e-ISSN: 2349-2678, p-ISSN:2961-6050

available online on www.ijpba.in

International Journal of Pharmaceutical and Biological Science Archive

NLM (National Library of Medicine ID: 101732687)

Index Copernicus Value 2022: 72.59

Volume 12 Issue 6; 2024; Page No. 127-135

To Describe the Pyrazolone Bases, Including Chalcones and Schiff Bases

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Article Info: Received: 16-09-2024 / Revised: 28-10-2024 / Accepted: 27-11-2024
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Conflict of interest statement: No conflict of interest

Abstract

The synthesis and characterization of heterocyclic molecules, particularly those containing nitrogen, have garnered significant attention due to their diverse biochemical activities and potential therapeutic applications. This research focuses on the development of novel nitrogen-containing heterocyclic compounds and the comprehensive evaluation of their biochemical activities The synthesized compounds were thoroughly characterized using a range of spectroscopic and analytical techniques, including NMR (Nuclear Magnetic Resonance) spectroscopy, FTIR (Fourier Transform Infrared) spectroscopy, mass spectrometry, and X-ray crystallography. These techniques confirmed the structures and purity of the compounds, providing detailed insights into their molecular configurations.

Keywords: Pyrazolone, Bases, Chalcones, Compound and Schiff Bases

Introduction

A chemical is considered heterocyclic if it has at least one heteroatom in its cyclic ring structure. The most common heteroatoms are nitrogen, oxygen, and Sulphur. Half of all organic compounds found in nature are heterocyclic compounds, which are present in many different kinds of plants and animals. Alkaloids, colours, medications, proteins, enzymes, and many other important heterocyclic compounds are found in nature.

Heterocyclic compounds may be easily classified by their electronic structures. Saturated and unsaturated groups predominate in heterocyclic molecules. Due to changes in their steric properties, saturated heterocyclic compounds operate similarly to their acyclic derivatives. Piperidine and Tetrahydrofuran are typical amines and ethers. Due to There has been a lot of research into unsaturated heterocyclic compounds with 5- and 6-member rings because of their unrestrained nature.

Pyridine, thiophene, pyrrole, furan, and those derived from them that are benzo fused are examples of unstrained unsaturated heterocyclic compounds. To name a few, benzothiophene, quinoline, indole, and benzofuran are notable benzo fused heterocycles. Pharmaceuticals, agrochemicals, and veterinary goods use heterocyclic molecules. Many heterocyclic molecules are vital to life. Heterocyclic compounds include hormones, alkaloids, antibiotics, vital components, including proteins, vitamins, haemoglobin, pigments, and dyes.

Compounds that are heterocyclic contain carbon, oxygen, and nitrogen, and sulfur in their cyclic rings. Pyrrole, furan, and thiophene are the simplest chemical types that include five carbon atoms and one heteroatom. Polycyclic molecules are the ideal natural chemicals for pharmacological purposes. Their unique ability to function as biomimetics and active cores in complex structures has made them essential inside the pharmaceutical sector. Heterocyclic derivatised compounds are many. The extent to which compounds are ionised at physiological pH may be affected by hetero-cyclic substitutions, changing their basicity and lipophilicity and affecting pharmacokinetic characteristics. Nitrogen heterocyclic molecules are more common and therapeutic.

Literature Review

Oluwakemi, Ebenezer et.al. (2022). Important in medicine, heterocyclic compounds are naturally occurring molecules with desirable properties. They are masters of deft biomimetics and possess a complicated structure that contains an active pharmacophore. This is why they are relevant to the field of medication development. The number of heteroatoms, ring type, and ring size all play a role in identifying heterocyclic compounds. The majority of these chemicals are heterocyclic nitrogen compounds. They have important pharmacological implications as well.

Kumar, Adarsh.et.al. (2023). There is a worldwide epidemic of cancer. The selectivity, safety, and lack of resistance are major issues with many anticancer drugs. Therefore, there is an immediate need for safer, more targeted anticancer medications. The majority of medications that have an effect on the body's physiology are heterocycles. The nitrogen heterocycle is the most common kind of heterocyclic framework. The biological features and list of FDA-approved heterocyclic nitrogen-containing medications are presented in this study. We have discovered heterocycles that include nitrogen, which are used in cancer therapy. These include pyrimidines, quinolones, carbazoles, imidazoles, benzimidazoles, triazoles, -lactams, indoles, pyrrolo-benzodiazepines, isatin, quinoxaline, and pyrido[2,3-d] pyrimidines. Additionally, we covered the procedures of pharmacological action and cellular targets.

Depa, Navaneetha et.al. (2022).

Heterocyclic chemistry has many everyday uses. Sulphur, nitrogen, and oxygen are heteroatoms in heterocyclic compounds. Many heterocyclic compounds containing Heteroatomic nitrogen is useful in biology and medicine. Compounds containing nitrogen that are heterocyclic have several uses in medicine. Combating cancer, infections, inflammation, and bacterial and viral infections are only a few of these purposes. The biological significance of indole, pyrazole, and triazole compounds incorporating novel moieties is examined in this research.

Bhardwaj, Nivedita et.al. (2019). Histerocytic compounds are a large and varied class of chemical compounds. The total the fast expansion of the market for heterocyclic compounds made from natural sources is being propelled by their high value. Many scientific disciplines rely on nitrogen-containing chemicals, such as medical and biochemical chemistry. Indole, carbazole, quinoline, isoquinoline, and benzthiazole are some of the nitrogen-containing heterocyclic compounds found in nature that are studied here. Antifungal, anti-inflammatory, antibacterial, antioxidant, anticonvulsant, antiallergic, herbicidal, and anticancer are just a few of the numerous beneficial characteristics possessed by these nitrogen heterocyclic molecules.

Gulati, Susheel et.al. (2021). In particular, heterocycles are useful as agrochemical and medicinal precursors due to their nor O-moieties. Synthesis of organic compounds relies on better techniques for preparing heterocycles, particularly those present in natural materials. The innovative,

environmentally conscious methods of organic synthesis have made it a welcome addition to green chemistry. Use of biocatalysts under moderate circumstances with environmentally acceptable solvents is green chemistry. Nitrogen and oxygen heterocycles, namely their biological activity and environmentally friendly synthesis techniques, were the primary foci of this study.

Research Methodology

This class of compounds includes the compound 4-acetyl-1-(4-methylphenyl) Triple-methylpyrazol-5(4H)-1H-pyrazolThe compounds 4-acetyl-1-(4-chlorophenyl) and -one pyrazolones. The compounds were synthesized using the previously described procedure. Benzaldehyde compounds of different kinds were obtained from the neighborhood store. We used analytical grade chemicals for everything else.

Acetyl pyrazolone, also known as the compound in question is This compound is known as 4-acetyl-1-(4-chlorophenyl)-3-methyl-1H-pyrazol-5(4H)-one. Synthesis was performed on the chemicals. using the previously described procedure. We got the different aniline derivatives from the neighborhood market. We used analytical grade chemicals for everything else.

Result

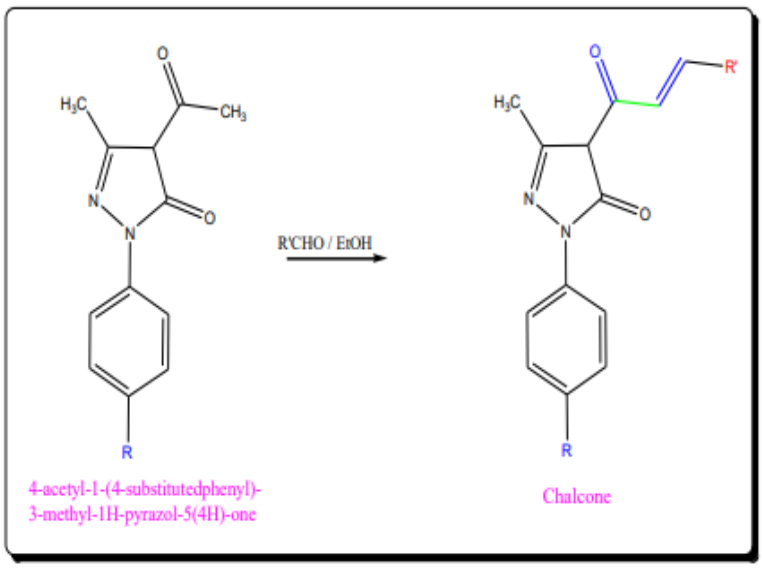
Purification of methyl-4-acetyl-1-(4-substitutedphenyl)-3-methyl compound(2a-h) and (3a-h) chalcones that are derived from -1H-pyrazol-5(4H)-one

Combining The compound 4-acetyl-1-(4-methylphenyl)-3-methylThe compound -1H-pyrazol-5(4H)-one (0.01mol) with a mixture of the reaction was carried out in RBF using 0.01mol of substituted aldehydes in EtOH as the media. After that, For the next day, the mixture was allowed to sit at room temperature and be stirred.

adding 5 40 millilitres of a potassium hydroxide solution. We were able to monitor the reaction's progress using TLC. The addition of HCl halted immediately after the reaction, the liquid was placed into a container of ice water. to cool. Isolation of the solid from the ethanol by filtering, drying, and recrystallization. The chalcones that form as a consequence are called 2a-h.

All of the chalcones 3a–h follows the same method of preparation.

Schema 1 shows the process of chalcone production.



Where R = $-CH_3$ & -Cl Where R'= a. phenyl

b. 4 - hydroxy phenyl

c. 4 - Nitro phenyl

d. 4 - methoxy phenyl

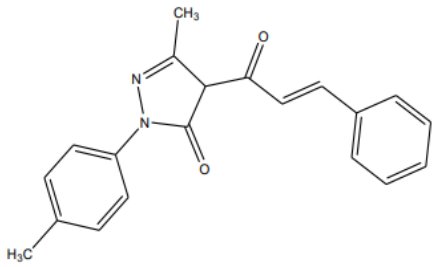
e. 2 - methyl phenyl

f. 4-chloro phenyl

g. 4 - bromo phenyl

h. 4-methyl phen

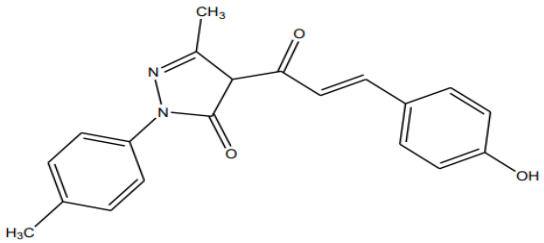
Compound -1a



6-methyl-4-(3-phenyl-acryloyl)-2-p-tolyl-2,4-dihydro-pyrazol-3-one is the compound in question.

Molecular formula: C20H18N2O2 Molecular weight: 318 gm/mol Melting point: 141-143 ^{0}C (uncorrected) Yield: 82%	**Elemental analysis** **%C** **% H** **% N** **Calculated** 75.45 5.70 8.80 **Found** 75.50 5.72 8.79
IR features around Cm^{-1} 2893 Aromatic C-H stretching 1669 C=O 1663,1593 α, β- unsaturated ketones 1605 C=N 1537 C=C	**^{1}H-NMR spectral features (δ-ppm)** 7.10-8.0 (9H,m, Ar-H) 6.88, 7.61 (2H,d, CH=CH) 3.2 (1H,s,Pyrazolone) 1.92 (3H,s,CH3) 2.4 (3H,s,CH3)

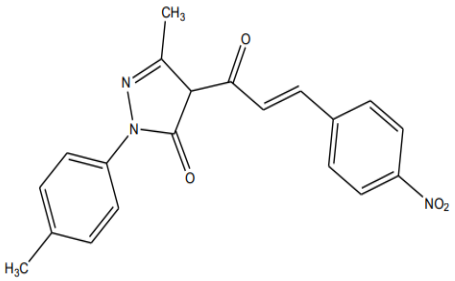
Compound -1b



4-[3-(4-hydroxy-phenyl)-acryloyl] is the formulation of the chemical. -5-methyl-2-p-tolyl-2,4-dihydro-pyrazol-3-one is the chemical formula.

Molecular formula: C20H18N2O3 Molecular weight: 334 gm/mol Melting point: 150-152 ^{0}C (uncorrected) Yield: 78%	**Elemental analysis** **%C** **% H** **% N** **Calculate** 71.84 5.43 8.38 **Found** 71.8 5.4 8.3
IR features around Cm^{-1} 3337 -OH (phenolic) 2896 Aromatic C-H stretching 1662 C=O 1658,1590 α, β- unsaturated ketones 1606 C=N 1542 C=C Ar	**^{1}H-NMR spectral features (δ-ppm)** 7.0-7.60 (8H, m, Ar-H) 6.91, 7.64 (2H, d, CH=CH) 3.40 (1H, s, Pyrazolone) 1.94 (3H, s,CH3) 2.35 (3H, s, CH3) 4.20 (1H, singlet, OH)

Compound -1c



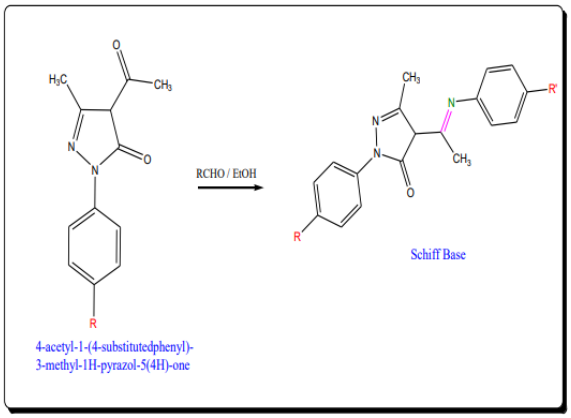
5-Methyl-4-[3-(4-nitro-phenyl)-acryloyl] 2-p-tolyl-2,4-dihydro-pyrazol-3-one are the compounds in question. -2-seven

Molecular formula: C20H17N3O4 Molecular weight: 363 gm/mol Melting point: 156-158 ^{0}C (uncorrected) Yield: 77%	**Elemental analysis** **%C** **% H** **% N** **Calculated** 66.11 4.72 11.56 **Found** 66.1 4.7 11.5
IR features around Cm^{-1} 2904 Aromatic C-H stretching 1674 C=O 1659,1596 α, β- unsaturated ketones 1609 C=N 1548 C=C conjugate	**^{1}H-NMR spectral features (δ-ppm)** 6.98-7.64 (8H, m, Ar-H) 6.94, 7.64 (2H, d, CH=CH) 3.35 (1H, s, Pyrazolone) 1.94 (3H,s,CH3) 2.37 (3H, s, CH3)

The Four-acetyl-1-(4-substitutedphenyl) compounds the compound -3-methyl-1H-pyrazol-5(4H) There are four Schiff bases, which are (4a-h), (5a-h), (6a-f), and (7a-f) were successfully isolated.

The phenyl group, 4-substituted, 3-methyl-1H-pyrazol-5(4H) After being subjected to a single molecule of a substituted radical, the amine in ethanol (0.01 mol), the reaction is refluxed for three to five hours. Refrigeration follows. A filtered, solid-yellow substance that has been washed with ethanol or methanol. Consequently, schiff bases 4a-h and 5a-h have been assigned. Similar procedures have been the various preparations were carried out thereafter 7a-h and 6a-h are Schiff bases.

Scheme 2 shows the formation of the Schiff base.



Compound -2a

Where R = -CH_3 & -Cl Where R'=

a. of phenyl

b. 4 - chloro phenyl

c. 3 - chlorophenyl

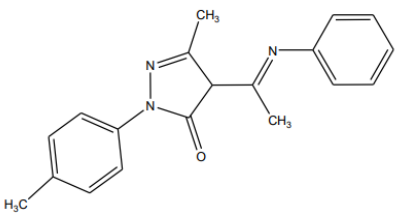
d. 4 - methyl phenyl

e. 4-nitro phenyl

f. isoniazide

g. 4 - methoxy phenyl

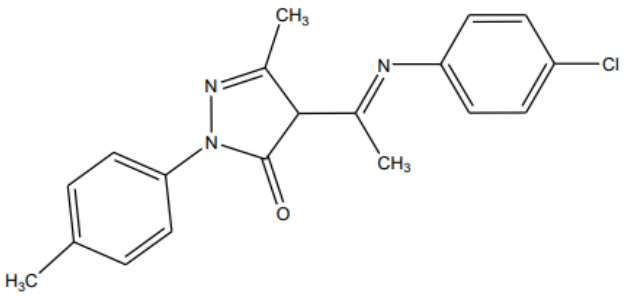
h.nicotinic acid



3-p-tolyl-2-methyl-4-(1-phenylimino-ethyl)-2, Four dihydropyrazol-3-one Five

Molecular formula : $C_{19}H_{19}N_3O$ Molecular weight : 305 gm/mol Melting point:212-214 ^{0}C (uncorrected) Yield: 82%	**Elemental analysis** **%C % H % N** **Calculated** 74.73 6.27 13.76 **Found** 74.7 6.3 13.78
IR features around Cm^{-1} 2893 Aromatic C-H stretching 1669 C=O 1605 C=N 1182 C-N str.	**^{1}H-NMR spectral features (δ-ppm)** 7.1-8.0 (9H,m, Ar-H) 2.4 (1H,s,Pyrazolone) 1.92 (6H,s,2CH_3) 2.30 (3H,s,CH_3)

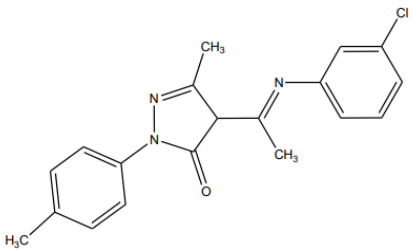
Compound -2b



Pyrazoline 4-[1-(4-chloro-phenylimino)-ethyl] is the name of the compound.3-one,5-methyl-2-p-tolyl-2,4-dihydro.

Molecular formula : $C_{19}H_{18}ClN_3O$ Molecular weight : 339 gm/mol Melting point:197-198 ^{0}C (uncorrected) Yield: 79%	**Elemental analysis** **%C % H % N** **Calculated** 67.15 5.34 12.37 **Found** 67.16 5.35 12.33
IR features around Cm^{-1} 2889 Aromatic C-H stretching 1672 C=O 1609 C=N 1186 C-N str. 763 C-Cl	**^{1}H-NMR spectral features (δ-ppm)** 7.35-7.80 (8H,m, Ar-H) 2.46 (1H,s,Pyrazolone) 1.94 (6H,s,2CH_3) 2.32 (3H,s,CH_3)

Compound -3c



the ethyl 4-[1-(3-chloro-phenylimino)]an alkyl2,4-dihydropyrazol-3-one -2-p-tolyl–

Molecular formula : $C_{19}H_{18}ClN_3O$ Molecular weight : 339 gm/mol Melting point:201-203 ^{0}C (uncorrected) Yield: 77%	**Elemental analysis** **%C** **% H** **% N** **Calculated** 67.15 5.34 12.37 **Found** 67.16 5.37 12.36
IR features around Cm^{-1} 2890 Aromatic C-H stretching 1666 C=O 1598 C=N 1180 C-N str. 766 C-Cl	**^{1}H-NMR spectral features (δ-ppm)** 7.37-7.82 (8H,m, Ar-H) 2.48 (1H,s,Pyrazolone) 1.94 (6H,s,2CH_3) 2.30 (3H,s,CH_3)

Conclusions

New pyrazole-ringed thiazole synthetic compounds and evaluated their antioxidant and antibacterial capabilities. These newly created chemicals P_{29} and P_{38} shown superior antibacterial Performance against all bacterial species at concentrations of 400 and 1000 µg/mL in compare and contrast with Streptomycin. With respect to Fluconazole, compounds P_{29} and P_{38} showed effectively inhibits the growth of all fungal strains at doses of 1000 and 500 microgrammes per millilitre, whereas others showed moderate activity. Six novel pyrazole-containing compounds have been developed. The compounds include pyrazoline, Triazole Schiff base, triazolothiadiazole, 1,3,4-oxadiazole, and thiazole. were used in the design.

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