

Chacone Application in Heterocyclic Synthesis: Synthesis of Isoxazolo, Thione, And Pyrimido Substituted Analogies Of 2-Benzylidene Cyclopentanone

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Abstract—New series of isoxazole and benzodizepine compounds were synthesised from chalcones and their antibacterial activity was evaluated. First, chalcones were created by reacting Utilising Claisen-Schmidt condensation, Benz aldehyde is combined with various acetophenones. In ethanol, chalcone was utilised to react with sodium acetate, hydroxylamine hydrochloride, and other isoxazole derivatives. In addition, piperidine was utilised to react with o-phenylenediamine in ethanol to produce derivatives of benzodizepine. The structures of the freshly synthesised isoxazole and benzodiazepine derivatives have been developed based on their spectrum data. The synthesised versions of the selected compounds' antibacterial efficacy were evaluated. Cyclopentanone was combined with a number of aromatic aldehydes to form chalcones. When urea, thiurea, and hydroxylamine hydrochloride are used to treat these chalcones.

Index Terms—chalcones, isoxazoles, pyrimido, thione, antimicrobial activity.

I. INTRODUCTION

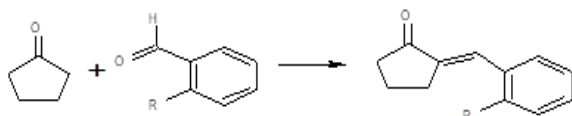
Chalcone is the name given to the often occurring - unsaturated ketone. Chalcone (Benzylidene acetophenone) and its derivatives belong to a unique class of secondary metabolites. Additionally, they serve as biosynthetic precursors for a number of natural products, including flavones, is flavones, isoflavanols, aurones, etc. Chalcones exhibit amazing biological activity as well. All of these factors make them desirable synthetic targets, and more crucially, they have been widely used as intermediates in the synthesis of hetrocyclic and carbocyclic systems. Among the many heterocycles that have been researched for creating significant medicinal

compounds are isoxazoles. Pyrimidinethiones and pyrimidinones have been crucial components of medicinal chemistry. Isoxazoles have been used in biological applications such as antileukemia, anticonvulsant (2) and antagonistic (3) and antagonistic (4) Pyrimidinethiones have been discovered to have ant-like properties. anticancer (5), hypoglycemic (6), and tubercular (7) actions. The potential of pyrimidinones to incorporate a variety of biological functions, such as anticancer (8), antibacterial (9), and analgesic (10), has been amply demonstrated during the past few years. We provide here a new series of isoxazoles, pyrimidine thiones, and pyrimidinone in light of the foregoing. By using the agar diffusion method, the synthesised compounds were tested for their Gram-negative bacteria are resistant to in vitro antibacterial activity *S. Paratyphi-B* (MTCC733) and *E. coli* (MTCC 443). In many different ways, heterocyclic compounds are vital to life and are extensively present in nature. Due to the extensive range of physiological actions connected to this class of chemicals, these molecules are very significant. Numerous substances, including the majority of the vitamin B complex members, antibiotics, chlorophyll, haemin(11), other plant pigments, amino acids, and proteins, as well as medicines, dyes, enzymes, and DNA, include heterocyclic rings. The constant search for innovative techniques for the creation of the heterocyclic units, namely isoxazoles and pyrazoles, is driven by the essential significance of heterocycles in natural product chemistry and pharmacology. These essential intermediate products, chalcones, which also have biological and pharmacological properties, were used to make the isoxazoles and pyrazoles.

II. PREPARATION METHOD

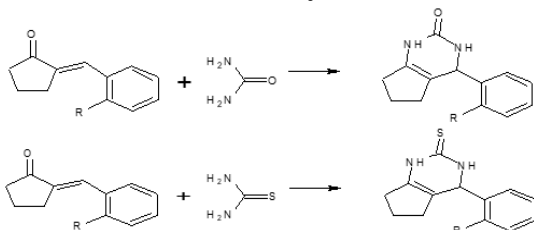
2.1. General Synthesis of Chalcone

Cyclopentanone (5 ml 0.01 mol) Aromatic aldehyde (5ml 0.01mol) and aq KOH (2 gm in 10 ml water) was added in ethanol (25 ml) and reaction was refluxed for 3 hour. After completion of reaction, mixture was poured into ice cold water, filtered and crystalize from ethanol.



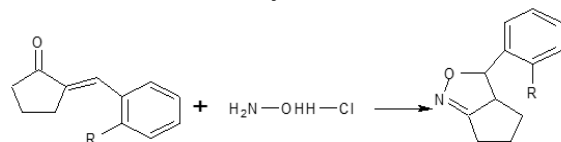
2.2. General Synthesis of Pyrimidine/Thione

Chalcone (0.01 mol, 1.7 gm), urea (0.2 mol, 1.2 gm)/thiourea (0.02 mol, 1.4 gm) and aq KOH (2 gm in 10 ml water) was added the reaction was refluxed for three hours in ethanol (25 ml). When the reaction was finished, the liquid was dumped into ice cold water and filtered. and crystalize from ethanol.



2.3. General Synthesis of Isoxazole

Chalcone (0.02 mole, 3.4 gm). Hydroxylamine hydrochloride (0.02 mol, 1.4 gm) and aq KOH (2 gm in 10 ml water) was added the reaction was refluxed for eight hours in ethanol (25 ml). When the reaction was finished, the liquid was dumped into ice cold water and filtered. and crystallizes from ethanol.



III. RESULT & DISCUSSION

3.1. (2E)-2benzylidenecyclopentanone

- The compound is yellow colour, crystalline solid with melting point 120°
- Elemental analysis of the product indicated the molecular formula of the compound to be molecular formula $C_{12}H_{12}O$

- IR data: (KBr, cm): 1706.43 (C=O Str.), 1625.29 (C=C Str.), 3054.53 (C-H Str.), 3020.52 (C-H Str.)
- ^1H NMR: -(CDCl₃) 8 7.3-7.5 (Ar-H), 82.3-3.01 (6H, Cyclopentanone), 8 2.9 (1H, -C=C-H)

Based on spectral and analytical data as well as chemical characteristics the compound was assigned as (2E)-2benzylidenecyclopentanone

3.2. (2E)-2-(2-chlorobenzylidene) cyclopentanone.

- The compound is yellow colour crystalline solid with melting point 115°.
- Elemental analysis of the product indicated the molecular formula of the compound to be molecular formula $C_{12}H_{12}OCl$
- IR data: (KBr, cm): 1687.41 (C=O str.), 1620, 31 (C-H str.), 3066, 55 (-C-H str.), 2957, 52 (C-H str.), 751, 21 (C-Cl str.)
- ^1H NMR: -(CDCl₃) 8 7.2-7.9 (Ar-H), 8 2.0-2.4 (6H, Cyclopentanone), 6 2.92 (1H, -C=C-H)

Based on analytical and spectral data & on the basis of chemical properties the compound was assigned as (2E)-2-(2-chlorobenzylidene) cyclopentanone

3.3. 4-phenyl-1,3,4,5,6,7-hexahydro-2H-cyclopenta[d]pyrimidin-2-one

- The compound is yellow colour, crystalline solid with melting point 90°.
- Elemental analysis of the product indicated the molecular formula of the compound to be molecular formula $CHNO$
- IR data: (KBr, cm): 1703.44 (C=O str.), 1624.38 (C-C str.), 1178.49 (C-N str.), 3406.62 (N-H str.), 3025.61 (C-H str.)

Depending on analytical, spectroscopic, and chemical characteristics data the compound was pyrimidin-2-one assigned as 4-phenyl-1,3,4,5,6,7-hexahydro-2H-cyclopenta [d]

3.4. 4-(2-chlorophenyl)-1, 3, 4, 5, 6, 7-hexahydro-2H-cyclopenta [d] pyrimidinone.

- The compound is yellow colour crystalline solid with melting point 95°
- Elemental analysis of the product indicated the molecular formula of the compound to be molecular formula $CH N_2 O Cl$
- IR data: (KBr, cm): 1703.37 (C=O str.), 1624.31 (C-C str.), 3405.53 (N-H str.), 3025.52 (C-H str.), 1178.41 (C-N str.)

Based on analytical a spectral data & on the basis of chemical properties the compound was 4-(2-chlorophenyl)-1, 3, 4, 5, 6, 7-hexahydro-2H-cyclopenta [d] pyrimidinone.

3.5. 4-phenyl-1, 3, 4, 5, 6, 7-hexahydro-2H-cyclopenta[d]pyrimidine-2-thione

- The compound is yellow colour crystalline solid with melting point 95°
- Elemental analysis of the product indicated the molecular formula of the compound to be molecular formula CH₄N₂S
- IR data: (KBr.cm):1700.56(C-S str.)1672.56(C=C str.)3026.55(C-H str.) 1180.45(C-N str.) str.) 3372.52(N-H)
- H¹NMR:-(CDC13)8 6.9- 7.5 (Ar-H). 8 1.2-2.17 (6H, Cyclopentanone), 8 5.28 (2H, -NH)

Based on analytical a spectral data & on the basis of chemical properties the compound was assigned as, 4-phenyl-1, 3, 5, 6, 7-hexahydro-2H4cyclopenta[d]pyrimidine-2-thione

3.6. 4-(2-chlorophenyl)-1, 3, 4, 5, 6, 7-hexahydro-2H-cyclopenta[d] pyrimidine-2thione

- The compound is yellow colour crystalline solid with melting point 160°
- Elemental analysis of the product indicated the molecular formula of the compound to be molecular formula C₁₂H₁₂SCI
- IR data: (KBr.cm):1701.47(C-S str.) 1625.52(C=C str.) 1181.45(C-N str.) 3391.53(N-Hstr.)3061.53(C-Hstr.)752.39(C-Clstr.)

Based on analytical a spectral data & on the basis of chemical properties the compound was assigned as, 4-(2-chlorophenyl)-1, 3, 4, 5, 6, 7-hexahydro-2Hcyclopenta[d]pyrimidine-2 thione

3.7. 3-phenyl-3a, 4, 5, 6-tetrahydro-3H-cyclopenta [c] [1,2] oxazole

- The compound is yellow colour, crystalline solid with melting point 85°.
- Elemental analysis of the product indicated the molecular formula of the compound to be molecular formula C₁₂H₁₂NO
- IR data: (KBr.cm):1690,28(C=N str.) 3055,23(C-H str.) 1179, 19(C-O str.) 1252,21(C-Cstr.)
- H¹NMR-(CDC)5 7.3- 7.6 (Ar-H), 5 2.0 2.6 (6H, Cyclopentanone), & 3.07 (1H, oxazoleH)

Based on analytical a spectral data & on the basis of chemical properties the compound was assigned as, 3-phenyl-3a, 4, 5, 6-tetrahydro-3H-cyclopenta [c] [1,2] oxazole

3.8. 3-(2-chlorophenyl)-3a,4,5,6-tetrahydro-3/1-

- The compound is yellow colour crystalline solid with melting point 85%
- Elemental analysis of the product indicated the molecular formula of the to be molecular formula CH NOCI
- IR data: (KBr.cm):1624,53 (C-N str.) 3065,45(C-H str.) 1125,48(C-O str.) 1257.51 (C-C str) 755,29(C-Cl str.)

Based on analytical a spectral data & on the basis of chemical properties the compound was assigned as 3-(2-chlorophenyl)-3a,4,5,6-tetrahydro-3/1-

IV. CONCLUSION

This study's main goals were to synthesise new isoxazoles, pyrimidinethiones, and pyridinone derivatives, purify them, and characterise them. Several identified chemicals, including [1.1, 1.2, 2.1, 2.2, 2.3, 2.4, 3.1, & 3.2], have been produced by the synthetic procedure. The yield of the synthesised compounds was estimated to be between 65% and 72%. Using analytical data from techniques like IR and ¹H NMR, the structures of synthesized substances were verified and described.

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