

Synthesis, Spectral Study, Physico-Chemical Properties and Biological Activity of Pyrrole Chalcone

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ABSTRACT: Pyrrole chalcones are open chain containing α, β unsaturated carbonyl group consisting of two aromatic rings. Pyrrole chalcone is synthesized by Claisen-Schmidt condensation method in alkaline solution. Spectroscopic characterization using Ultra-Violet visible spectra, Infrared absorption, optical property, chemical tests and biological activity has been studied for pyrrole chalcone. Physico-chemical properties study of this compound shows that it is novel pyrrole chalcone.

KEYWORDS: Pyrrole chalcone, Claisen-Schmidt condensation method, Ultra-violet spectrum, Infrared spectrum, Biological activity, physico-chemical property.

I. INTRODUCTION

The chemistry of chalcones has generated intensive scientific studies throughout the world. Especially interest has been focused on the synthesis and biodynamic activities of chalcones. The name chalcone is given by Kostanecki and Tambar [1]. The chalcones (1,3-di-aryl-2-propenones) and their derivatives are important intermediates in organic synthesis [2-4]. They serve as starting materials for the synthesis of variety of heterocyclic compounds which are due to the presence of enone functionality in chalcone moiety confers biological activity up on it, like anti-inflammatory [5], antifungal [6], antioxidant [7], antimalarial [8]. Chalcones are open chain containing α, β -unsaturated carbonyl group consisting of two aromatic rings (ring A & B) having diverse any of substituent's [9]. In this paper we synthesize substituted pyrrole chalcone by Claisen-Schmidt condensation method and characterize it by Infra red, Ultra violet spectra, Wilsons test, FeCl₃ test, unsaturation test with KMnO₄, optical activity and biological activity of pyrrole chalcone.

II. Materials and Methods

Pyrrole chalcone is synthesized by Claisen-Schmidt condensation of pyrrole-2-carbaldehyde and 2,6-dihydroxy acetophenone by base or acid catalyzed followed by dehydration to yield pyrrole chalcone [10-11]. The chemicals used for preparation of pyrrole chalcone are of A.R. grade. The mixture of 2,6, dihydroxy acetophenone (0.01 mol) and pyrrole-2-carbadehyde (0.01 mol) are dissolved in ethyl alcohol (25ml) and then potassium hydroxide 10ml(40%) were added to it. The reaction mixture was heated for 3 hours till blackish brown color was obtained. The progress of reaction was monitored by TLC. After completion of reaction the contents were poured into ice water and then acidified by dil. HCL. The solid obtained was filtered and crude product was recrystallized from ethyl alcohol to give the pyrrole chalcone [12]. The reaction for formation of pyrrole chalcone is given in figure (1). The melting point of the pyrrole chalcone is determined by an open capillary tube and is unconfirmed. Infra red spectra are recorded using

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FT-IR spectrophotometer, UV-visible spectrum of pyrrole chalcone measured on SL159, single beam UV-VIS spectrophotometer. The purity of compound is checked by TLC plate, which were precoated with silica gel using solvent ethyl acetate and petroleum ether (3:7). The chemical parameters are measured on colorimeter. The biological activity of the pyrrole chalcone is given below.

III. RESULTS AND DISCUSSION

The pyrrole chalcone having IUPAC name 1-(2, 6-di-hydroxyphenyl)-3-(1 H-pyrrole-2-yl) prop-2-en-1-one has been synthesized by Claisen-Schmidt method and its structure is stable at room temperature, insoluble in water and is soluble in organic solvent (ethyl alcohol). The stoichiometry of the compound may be represented as 1:1 substituted pyrrole and 2,6-dihydroxy acetophenone ratio. The physico-chemical properties of pyrrole chalcone are given in, table (1) and (2). The completion of reaction was checked by thin layer chromatography, Wilsons test, FeCl₃ test are positive for pyrrole chalcone. The reaction between pyrrole-2-carbaldehyde and 2,6-dihydroxy acetophenone is shown in figure (1). From the reaction mechanism it is observed that condensation of aldehyde group of pyrrole and ketone group of 2,6-dihydroxy acetophenone takes place in the presence of alkali catalyst.

Infra red spectrum:

The Fig (a) IR spectrum of α , β -unsaturated carbonyl group has characteristic bands of chalcone at prominent bands between 1625 to 1650 per cm. The characteristic infra red peaks give the presence of particular functional group. The region at which other absorption bands appear depends on the type of aromatic / hetero-aromatic rings as well as the substituent present on these rings. The characteristic bands of chalcone are observed in pyrrole chalcone as (per cm):

3065-Ar-H, 1658-C=C, 1650- C=O, 1230-C-O-C, 3136-(OH), 3156-(OH), 3215(-N-H)

Ultra Violet -visible spectrum of pyrrole chalcone

The Ultra Violet visible spectrum of pyrrole chalcone shows that major absorption bands usually occurs in the range 230 to 490 nm. Molecules containing π -electrons or nonbonding electrons can absorb energy in the form of Ultra Violet -visible light to excite the electron to higher anti bonding molecular orbital (i.e. lower energy gap between the HOMO and LUMO) the longer the wavelength of light it can absorb [12] The energy required for various transitions obeys the following order

$$\sigma - \sigma > n - \sigma^* > \pi - \pi^* > n - \pi^*$$

Biological activity

Antibacterial activity:

The -ve shows that pyrrole chalcone has no antibacterial activity. Zone of inhibition in mm is not mentioned.

Antifungal activity:-

The -ve growth shows that more than 90% reduction in growth pyrrole chalcone shows the antifungal activity. The reduced growth shows that there is more than 50% and less than 90% reduction in growth it shows antifungal activity.

IV. CONCLUSION

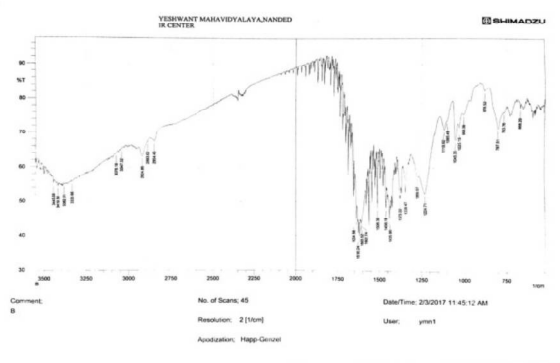
The pyrrole chalcone having IUPAC name 1-(2, 6-di-hydroxyphenyl)-3-(1 H-pyrrole-2-yl) prop-2-en-1-one has been synthesized by Claisen-Schmidt method and its structure is confirmed by Infra red, Ultra Violet visible, optical activity, Wilsons test, FeCl₃ test, and unsaturation test with KMnO₄ are positive for this novel pyrrole chalcone. The reaction mechanism for the formation of pyrrole chalcone shows condensation of aldehyde group of pyrrole and ketone group of 2, 6-di-hydroxy acetophenone takes place. The pyrrole chalcone shows antifungal activity but does not shows antibacterial activity.

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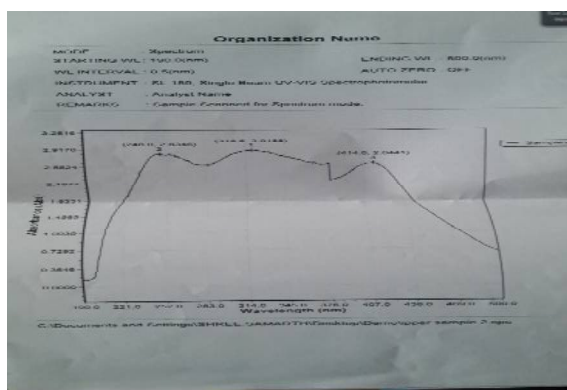
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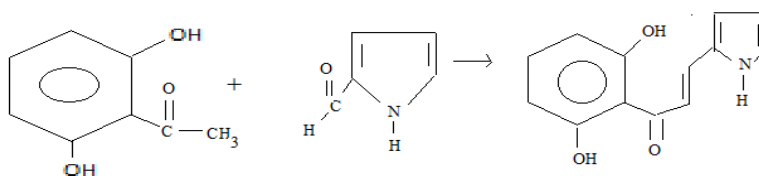
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(a)



(b)



(c)

Figure1:

(a) Infrared spectrum (b) Ultra Violet-visible spectrum of pyrrrole chalcone (c) Reaction of pyrrrole chalcone

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Table (1):

Property	color	M.P.	Yield	Chemical name	Chemical formula	Molecular weight	phase
Observation	Blackish brown	>250 ⁰ c	90%	Pyrrole chalcone	C ₁₃ H ₁₁ O ₃ N	229	Solid(Blackish brown crystals)

(a)

Absorption spectra	Wavelength
absorption	λ(nm)
2.1275	231.5
1.7767	272.0
0.6273	355.5
0.3379	497.5

(b)

Sr no	compound	Escherichina coli	Salmonella typhi	Staphylococcus aureus	Bacillus subtilis
01	Pyrrole chalcone	-ve	-ve	-ve	-ve

(c)

Sr no	compound	Aspergillus niger	Penicillium chrysogenum	Fusarium moneliforme	Aspergillus flavus
01	Pyrrole chalcone	RG	RG	-ve	RG

(d)

Table(1):

(a) Physico-Chemical properties of pyrrole chalcone (b) Optical activity (c) Antibacterial activity (d)Antifungal activity

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