring at chemical displacement is 169.61 ppm and conjugated ketones are 190.61 ppm.

Adsorption related to tensile vibrations of nitro NO2 group has been done in 1345 and 1522 cm-1. Studies have shown that the results are new and the compounds have shown standard behavior in the tests and prepare the appropriate ground for the use of this combination in various industries. As you know, the use of this compound in microbiology and their destructive effect on microorganisms is of particular importance. Now these results are a part of our study in a comprehensive research. This article will continue in the biological sections (antimicrobial and antifungal). We will also share the results and publish them.

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Introduction

Cyclic compounds in chemistry can be studied from several perspectives. If these particles are composed only of carbon groups, the resulting compounds and rings are called carboxylic, but if in these rings other groups besides carbon, such as nitrogen, oxygen, and sulfur or metal groups are involved, the resulting rings are called Heterocycles. A heterocyclic compound or ring structure is a ring compound in which there are at least two different elements as members of the ring. Chemistry of heterocyclic compounds is a branch of organic chemistry that describes the synthesis, properties and applications of this type of compounds. Examples of heterocyclic compounds include nucleic acids, many drugs, biomass, and many natural and synthetic dyes [1-6]. If the heterocyclic rings have no carbon, we will have a mineral heterocycle such as borazin or mineral benzene. Figure 1.

Application of Heterocycles

Heterocyclic compounds have a wide range of applications from the pharmaceutical industry to other large industries such as foodstuffs. They are also used as starting material in the synthesis of organic compounds. The table 1 lists some of these applications [7-13].

Heterocycles and Their Synthesis

There are various methods for the synthesis of heterocycles, many of which are classical, and there are many new examples that these compounds are of particular importance in terms of biological activity and medicinal properties. [14]

Types of reactions often used in the synthesis of heterocyclic rings

The most commonly used process is to add a nucleophile to a carbonyl carbon (Or o-protonated carbonyl reactive carbon) When the reaction results in the formation of a c-c bond, the nucleophile β-carbon is an enol ion or an enolate anion or an anamine. [15]

Isatin

Isatin is an indole derivative that contains the ketone group at positions 2 and 3 of the ring. The structural form of isatin consists of a pyrrole ring combined with a benzene ring. It looks like an red-orange powder with a high melting point that produces an aldol condensation product or forms an imine or anamine [16]. Isatin is an important group of heterocyclic compounds. Isatin derivatives are important synthetic substrates used for the synthesis of various heterocyclic compounds as well as as raw materials for the synthesis of various drugs. Recently, isetine derivatives have received attention due to their potent biological and pharmacological activities. [17] Isatin can be attacked by nucleophiles and electrophils by having two functional groups, amide and ketone [11].

General Methods of Isatin Synthesis

Sandmeyer method [17-24]

Martinet method [40, 41]

Stolle method [25-33]

Gassman method [34-39]

Method of metals of anilide derivatives [40]

Chalcones

Chalcone and its related compounds (chalconoids) are aromatic ketones that form the core of various important biological compounds. They have different activities.

Types of Synthesis of Chalcones

1. The Claisen Schmidt condensation method [41,42]
2. Aldoli condensation method [43-46]

Materials and Methods

Material

In this research, we study the physical properties of the newly synthesized heterocycle, which is in fact a new method for synthesis and product development. In the following, we will review the materials and methods used in this study. Tab 2.

Equipment

IR Spectrometer: All spectra listed in this article have been taken by Scientific-Nicdet 6700 FTIR.

HNMR spectrometer: All NMR spectra have been registered by BRUKER ULTRASHIELD 400 ADVANCE III, (chloroform and DMSO have been used as solvents).

Heater device: Heidolph Germany mixer and heater has been used to perform the reactions.

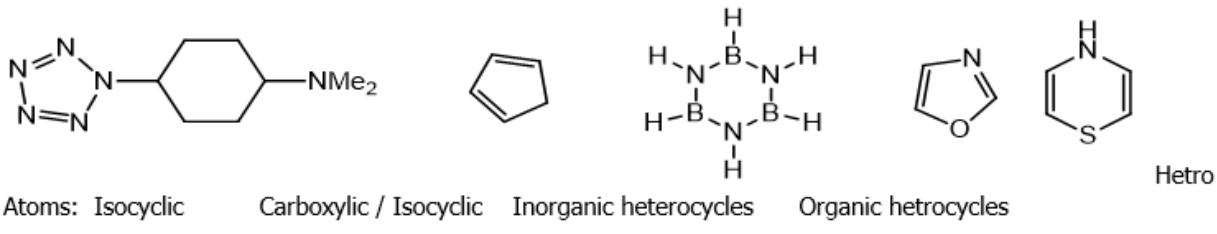


Figure 1. examples of several types of heterocycles

Table 1. Investigation of the use of heterocycles

Industry	Material	Application
Medicine	90% of pharmaceutical hetrocycles	Penicillin, Quinoline, Pain killer, anti-tumors
Foodstuffs	Caffeine in coffee	In food and energy drinks
Textile	Sulfolane	Solvent for all fabrics
Paint industries	Pyridine	Paint and coloring
Bioengineering	Adenine, guanine, cytosine, thymine	Nitrogen bases in DNA (genetic units)

Table 2. Names and specifications of materials used in this research

Manufacturer	Formula or acronym	Material
Exir Austria	$C_8H_4ClNO_2$	5-Chloroisatin
Sigma	$(C_2H_5)_2NH$	Dimethylamine
Merck	$(C_2H_5)_3N$	Triethylamine
Merck	$CH_3COC_6H_5$	Acetophenone
Merck	$O_2NC_6H_4COCH_3$	4-Nitroacetophenone
Merck	$C_9H_{10}O_2$	4-Metoxyacetophenone
Merck	$ClC_6H_4COCH_3$	4-Chloroacetophenone
Merck	$BrC_6H_4COCH_3$	4-Bromoacetophenone
Merck	HCL	Hydrochloric acid
Merck	CH_3COOH	Glacial Acetic Acid
Merck	CH_3CH_2OH	Ethanol
Merck	CH_3COCH_3	Acetone
Merck	TLC	Thin-layer chromatography (TLC)
Iran	$CHCl_3$	chloroform
Iran	C_6H_{14}	n-Hexan
Iran	$C_4H_8O_2$	Ethyl Acetat
Iran	H_2O	Distilled water - deionized

UV lamp device for TLC test.

Oven

Scales

Magnetic stirrer

Glass reflux

Methods

The Synthesis Method of β-hydroxy Ketone

Synthesis of 5-chloro-3-hydroxy-3- (2-oxo-2-phenyl ethyl) indoline-2-one Fig 2.

To produce β-hydroxy ketone, 0.005 mol of raw material is weighed. 0.9 g of 5-chloroisatin and 0.7 ml of acetophenone were mixed with 1 ml of triethylamine and 1 ml of dimethylamine for 1-2 hours at room temperature to react. The color changes of the solution were as follows: first it changed from orange to green and mustard, and after half an hour it changed color to brown and finally to light brown color. Every 15 minutes, reaction changes were observed and analyzed by TLC and UV lamp. After two hours, the completion of the reaction was determined using TLC test. After the precipitate dried and the excess amount of acetophenone evaporated, it was washed with 5% solution of water and ethanol and 1 drop of concentrated hydrochloric acid and the precipitate was dried in an oven. Fig 3.

The Method of Synthesis of Chalcone Acetophenone

Synthesis of 5-chloro-3- (2-oxo-2-phenylethylenidine) indoline-2-one: Fig 4.

Deposition of β-hydroxy ketone acetophenone and 30 ml of glacial acetic acid with a magnetic stirrer at 100 ° C put on the heater to completely be solved in the acid. After 14 minutes, when the solution was completely hot, about 2 drops of concentrated hydrochloric acid were added and wait for it to precipitate over time.

Every half hour, reaction changes were observed and analyzed by TLC and UV lamp. After half an hour, two more drops of concentrated hydrochloric acid were added and put the solution at the rest. And after a few hours when the solution cooled, sediments appeared at the bottom of the container. To dry little by little, the solution and sediment were poured onto the watch glass and evaporated on the excess acid heater with a little heat, and the precipitate remained. The precipitate was placed in the oven for complete drying. After drying, it was washed with water and 5% ethanol. Fig 5.

IR, HNMR and CNMR spectra were taken from the synthesized precipitate.

Synthesis of β-hydroxy ketones 4-Nitroetophenone:

Synthesis of 5-chloro-3-hydroxy-3- (2- (4-nitrophenyl) -2-exoethyl) indoline-2-one:

0.001 mol of raw materials are weighed to produce β-hydroxy ketone 4-nitrostophenone. 0.18 g of 5-chloroisatin and 0.165 g of 4-nitrostophenone were mixed with 1 ml of dimethylamine and 1 ml of triethylamine for 3 hours at room temperature to react. Every quarter hour, reaction changes were observed and analyzed by TLC chromatography and UV lamp. After the reaction was complete and the excess evaporation was complete, the precipitate was placed in an oven and dried. After the precipitate dried, it was washed with 5% water and ethanol and a drop of concentrated hydrochloric acid, and the precipitate was dried in an oven. Fig 6.

Synthesis of Chalcone 4-nitroetophenone

5--Chloro-3- (2- (4-nitrophenyl) -2-oxoethylenidine) indoline-2-one

Deposition of β-hydroxy ketone 4-nitroetophenone with 30 ml of glacial acetic acid and a magnetic stirrer at 100 ° C on the heater in order to the precipitate to be solved completely in the acid.

After a quarter of an hour, when the solution was completely hot, about 2 drops of concentrated hydrochloric acid were added and it waited for it to precipitate over time. Every half hour, reaction changes were observed and analyzed by TLC chromatography and UV lamp. After half an hour, two more drops of concentrated hydrochloric acid were added.

During the reaction, simultaneously performed TLC test. If the reaction is not complete, add another two drops of concentrated hydrochloric acid to the solution after one hour, and after performing the TLC test and completing the reaction, put the solution at rest and wait for the solution to cool and precipitate.

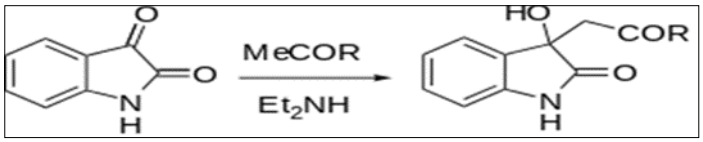


Figure 2. synthesis of β-hydroxy ketone

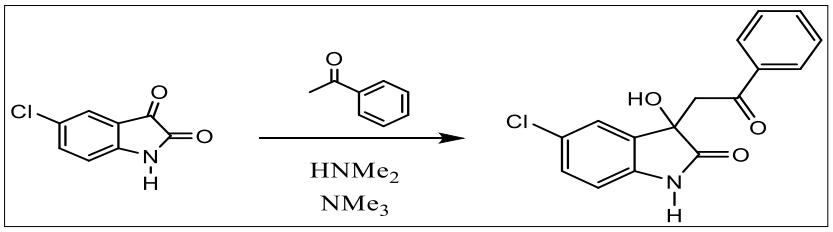


Figure 3. 5-chloro-3-hydroxy-3-(2-oxo-2-phenylethyl) indolin-2-one

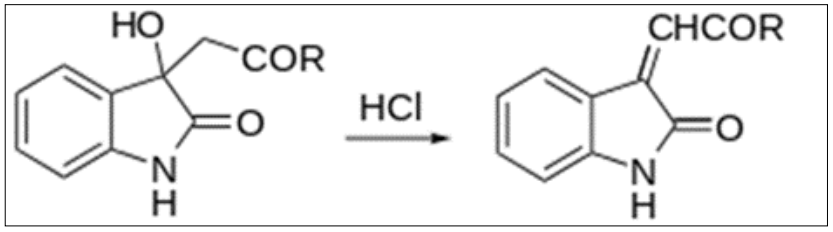


Figure 4. synthesis of Chalcone

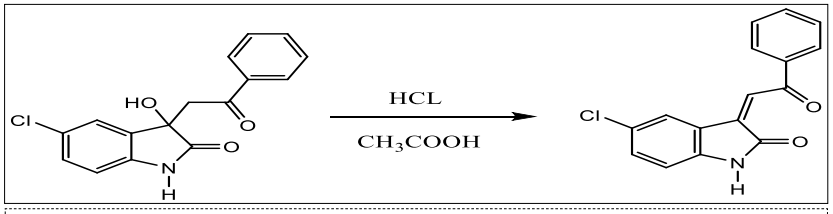


Figure 5. (Z)-5-chloro-3-(2-oxo-2- phenylethylidene) indolin-2-one

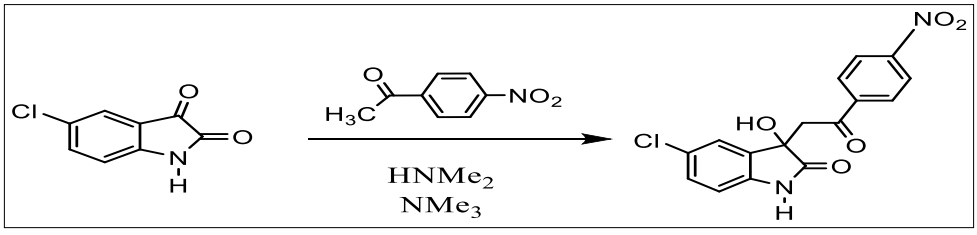


Figure 6. chloro-3-hydroxy-3-(2-(4-nitrophenyl)-2-oxoethyl)indolin-2-one

For drying little by little, the solution and precipitate were poured onto the watch glass on the heater and the excess acid was evaporated with a little heat, and the precipitate remained. The precipitate was placed in the oven for complete drying. After drying, it was washed with water and 5% ethanol. Fig 7.

Synthesis of β-hydroxy Ketone 4-methoxy Acetophenone

Synthesis of 5-chloro-3-hydroxy-3- (2- (4-methoxyphenyl) -2-oxoethyl) indoline-2-one:

To produce β-hydroxy ketone 4-methoxetophenone, 0.001 mol of raw materials are weighed. 0.18 g of 5-chloroisatin and 0.16 g of 4-methoxetophenone with 1 ml of dimethylamine and 1 ml of triethylamine stir at room temperature for 2 hours to react.

Every quarter hour, reaction changes were observed and analyzed by TLC test and UV lamp. After completion of the reaction and evaporation of the excess base, the precipitate was placed in the oven and dried. After the precipitate dried, it was washed with 5% water and ethanol and a drop of concentrated hydrochloric acid, and the precipitate was dried in an oven. Fig 8.

Chalcone Synthesis 4-methoxy Acetophenone

Synthesis of 3- (2- (4-methoxyphenyl) -2-oxoethylenidine) -5-chloro-indoline-2-one:

Deposition of β-hydroxy ketone 4-methoxy acetophenone with 30 ml of glacial acetic acid and a magnetic stirrer at 100 ° C on the heater in order to be solved completely the in the acid. After a quarter of an hour, when the solution was completely hot, about 2 drops of concentrated hydrochloric acid were added and it waited for it to precipitate over time. Every half hour, reaction changes were observed and analyzed by TLC chromatography and UV lamp.

After half an hour, two more drops of concentrated hydrochloric acid were added and the TLC test was performed at the same time. After performing the TLC test and completing the reaction, put the solution at rest and wait for the solution to cool and precipitate. The reaction was complete in about two hours. To dry little by little, the solution and sediment were poured onto the watch glass and evaporated on the excess acid heater with a little heat, and the precipitate remained. The precipitate was placed in the oven for complete drying. After drying, it was washed with water and 5% ethanol. Fig 9.

IR and HNMR spectra were taken from the synthesized precipitate.

Synthesis of β-hydroxy Ketone 4-Chlorostophenone:

Synthesis of 5-chloro-3-hydroxy-3- (2- (4-chlorophenyl) -2-oxoethyl) indoline-2-one:

To produce β-hydroxy ketone 4-chlorostophenone, 0.001 mol of raw material is weighed 0.18 g of 5-chloroisatin and 0.13 ml of 4-chloropetophenone plus 1 ml of dimethylamine and 1 ml of triethylamine Stir at room temperature for 3-4 hours to react.

Every quarter hour, reaction changes were observed and analyzed by TLC test and UV lamp. After completion of the reaction and evaporation of the excess base, the precipitate was placed in the oven and dried. After the precipitate dried, it was washed with 5% water and ethanol and a drop of concentrated hydrochloric acid, and the precipitate was dried in an oven. Fig 10.

Chalcone Synthesis 4-Chlorostaphenone

Synthesis of 5-chloro-3- (2- (4-chlorophenyl) -2-oxoethylenidine) indoline-2-one:

Deposition of β-hydroxy ketone 4-chlorostophenone with 30 ml of glacial acetic acid and a magnetic stirrer at 100 ° C on the heater to completely dissolve the precipitate in the acid. After a quarter of an hour, when the solution was completely hot, about 2 drops of concentrated hydrochloric acid were added and it waited for it to precipitate over time.

Every half hour, reaction changes were observed and analyzed by TLC chromatography test and UV lamp. After half an hour, two more drops of concentrated hydrochloric acid were added and the TLC test was performed at the same time. After performing the TLC test and completing the reaction, put the solution at rest and wait for the solution to cool and precipitate. The reaction was complete in about two hours. To dry little by little, the solution and sediment were poured onto the watch glass and evaporated on the excess acid heater with a little heat, and the precipitate remained. The precipitate was placed in the oven for complete drying. After drying, it was washed with water and 5% ethanol. Fig 11.

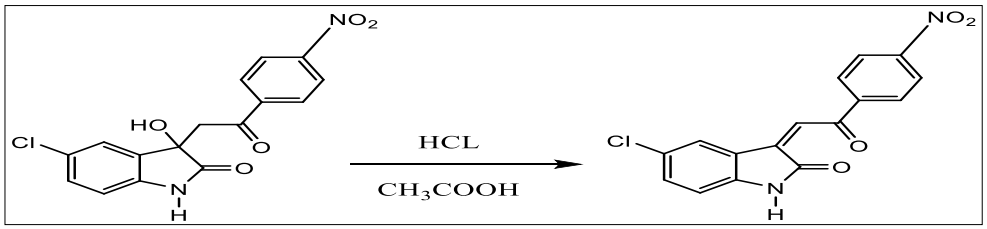


Figure 7. (Z) 5-chloro-3-(2-(4-nitrophenyl)-2-oxoethylidene) indolin-2-one

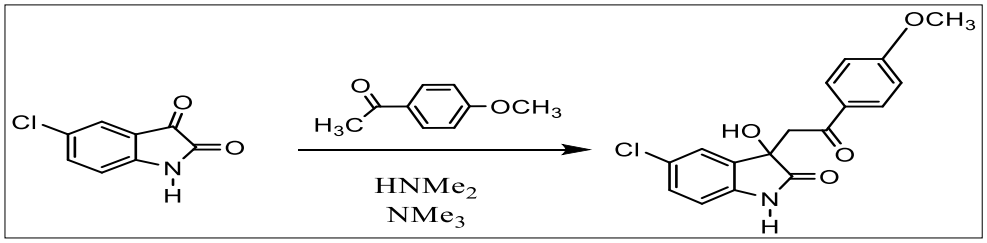


Figure 8. chloro-3-hydroxy-3-(2-(4-methoxyphenyl)-2-oxoethyl)indolin-2-one

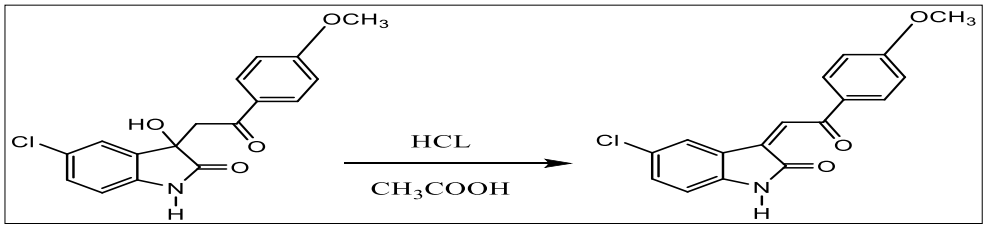


Figure 9. (Z)-5-chloro-3-(2-(4-methoxyphenyl)-2-oxoethylidene)indolin-2-one

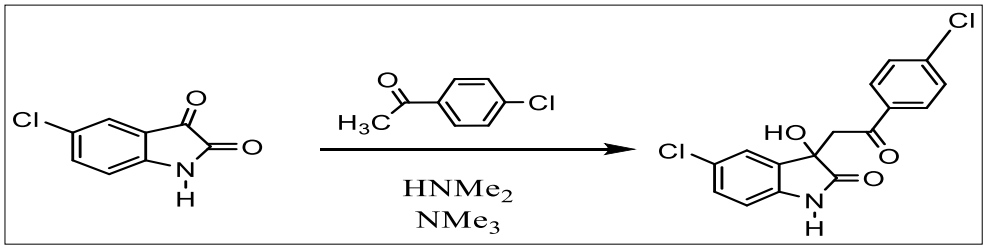


Figure 10. 5-chloro-3-(2-(4-chlorophenyl)-2-oxoethyl)-3-hydroxyindolin-2-one

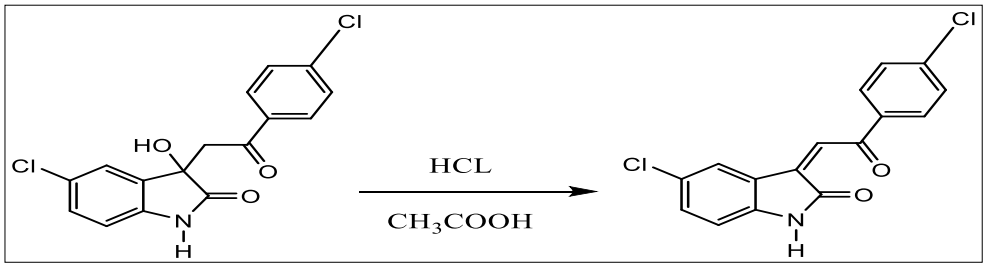


Figure 11. (Z)-5-chloro-3-(2-(4-chlorophenyl)-2-oxoethylidene)indolin-2-one

Synthesis of β-hydroxy Ketone Bermostophenone

Synthesis of 3- (2- (4-bromophenyl) 2-oxoethyl) 5- chloro-3-hydroxy-indoline-2-one:

To produce β-hydroxy ketone 4-bermothophenone, 0.001 mol of raw materials are weighed. 0.18 g of 5-chloroisatin and 0.199 g of 4-bermostophenone with 1 ml of dimethylamine and 1 ml of triethylamine were stirred for 2 hours at room temperature to perform the reaction.

Every quarter hour, reaction changes were observed and analyzed by TLC chromatography test and UV lamp. After the reaction was complete and the excess base evaporation was complete, the precipitate was placed in an oven and dried. After the precipitate dried, it was washed with 5% water and ethanol and a drop of concentrated hydrochloric acid, and the precipitate was dried in an oven. Fig 12.

Synthesis Chalcone 4-Bermostofenone

Synthesis of 3- (2- (4-bromophenyl) -2-oxoethylenidine) -5-chloro indoline-2-one:

Deposition of β-hydroxy ketone 4-bermostophenone with 30 ml of glacial acetic acid and a magnetic stirrer at 100 ° C on the heater to completely dissolve the precipitate in the acid. After a quarter of an hour, when the solution was completely hot, about 2 drops of concentrated hydrochloric acid were added and it waited for it to precipitate over time.

Every half hour, the reaction changes were observed and analyzed by TLC chromatography test and UV lamp. After half an hour, two more drops of concentrated hydrochloric acid were added and TLC test was performed at the same time. Put and wait the solution to cool and precipitate.

The reaction was complete in about two hours. For drying little by little, the solution and sediment were poured onto the watch glass and evaporated on the excess acid heater with a little heat, and the precipitate remained. The precipitate was placed in the oven for complete drying. After drying, it was washed with water and 5% ethanol. Fig 13.

Results

All results are shown in Tables 3 and 4 for prepared materials from 5a to 5e. The samples were examined for IR testing in the form of KBr tablets and for NMR dimethyl sulfoxide (DMSO) or Chloroform solvents were used.

In this research, the synthesis of new chalcones has been performed using of 5-chloroisatin as a primary substance, by the method of single-container synthesis, which is without solvent. The compounds created or the products are 3a, 3b, 3c, 3d, 3e, respectively, each in terms of melting point, efficiency, IR spectrum, HNMR, CNMR have been measured.

The first product, or 3a, has an efficiency of 92% and a melting point of 190 ° C. In the FTIR spectrum, this combination of tensile vibrations of alkene and aromatic C-H bonds at an absorption frequency of 3100 cm^{-1}.

Tensile vibration of N-H bond at 3194 cm^{-1}, C = O amide carbonyl group at 1772 cm^{-1}

Conjugated ketones appeared at 1662 $^{cm-1}$, and C = C group tensile vibrations at 1600, 1620 and 1450 cm^{-1}.The second product, or 3b, with 88% efficiency and melting point of 180 ° C in the IR spectrum, had tensile vibrations at points 3444-1716-1616-1473.

The third product or 3c with 91% efficiency and melting point of 195 ° C in the IR spectrum in the points 3067 - 3299 - 1746 - 1709 - 1617 - 1587 - 1475 had a tensile vibration.

The fourth product or 3d with 89% efficiency and a melting point of 185 ° C showed tensile vibrations at points 3056 - 2800-2900 - 3226 - 1720 - 1679 - 1600 - 1477 for the IR spectrum.

The final product of 3e with 86% efficiency and melting point of 195 ° C showed tensile vibrations at points 3100 - 3377 - 1716 - 1670 - 1592 - 1473 - 1345 - 1522 for the IR spectrum.

HNMR and CNMR spectra were performed for product 3a as shown in the table. The 3d product was also measured in terms of HNMR spectrum, which showed the results and peaks of tensile vibration in the table.

Conclusion

The aim of this study was to synthesize new derivatives of 5-chloroisatin that are the basis for the synthesis of many other heterocyclic compounds such as pyrazolines, tryptanes, acridine derivatives and pyran derivatives.

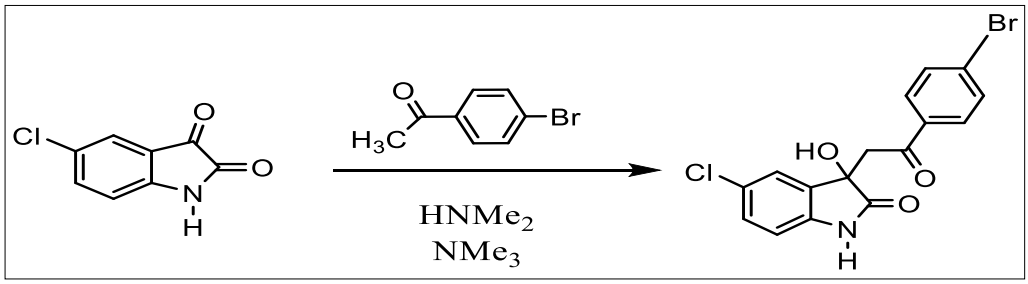


Figure 12. 3-(2-(4-bromophenyl)-2-oxoethyl)-5- chloro-3-hydroxyindolin-2-one

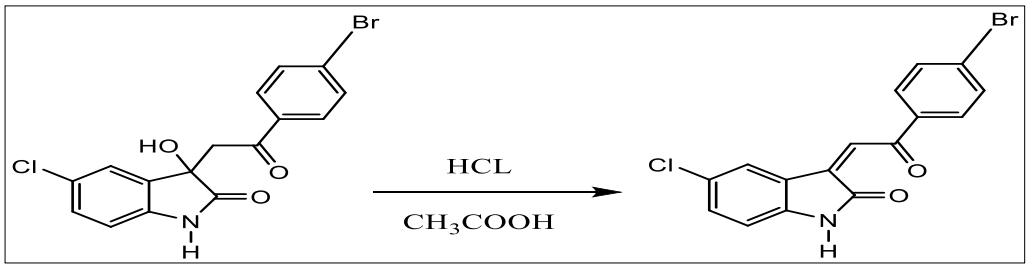


Figure 13. (Z)-3-(2-(4-bromophenyl)-2-oxoethylidene)- 5-chloroindolin-2-one

Table 3. Physical and spectral information of IR related to synthesized derivatives.

Compound	Ar	melting point Not corrected	Efficiency	IR spectrum results (Wave numbers in cm-1)
3a	Acetophenone	190	92	1450-1620-1600-1662-1722-3194-3100
3b	4-bromoacetophenone	180	88	1473-1616-1716-3444
3c	4-chloroacetophenone	195	91	1475-1587-1617-1709-1746-3299-3067
3d	4-methoxyacetophenone	185	89	1477-1600-1679-1720-3226-2900-2800-3056
3e	4-nitroacetophenone	195	86	1522-1345-1473-1592-1670-1716-3377-3100

Table 4. Physical and spectral information of HNMR related to synthesized derivatives

Compound	HNMR spectroscopy (δ Chemical displacements in ppm)
3a	Aromatic hydrogens (6.38-8.40) , Alkene hydrogens =C-H (7.93) , H N-H (8.72)
3d	Aromatic hydrogens (6.82- 8.50) , Alkene hydrogens =C-H (7.91) , H N-H (8.55) , H of Methyl methoxy group (3.93)

Table 5. Physical and spectral information of CNMR related to synthesized derivatives

Compound	CNMR spectroscopy (δ Chemical displacements in ppm)
3a	C of Aromatic and Alkene group (111.11- 141.68) , C of carbonylamide group in the indoline ring (169.61) , C of conjugated ketone (190.61)

One of the advantages of this method is the synthesis of a single container, which can be done without a solvent. These compounds have various biological properties including anti-cancer, anti-tumor, anti-virus, anti-bacterial and anti-fungal.

In this study, some new chalcone derivatives 3a-e of 5-chloroisatin 1 have been synthesized solvent freely by the reaction between 5-chloroisatin 1 and acetophenones 2a-e in basic media of dimethylamine and then, dehydration in the presence of HCl and AcOH mixture. The chemical structures of these chalcones were elucidated from their FTIR and NMR spectroscopic data. Fig 14

Spectral Analysis of New Derivatives of Synthesized Chalcones

The chemical structure of chalcone derivatives obtained from 5-chloroisatin reaction and acetophenone derivatives was determined by FTIR, ^{1}HNMR and ^{13}C NMR spectral analysis methods

Investigation of the Structure of the Compound 5-chloro -3- (2-oxo-2-phenylethylenidine) Indoline-2-one (3a) Fig 15.

In the FT IR spectrum of this compound (Figure 16) the tensile vibrations of alkene and aromatic CH bonds at the absorption frequency of 3100 cm^{-1}, the tensile vibration of the NH bond at 3194 cm^{-1}, the carbonyl group C = O amide at 1722 cm^{-1} and the conjugated ketone at 1662 cm^{-1} and the tensile vibrations of the C = C groups appear at 1600, 1620 and 1450 cm^{-1}.

Examination of the ^{1}H NMR spectrum (Figure 17) shows δ aromatic hydrogens in the range of 6.83 to 8.40 ppm with a total of 8 integrals. Alkene hydrogen of group H-C= appeared in the chemical displacement of 7.93 ppm and as a single branch with integral 1. N-H hydrogen in chemical displacement is 8.72 ppm.

Examination of the ^{13}C NMR spectrum (Figure 18) shows aromatic and alkene group carbons in the range of 111.11 to 141.68 ppm. The absorption of carbon of the carbonylamide group into the indoline ring at chemical displacement is 169.26 ppm and the conjugated ketone at 190.61 ppm.

Investigation of the structure of the Compound 3- (2- (4 -bromophenyl) -2-oxoethylenid) -5-chloro Indoline-2-one (3b) Fig 20

In the FT IR spectrum of this compound (Figure 19) the tensile vibrations of the N-H bond at 3444 cm^{-1}, the carbonyl group of C = O amide at 1716 cm^{-1} and the tensile vibrations of the C=C groups at 1616 and 1473 cm^{-1}, respectively.

In the FTIR spectrum of this compound (Figure 21) the tensile vibrations of alkenic and aromatic C-H bonds at the absorption frequency of 3067 cm^{-1}, the tensile vibration of the NH bond at 3299 cm^{-1}, the carbonyl group C = O amide at 1746 cm^{-1} and the conjugated ketone at 1709 cm^{-1} and the tensile vibrations of the C = C groups appear at 1617, 1587 and 14750 cm^{-1}.

Investigation of the structure of the compound 3-(2-(4-methoxyphenyl) -2-oxoethylidene) -5-chloro-indoline-2-one (3d) Fig 22.

In the FTIR spectrum of this compound (Figure 23), the tensile vibrations of alkene and aromatic C-H bonds at the absorption frequency of 3056 cm^{-1}, the C-H bonds of the methyl group in the range of 2800 and 2900 cm^{-1}, the tensile vibration of the N-H bond at 3226 cm^{-1}, the carbonyl group C = O amide at 1720 cm^{-1} and conjugated ketone at 1679 cm^{-1} and the tensile vibrations of the C = C groups at 1600 and 1477 cm^{-1}.

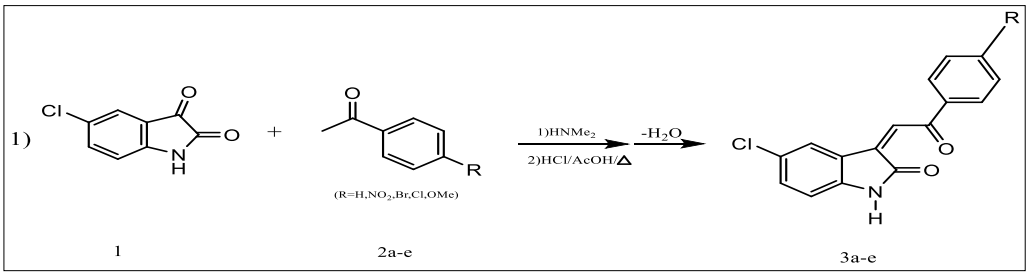


Figure 14. Investigation of the synthesis of new chalcone derivatives in alkaline environment.

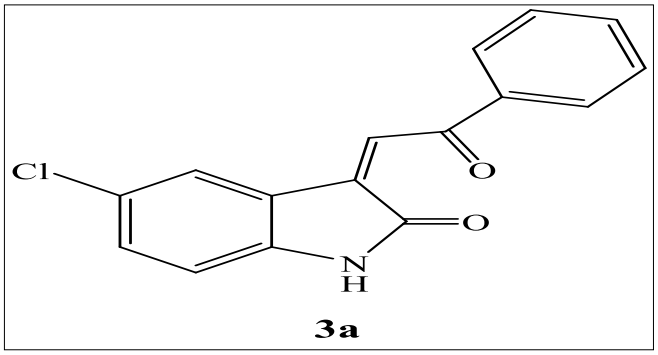


Figure 15. schematic of 3a

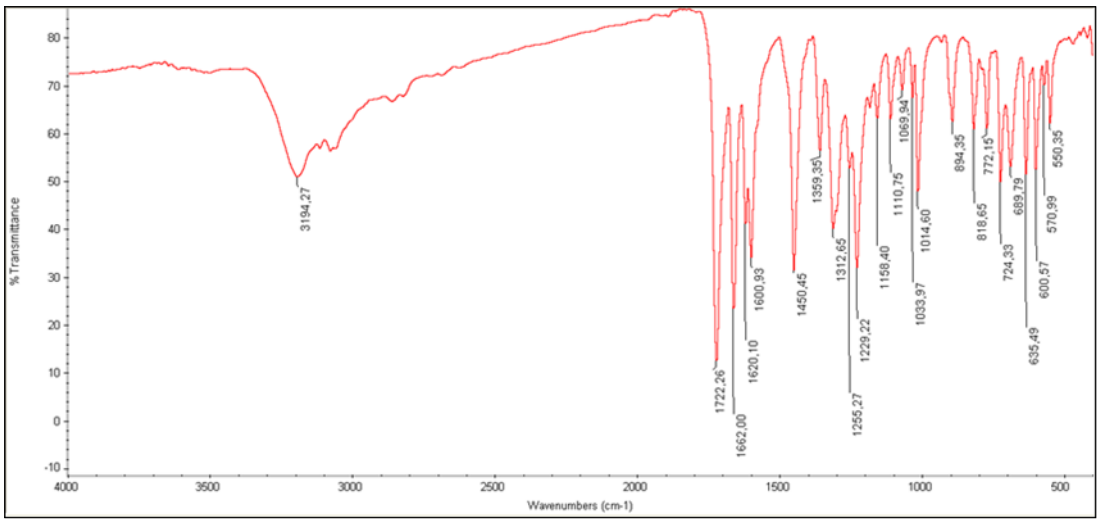


Figure 16. FTIR Spectrum of 3a compound

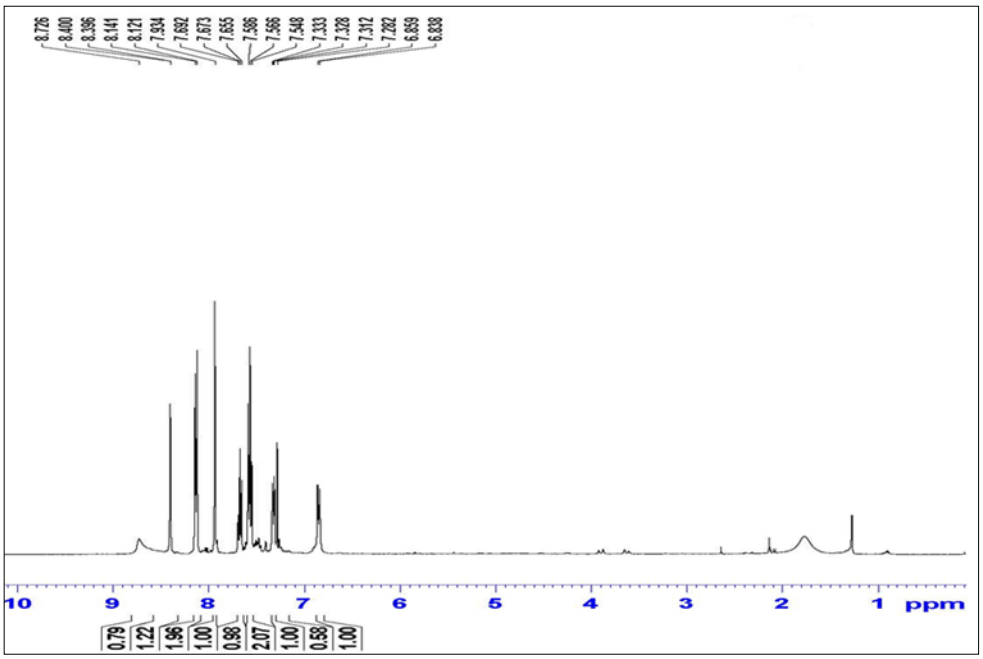


Figure 17. ^{1}HNMR Spectrum of 3a compound

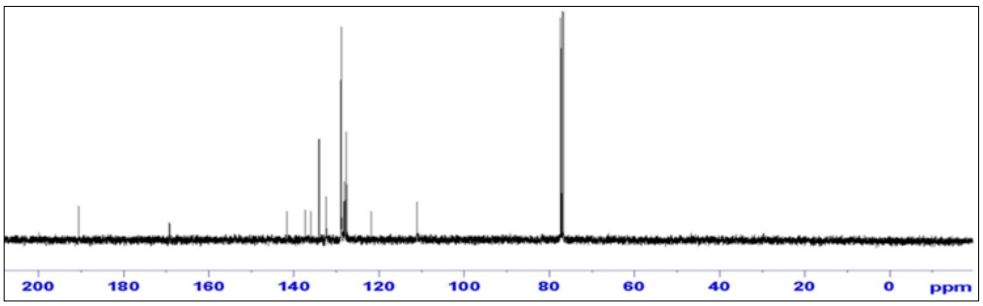


Figure 18. ^{13}C NMR spectrum of 3a compound

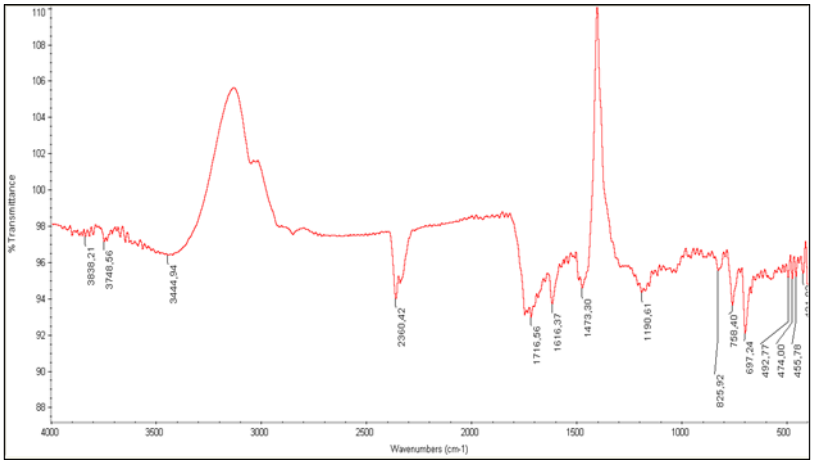


Figure 19. FTIR spectrum of 3b compound

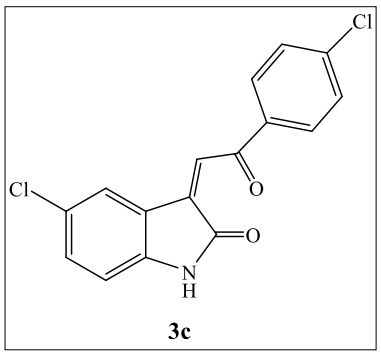


Figure 20. schematic of 3c

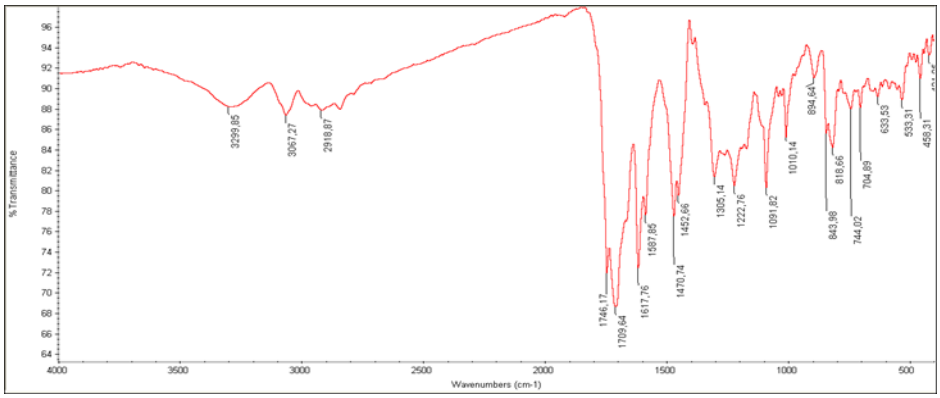


Figure 21. FTIR spectrum of 3c compound

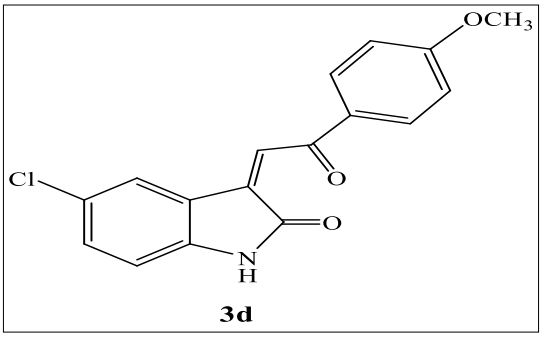


Figure 22. schematic of 3d

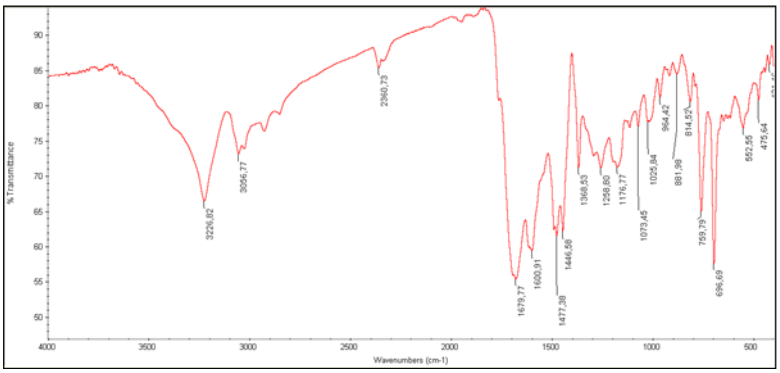


Figure 23. FTIR spectrum of 3d compound

Examination of the ^{1}HNMR spectrum (Figure 24) shows δ aromatic hydrogens in the range of 6.82 to 8.50 ppm with a total of 7 integrals. Alkene hydrogen of group H-C = appeared in chemical displacement at 7.91 ppm and as a single branch with integral 1. N-H hydrogen is flattened at a chemical displacement of 8.55 ppm. Methyl hydrogens of the methoxy group is found in 3.93 δ with integral 3.

Investigation of the structure of 5-chloro-3- (2- (4-nitrophenyl) -2-oxo ethylened) indoline-2-one (3e) Compound Fig 25.

In the FT IR spectrum of this compound (Figure 26) the tensile vibrations of alkene and aromatic C-H bonds in the absorption frequency range 3100 cm^{-1}, the tensile vibration of the N-H bond in 3377 cm^{-1}, the carbonyl group C = O amide in 1716 cm^{-1} and conjugated ketones in 1670 cm^{-1} and the tensile vibrations of the C = C groups appear at 1592 and 1473 cm^{-1}. Adsorption related to tensile vibrations of nitro NO2 group has been done in 1345 and 1522 cm^{-1}.

Discussion

Chalcones and their derivatives are becoming increasingly popular due to their various pharmacological effects. In the present study, the physical and chemical properties of our compounds were investigated that some of them were reported. Now the results are new in their group. We are also investigating the antimicrobial and antifungal effects of these compounds. We definitely hope the results are better than before. We will also apply the effect of different doses in the samples to be more complete than before. On the other hand, another factor considered

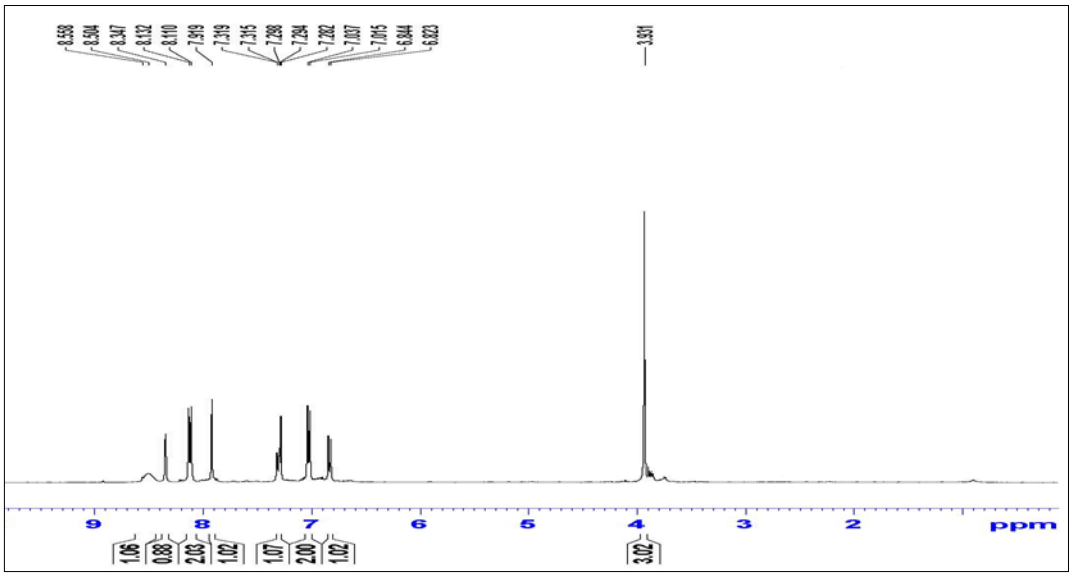
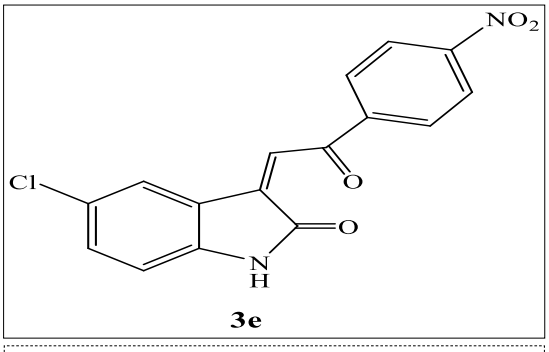


Figure 24. ^{1}HNMR spectrum of 3d compound



3e

Figure 25. schematic of 3e

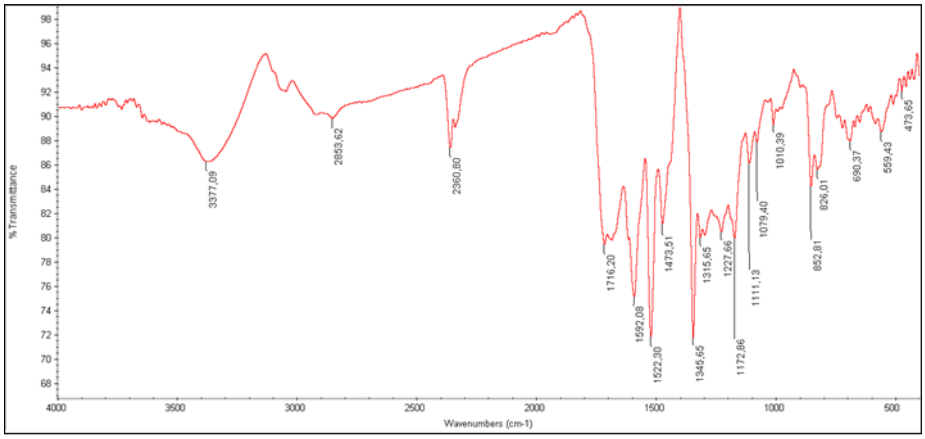


Figure 26. FTIR spectrum of 3e compound

and studied is the high lipophilicity of the compounds. As a result, new chalcons can be a suitable alternative to classic chalcons.

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