



Synthesis and Biological Activity of 3-Nitro 5-Chloro Chalcone and Their Pyrazole and Isoxazole Derivatives

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Abstract:

The heterocyclic compounds and their derivatives hold significant importance in chemistry due to their diverse biological activities, which attract researchers to explore them further. The chalcone structure consists of two aromatic rings connected by a three-carbon aliphatic chain, containing an α,β -unsaturated ketone with a reactive ethylenic group. In the Claisen-Schmidt condensation, equimolar amounts of an aromatic aldehyde (lacking α -hydrogen) and an aromatic ketone (with an active $-\text{CH}$ group) react in the presence of a condensing agent. In the current study, 3-nitro-5-chloro benzaldehyde reacts with 1,4-benzodioxane-6-yl methyl ketone in the presence of potassium hydroxide to form 3-nitro-5-chloro chalcone. The chalcone product was identified using thin-layer chromatography (TLC). The newly synthesized 3-nitro-5-chloro chalcone was then reacted with hydroxylamine hydrochloride and hydrazine hydrate in the presence of sodium acetate in ethanol under reflux conditions. This reaction led to the formation of isoxazole and pyrazole derivatives of the 3-nitro-5-chloro chalcone, and these derivatives were confirmed using TLC.

Keywords: *Derivative, Nitro Chalcone, Pyrazole, Isoxazole.*

Introduction:

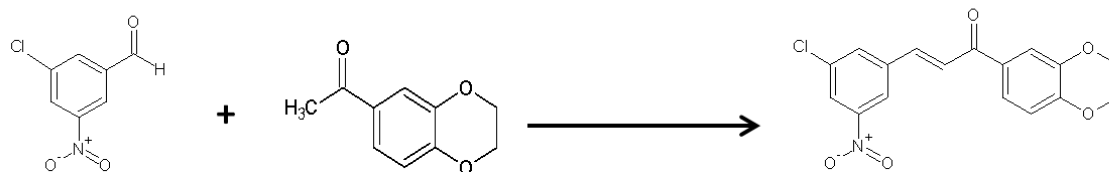
In the field of organic chemistry, the synthesis of heterocyclic compounds is an increasingly important area of research. Among these, the synthesis of chalcones stands out as a particularly interesting topic. The most convenient and widely applied method for chalcone synthesis is the Claisen-Schmidt condensation process, a condensation reaction that involves the reaction of an aromatic aldehyde with an aromatic ketone in the presence of a suitable condensing reagent, leading to the formation of chalcones.

A review of the literature reveals that chalcones and their derivatives have a broad range of applications in both the medicinal and industrial fields. These compounds exhibit a variety of biological activities, which are of great interest in pharmaceutical

research. Various chalcone derivatives display significant pharmacological effects, demonstrating their versatility and potential as therapeutic agents. Given the diverse biological and pharmacological activities of chalcones and their derivatives, the synthesis of new chalcones and their derivatives has become a key area of focus. This is crucial for the discovery of new heterocyclic compounds, which could increase the likelihood of finding novel drugs with diverse biological and pharmacological properties. Thus, the synthesis of chalcones and their derivatives remains an important research topic in the quest for new therapeutic agents.

Experimental Procedure:**Procedure for the synthesis of Nitro Chloro Chalcones:**

A mixture of 3-Nitro,5-Chloro Benzaldehyde react with 1,4-benzodioxane-6-yl methyl ketone (0.01 mol) were dissolved in ethanol (25 ml) and 10% sodium hydroxide solution (25 ml) was added slowly and the mixture was stirred for near about 4 hrs then it was poured in to 400 ml of water with constant stirring and left overnight in refrigerator. The precipitate as obtained after that it was neutralized by 10 % HCL solution and cheked it by PH paper



Melting points of the compounds was determined in open capillary tubes and are uncorrected. Identification of chalcone compound with the help of thin layer chromatography was performed on TLC plate and spots were visualized by iodine vapor.

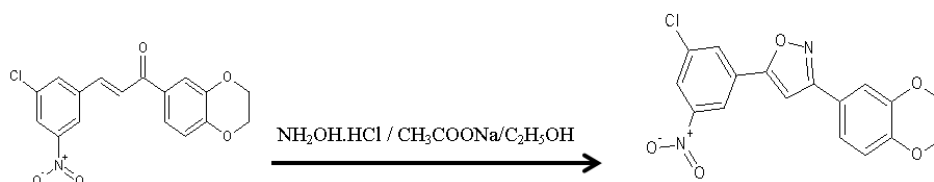
and litmus paper also and after that it was re-crystallized with the ethanol.and we get pure compound and it cheked with the help of TLC.

Reaction:

When equimolar mixture of 3-Nitro,5-Chloro benzaldehyde react with 1,4-benzodioxane 6-yl methyl ketone in the presence of base NAOH we get (3- N Cl C) (2E)-3-(3-chloro-5-nitrophenyl)-1-(2,3-dihydro-1,4-benzodioxin-6-yl)prop-2-en-1-one

Methods for synthesis of Isoxazole**Derivative:**

A mixture of 3-Nitro,5-Chlorochalcone (0.02 mol) react with hydroxylamine hydrochloride (0.02 mol) and sodium acetate in ethanol (25 ml) was refluxed for 6 hrs. The reaction mixture was poured in to ice water (50 ml).the precipitate obtained was filtered washed and recrystallized from ethanol.Completion of the reaction was monitored by TLCs.

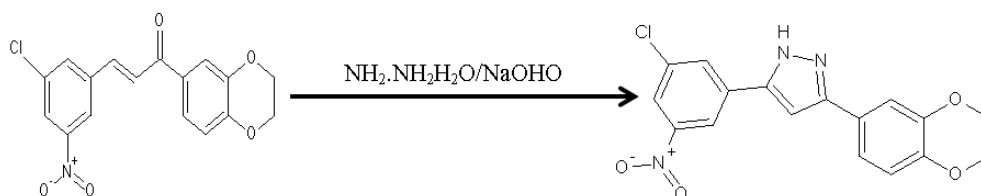
A) Synthesis of Isoxazole Derivatives:

(2E)-3-(3-chloro-5-nitrophenyl)-1-(2,3-dihydro-1,4-benzodioxin-6-yl)prop-2-en-1-one

B) Synthesis of Pyrazole Derivative:

A mixture of 3-Nitro 5-Chloro chalcone (0.02 mol) react with hydrazine hydrate (0.02 mol) and sodium acetate in ethanol (25 ml) was refluxed for 6 hrs. The

reaction mixture was poured in to ice water (50 ml).the precipitate obtained was filtered washed and recrystallized from ethanol.Completion of the reaction was monitored by TLCs.



5-(3-chloro-5-nitrophenyl)-3-(2,3-dihydro-1,4-

benzodioxin-6-yl)-1H-pyrazole

Biological Activity:

The Synthesized derivative of Isoxazole and pyrazole to checked the Antibacterial Activity we found that it shows antibacterial activity. 3-Nitro, 5-Chloro

Chalcone Observed that E.coli is 14 mm and S.aureus is 09 mm 3-Nitro Pyrazole Observed that E.coli is 13 mm and S.aureus is 12 mm and 3-Nitro Isoxazole Observed that E.coli is 09 mm.

S.N	Samples	Zone of Inhibition (In mm)	
		<i>E. coli</i>	<i>S. aureus</i>
1	Sample 7	14 mm	09 mm
2	Sample J	13 mm	12 mm
3	Sample K	9 mm	---

Result:

The Synthesized 3-Nitro 5-Chloro chalcone and its pyrazole and Isoxazole derivatives clearly shows Anti-bacterial Activities against two bacteria that is E.coli and S.aureus. Pyrazole & Isoxazole Derivative shows Antibacterial Activities and it is Important property to show that compound. The newly synthesized ((3-N,5-Cl C) (2E)-3-(3-chloro-5-nitrophenyl)-1-(2,3-dihydro-1,4-benzodioxin-6-yl)prop-2-en-1-one compounds were characterized by thin layer chromatography for the reacting 3-Nitro5-Chloro benzaldehyde (Rf value – 0.67) with 1,4-benzodioxane-6-yl-methyl ketone (Rf value – 0.49) and the produced ((3-N,5-Cl C) (2E)-3-(3-chloro-5-

nitrophenyl)-1-(2,3-dihydro-1,4-benzodioxin-6-yl)prop-2-en-1-one (Rf value 0.79) were noted. This gives evidence for formation of the product. The product ((3-N,5-Cl C) (2E)-3-(3-chloro-5-nitrophenyl)-1-(2,3-dihydro-1,4-benzodioxin-6-yl)prop-2-en-1-one also showed the Wilson's test for chalcone. Melting point of concerning compound was detected in open capillary tube. The M.Pt.of ((3-N,5-Cl C) (2E)-3-(3-chloro-5-nitrophenyl)-1-(2,3-dihydro-1,4-benzodioxin-6-yl)prop-2-en-1-one was 177^o.

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