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A comprehensive review on the pharmacological activities of pyrazoline derivatives

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Abstract
Pyrazoline derivatives represent an important class of five-membered nitrogen-containing heterocyclic compounds that have attracted considerable attention in medicinal chemistry because of their broad spectrum of pharmacological activities and favorable structural versatility. The pyrazoline scaffold serves as a valuable pharmacophore for the development of novel therapeutic agents through structural modifications that enhance biological activity, selectivity, and pharmacokinetic properties. This review provides a comprehensive overview of the pharmacological potential of pyrazoline derivatives, highlighting recent advances in their medicinal applications and structure-activity relationships. The reported literature demonstrates that pyrazoline-based compounds exhibit diverse biological activities, including anticancer, antimicrobial, anti-inflammatory, antioxidant, antitubercular, antiviral, antidiabetic, anticonvulsant, analgesic, antidepressant and antiparasitic effects. The review also discusses the influence of different substitution patterns on the pyrazoline nucleus in determining pharmacological efficacy and target specificity. Furthermore, recent developments in computational approaches, including molecular docking, molecular dynamics simulations, quantitative structure-activity relationship (QSAR) studies, and *in-silico* pharmacokinetic and toxicity predictions, are summarized to illustrate their role in the rational design and optimization of pyrazoline-based drug candidates. The integration of synthetic chemistry with biological evaluation and computational techniques has significantly accelerated the identification of promising lead molecules with improved therapeutic profiles. Despite the considerable progress achieved, challenges related to bioavailability, selectivity, toxicity and clinical translation remain to be addressed. Overall, pyrazoline derivatives continue to emerge as versatile and promising scaffolds for modern drug discovery, offering substantial opportunities for the development of safer and more effective therapeutic agents. This review aims to provide researchers with a comprehensive understanding of the pharmacological significance of pyrazoline derivatives and to highlight future research directions for their successful advancement into clinical applications.

Keywords: Pyrazoline derivatives, Pharmacological activities, Structure–activity relationship, Therapeutic agents

Introduction

Heterocyclic compounds constitute one of the most important classes of organic molecules in medicinal chemistry owing to their remarkable structural diversity and wide range of biological activities [1]. Among them, pyrazoline derivatives, characterized by a five-membered ring containing two adjacent nitrogen atoms, have emerged as privileged scaffolds for the discovery and development of novel therapeutic agents. Their unique chemical architecture allows extensive structural modifications, enabling the synthesis of derivatives with enhanced pharmacological efficacy, selectivity, and favorable pharmacokinetic properties [2]. Consequently, pyrazoline-based compounds have attracted considerable interest from researchers in pharmaceutical, medicinal, and synthetic chemistry.

Over the past few decades, numerous studies have demonstrated that pyrazoline derivatives possess a broad spectrum of pharmacological activities, including anticancer, antimicrobial, anti-inflammatory, antioxidant, antiviral, antitubercular, antidiabetic, anticonvulsant, analgesic, antidepressant, and antiparasitic properties. These diverse biological effects are primarily attributed to the ability of the pyrazoline nucleus to interact with multiple molecular targets involved in various pathological processes. Furthermore, the incorporation of different electron-donating or electron-withdrawing substituents into the pyrazoline framework has been shown to significantly influence biological activity, making structure–activity relationship (SAR) studies an essential component of pyrazoline-based drug development [3-4].

Recent advances in synthetic methodologies, computational drug design, and biological screening have further accelerated the identification of potent pyrazoline derivatives with improved therapeutic potential. Modern in silico techniques, including molecular docking, molecular dynamics simulations, quantitative structure–activity relationship (QSAR) analysis, and pharmacokinetic prediction, have become indispensable tools for optimizing lead compounds prior to experimental evaluation. These integrated approaches have enhanced the efficiency of drug discovery while reducing the time and cost associated with conventional drug development [5-7].

The present review aims to provide a comprehensive overview of the pharmacological activities of pyrazoline derivatives by summarizing recent literature on their medicinal applications, synthetic developments, and structure–activity relationships. In addition, the review highlights emerging computational strategies and discusses the challenges and future prospects associated with the development of pyrazoline-based therapeutics. Collectively, this review serves as a valuable resource for researchers seeking to advance the design and development of

pyrazoline derivatives as promising candidates for the treatment of a wide range of human diseases.

Chemistry of Pyrazoline

Pyrazoline is a five-membered nitrogen-containing heterocyclic compound composed of three carbon atoms and two adjacent nitrogen atoms within the ring. It is a partially saturated analogue of pyrazole, containing one endocyclic double bond, and exists as three Regio isomeric forms: 1-pyrazoline, 2-pyrazoline, and 3-pyrazoline [8-11]. Among these, 2-pyrazoline is the most stable and extensively investigated because of its remarkable pharmacological potential and synthetic versatility. The pyrazoline nucleus serves as a privileged scaffold in medicinal chemistry, allowing the introduction of diverse electron-donating and electron-withdrawing substituents that significantly influence its physicochemical and biological properties [12-14]. Pyrazoline derivatives are commonly synthesized through the cyclization of α,β-unsaturated ketones (chalcones) with hydrazine or substituted hydrazines under acidic or basic conditions. The presence of nitrogen atoms and the flexible substitution pattern enable pyrazoline derivatives to interact effectively with various biological targets through hydrogen bonding, hydrophobic interactions, and π–π stacking. These structural characteristics have made pyrazoline derivatives attractive candidates for the development of novel therapeutic agents with diverse pharmacological applications [15].

Pharmacological Activities

Lamya Al-Wahaibi H *et al*., (2023) they reported that new Bis-pyrazoline hybrids were designed, performed molecular docking studies against EGFR and BRAF ^{V600E}, synthesized using conventional methods and screened for *in-vitro* anticancer activity against four cell lines MCF-7(breast cancer cell line), Panc-1(pancreatic cancer cell line), A-549(lung cancer cell line) and HT-29(colon cancer cell line) by MTT assay method. Among those Compound 1 shows potent activity for all the cell lines with IC_{50} value of 1.05 µM when compared with the standard drug Erlotinib [16].

Monica Kamel G *et al.,* (2024) they reported new pyrazole derivatives were synthesized by using conventional method and screened for *in-vitro* anticancer activity against pancreatic cancer (PaCa-2), breast cancer (MCF-7), prostate cancer (PC3) and normal cell lines (BJ1) by comet assay method. Among those Compound 2 shows

Potent activity for all the celllines when compared with Doxorubicin as a standard drug with IC_{50} value 28.3mg/mL[-117].

Manar Salem G *et al., (*2024) they reported new pyrazole derivative were designed, performed molecular docking studies against VEGFR2/CDK-2 inhibitors synthesized using conventional method screened for both *in-vitro* and *in-vivo* as anticancer activity HepG2 cancer cells by MTT assay method. Among those Compound 3 shows potent activity for all the cell IC50 value of 4.18 µM when compared with Sorafenib and Roscovitine as a Standard drug [18].

Devidas Pawar C *et al*., (2022) they reported Pyrazole-3,5 diamine Derivatives synthesized using conventional method and screened for *in-vitro* anti-tubercular activity against *Mycobacterium tuberculosis* H37RV strain by MTT assay method. Among those Compound 4 shows excellent activity for all the cell with IC_{50} value of 12.5±0.61µg/ml when compared with Pyrazinamide, Isoniazid, Ethambutol and Streptomycin as a standard drug [19].

Saritha Keerthi *et al*., (2025) they reported Novel Pyrazole Derivatives synthesized using conventional method screened for *in-vitro* anti-tubercular activity against *Mycobacterium tuberculosis* H37Rv by MTT assay method. Among those Compound 5 shows potent activity for all the cell with IC_{50} value of 1.56mg/mL when compared with the standard drug Ethambutol [20].

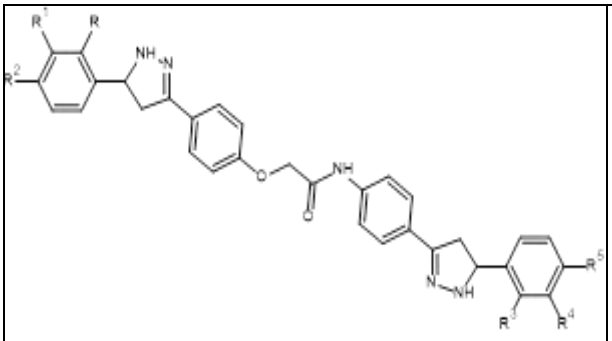
Kok Tong Wong *et al., (*2022) they reported New 3,5-Disubstituted pyrazole-1- Carbothioamides were designed performed molecular docking studies against dihydrofolate reductase, synthesized using conventional methods screened for *in vitro* anti-tubercular activity against *Mycobacterium tuberculosis* H37Ra by using Tetrazolium microplate assay (TEMA) method. Among those Compound 6 shows potent activity for all the cell with IC_{50} 650–530µM when compared with the standard drug Isoniazid [21].

Suhailah Aljameel S *et al., (2026)* they reported multi-targeted pyrazole scaffolds synthesized using conventional methods screened for *in-vitro* anti-inflammatory activity against Hela cells by using MTT assay method. Among those Compound 7 shows potent activity for all the cell IC_{50} 62.5 µg/mL when compared with the standard drug Aminophenazone [22].

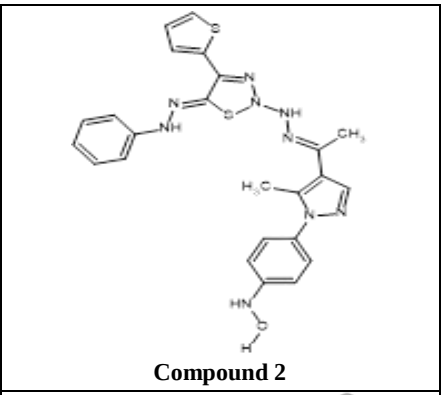
Monika Sihag *et al., (2024*) they reported pyrazole and pyrazoline derivatives were designed performed molecular docking studies against COX-II enzyme using conventional methods screened for *in-vitro* anti-inflammatory activity against VERO cell line by using bovine serum albumin assay. Among those Compounds 8 shows potent activity for all the cell IC_{50} 0.5 mg/mL when compared with the standard drug Celecoxib [23].

Sucheta Singh *et al., (2022)* they reported bispyrazole derivatives synthesized using conventional methods screened for *in-vitro* anti-inflammatory activity against micro-organisms, pro-oxidants by using protein albumin denaturation assay. Among those Compound 9 shows potent activity IC_{50} =63.78mol/L when compared with the standard drug Aspirin [24].

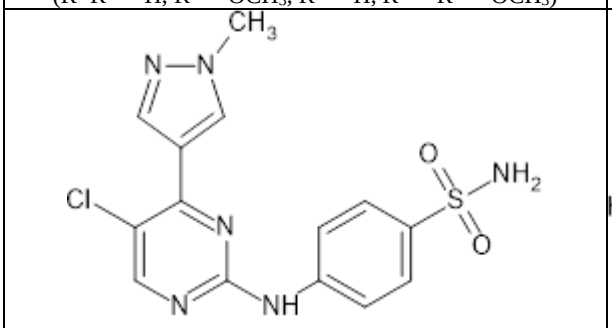
10. Christina Zalaru *et al., (2026)* they reported Novel Pyrazole Derivatives synthesized conventional methods screened for *in-vitro* anti-microbial activity against planktonic microbial cells by using MTT assay. Among those Compound 10 shows potent activity IC_{50} 0.046 µg/mL when compared with the standard drug Sulfaphenazole [25].



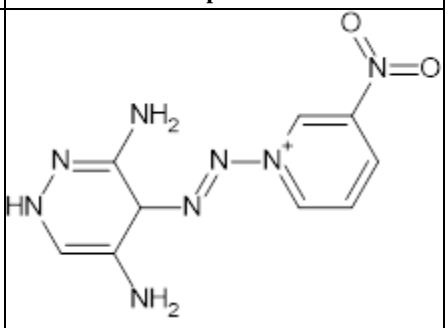
Compound 1
(R=R [1]=H, R [2]=OCH_3, R [3]=H, R [4]=R [5]=OCH_3)



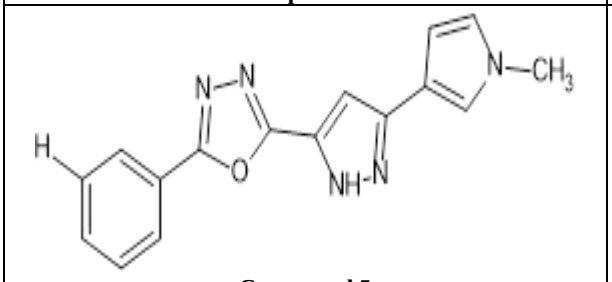
Compound 2



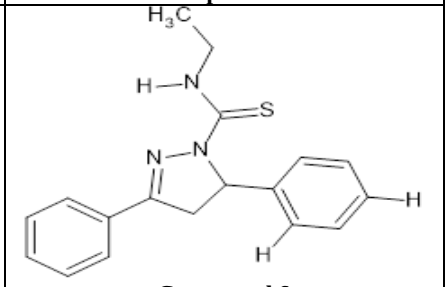
Compound 3



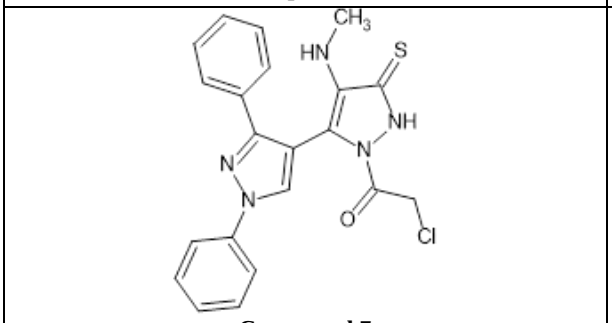
Compound 4



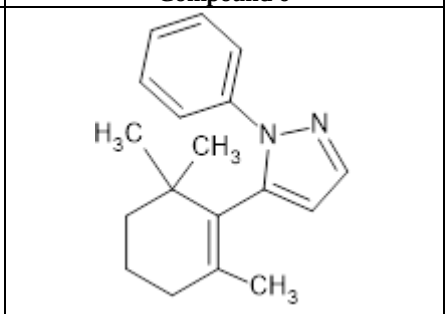
Compound 5



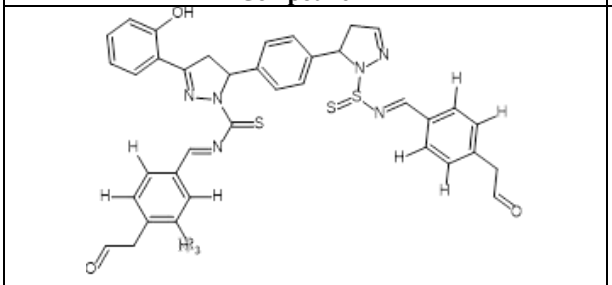
Compound 6



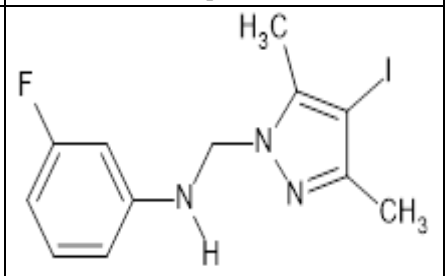
Compound 7



Compound 8



Compound 9



Compound 10

Idhayadhulla Akbar *et al., (2023)* they reported pyrazolo[3,4-c] pyrazole derivatives were designed performed molecular docking studies against dihydrofolate reductase enzyme, synthesized using conventional methods and screened for *in-vitro* anti-microbial activity against *Escherichia Coli* by MTT assay. Among those Compound shows potent activity IC_{50} 10mgmL $^{-1}$ when compared with the standard drug Ciprofloxacin [26].

Ahmed Raga *et al.,* (2023) they reported Novel Pyrazole and Pyrazolo[1,5-a] pyrimidine derivatives were designed performed molecular docking studies, synthesized using conventional methods and screened for *in-vivo* anti-microbial activity against six clinically isolated multidrug resistance by MTT assay. Among those Compound 12 shows potent activity IC_{50} 92.34nM when compared with the standard drug Erythromycin and Amikacin [27].

Ahmed El-Sewedy *et al*., (2025) they reported newly synthesized pyrazole derivatives were designed performed molecular docking studies against targeting immune receptor TLR4 protein revealed that compound 13 achieved the highest docking score, Synthesized using conventional methods and screened for *in vitro* anti-viral activity against NDV by assessing their ability to inhibit virus-induced haemagglutination by MTT assay. Among those Compound 13 shows potent activity IC_{50} 200 to 800 µL when compared with standard drug Amantadine [28].

Zhi-Wei Lei *et al., (2022)* they reported Synthesized Novel Sulfonate scaffold-Containing Pyrazole carbamide Derivatives, synthesized using conventional methods and screened for *in-vivo* anti-viral activity against four plant pathogens *C. Camelliae*, *P. theae*, and *R. solani* by bioassay. Among those Compound 14 shows excellent activity IC_{50} 0.45mg/L when compared with standard drug Ningnanmycin [29].

Abdulmalik Shehu *et al*., (2026) they reported Heteroaryl p-Methyl N-Acetyl

Pyrazoline Derivatives synthesized using conventional methods and screened for *in-vitro* anti-oxidant activity against 2,2-diphenyl-2 picrylhydrazyl by DPPH assay. Among those Compound 15 shows potent activity IC_{50} 5.35±0.60 µM when compared with standard drug Ascorbic acid [30].

Wafaa Yusuf Khalaf *et al., (2023)* they reported New Coumarin-Pyrazoline Derivatives synthesized using conventional methods and screened for *in-vitro* anti-oxidant activity by ABTS assay. Among those Compound 16 shows potent activity IC_{50} 12.76 µg/ml when compared with standard drug Ascorbic acid [31].

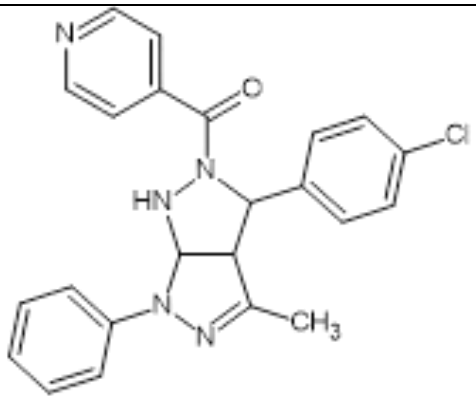
Wesam Shehab S *et al.,* (2025) reported the synthesis of new fused pyrazole derivatives and evaluated for their *in-vitro* anti-bacterial, anti-fungal, antioxidant activity.

The Compound 17 showed strong antioxidant capacity (87.6 % ABTS inhibition) compared to Ascorbic acid as a standard drug by using ABTS method and also showed antifungal activity against *Candida albicans* (15.6 mm/mg) and *Aspergillus flavus* (7.8 mm/mg) as compare to Ampicillin and Clotrimazole (5.8 ± 0.07 3.9 ± 0.23mm/mg) by using Kirby-Bauer diffusion method [32].

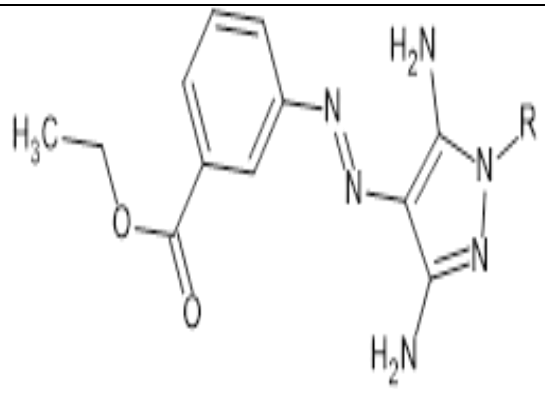
Maria Isabel Murillo *et al., (2025)* they reported Pyrazole Derivatives, were designed performed molecular docking studies against potential targets synthesized using conventional methods and screened for *in vitro* anti-fungal activity against *C. albicans* and *C. neoformans* by MTT assay. Among those Compounds 18 shows potent activity IC_{50}6.83 µg/mL compared with standard drug Amphotericin B [33].

Chandra Shekhar Yadav *et al., (2025)* they reported Synthesis, characterization and bio-evaluation of novel series of pyrazoline derivatives were designed performed molecular docking studies synthesized using conventional methods and screened for *in-vitro* anti-fungal activity against five bacterial strains (*Pseudomonas aeruginosa*, *Klebsiella pneumoniae*, *Escherichia coli*, *Staphylococcus aureus*, and *Acinetobacter baumannii*) and three fungal strains (*Candida tropicalis*, *Candida parapsilosis*, and *Candida albicans*) by Haemolysis assay. Among those Compounds 19 shows potent activity MIC value of 6.25 µg/mL when compared with the standard drug Fluconazole [34].

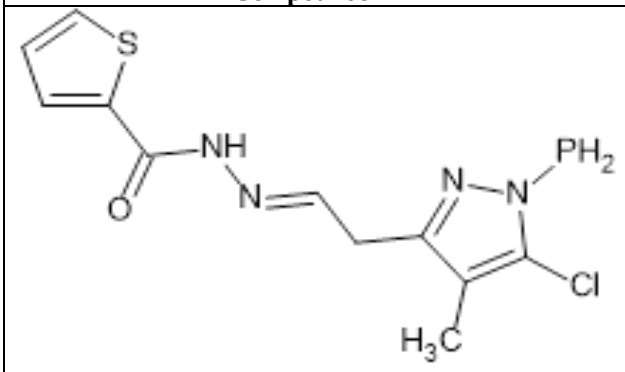
Oluwakemi Ebenezer *et al., (2022)* they reported Pyrazole Derivatives Synthesis and Biological Evaluations of Pyrazole Derivatives were designed performed the synthesized by using conventional methods and screened with *in-vivo* antifungal activity Among those Compounds 20 shows potent activity in IC_{50} 71.00 µM when it compared with the standard drug Cycloheximide [35].



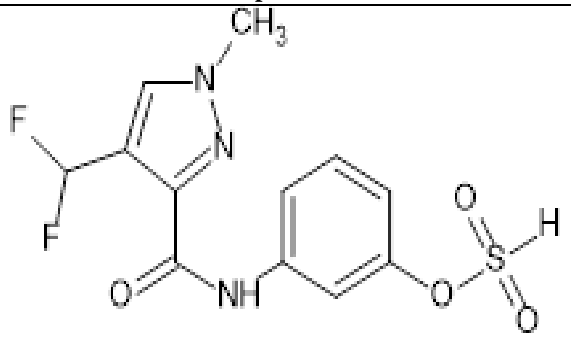
Compounds 11



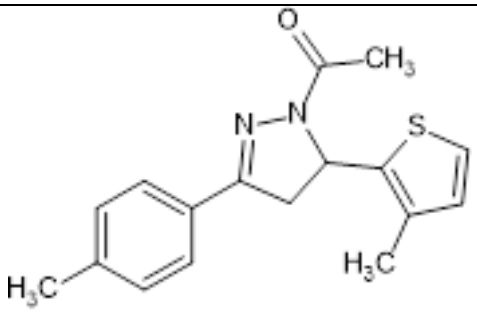
Compounds 12



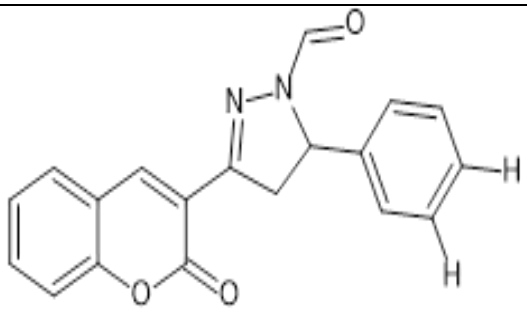
Compounds 13



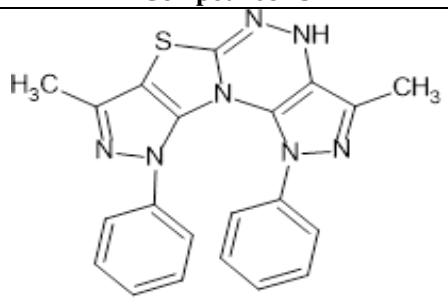
Compounds 14



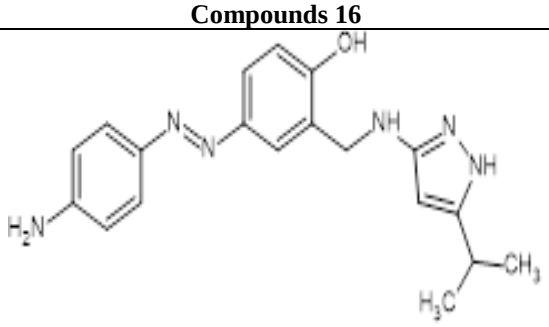
Compounds 15



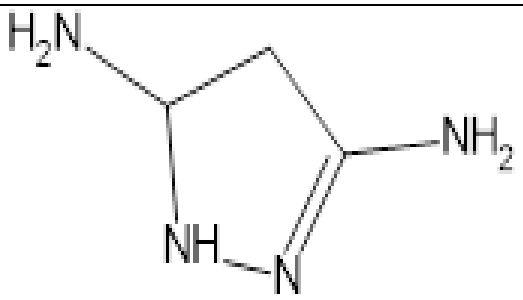
Compounds 16



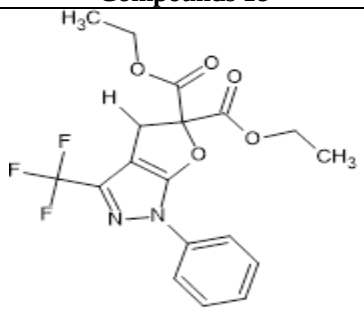
Compounds 17



Compounds 18



Compounds 19



Compounds 20

Halimah Syaadiyah *et al.,* (2026) they reported pyridine-containing N-phenyl pyrazoline derivatives were designed performed docking study was conducted to investigate interactions between all compounds and the PfENR receptor as an antimalarial target by using conventional methods and *in vitro* anti-malarial activity evaluation against *P. falciparum* 3D7 and FCR-3 strains by MTT assay. Among those Compounds 21 shows potent activity IC_{50} of 6.70 µ M compared with standard drug Chloroquine [36].

Adnan Bekhit A *et al*., (2021) they are reported Antileishmanial Agents Derivatives were designed performed synthesized using conventional methods and screened for both *in-vitro* and *in-vivo* antimalarial activity against MTT assay. Among those Compound 22 show the potent activity IC_{50} 1.6622 µ M compared with standard drug Amphotericin [37].

Viktor Zapols kii A *et al.,* (2022) they reported persubstituted chloroquinolinyl-1H-
pyrazoles and evaluation of their antimalarial, anti-SARS-CoV-2, antibacterial and cytotoxic derivatives were designed performed by using conventional methods *in vitro* anti-malarial activity against the protozoan malaria parasite *Plasmodium falciparum* by ABTS assay. Among those Compounds 23 shows potent activity EC_{50} of 0.2 ± 0.1 µM compared with standard drug Chloroquine [38].

Bedriye Seda Kursun Aktar *et al., (2025)* they reported Novel Pyrrolidine-Based Pyrazolines derivatives were designed performed molecular docking studies synthesized using conventional methods and screened for *in-vitro* anti diabetic activity against α-amylase and α-glucosidase by α-amylase assay. Among those Compound 24 shows potent activity IC_{50} value of 52.79±6.00µM when compared with the standard drug Acarbose [39].

Mohamed Amine Ben Abdallah *et al.,* (2025) they reported novel pyrazoles and pyrazolines derivatives were designed performed molecular docking studies synthesized using conventional methods and screened for *in-vitro* anti diabetic activity against human lysosomal acid α-glucosidase (HLGAA) proteins with PDB IDs: 5NN5, 5NN6 and 5NN8 *in-vitro* enzyme inhibition assay. Among those Compound 25 shows potent activity binding affinities, ranging from –7.0 to –10.2 kcal/mol when compared with the standard drug Acarbose [40].

Ahmed Naglah M *et al., (2024)* they reported Pyrazole-Based Schiff Bases derivatives were designed and performed synthesized using conventional methods and screened for *in-vitro* anti-diabetic activity against α-amylase and α-glucosidase Enzymatic assay Among those Compound 26 shows potent activity inhibitory effect 31.24 ± 0.05 when compared with the standard drug Acarbose [41].

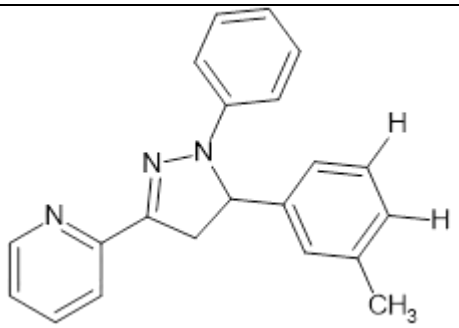
Jitendra Kumar Chaudhary *et al.,* (2021) they reported New 1,3,5 Trisubstituted-2-Pyrazolines Derivatives were designed performed the synthesized using conventional methods and screened for *in-vivo* anti analgesic activity. Among those Compound 27 shows the potent activity and they shows the hot plate test in 9.10 when compared with the standard drug pentazocine [42].

Adnan Bekhit A *et al.,* (2022) they reported pyrazole derivative were designed and performed the synthesized by conventional methods and screened both *in-vitro* anti

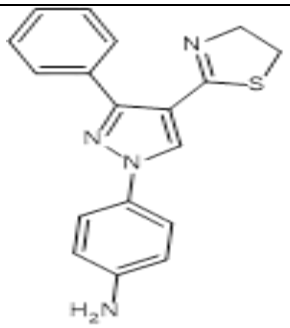
analgesic activity. Among those Compound 28 shows the potent activity and compared with standard drug is Methacin [43].

Vishal S *et al* (2022) they reported Analgesic activities of Some Pyrazolo[3,4-c],

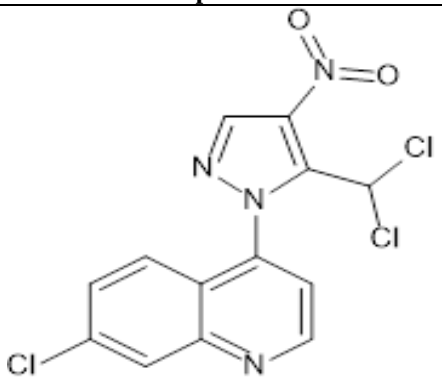
Pyrazole derivatives performed the synthesized by conventional methods and screened both *in-vitro* and *in-vivo* anti analgesic activity. Among those Compound 29 shows the potent activity and compared with standard drug is pentazocine [44].



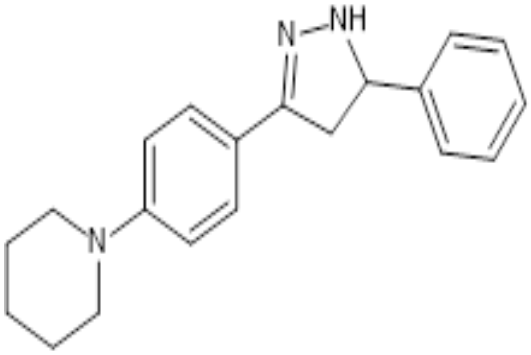
Compound 21



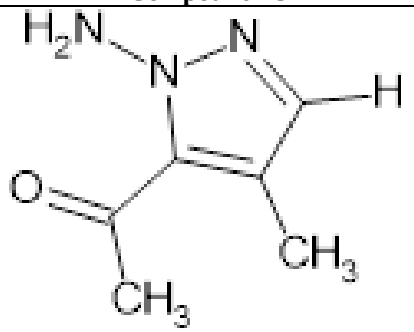
Compound 22



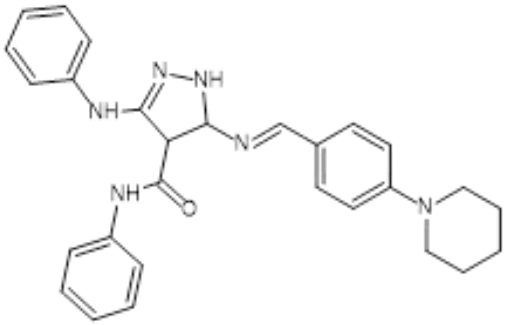
Compound 23



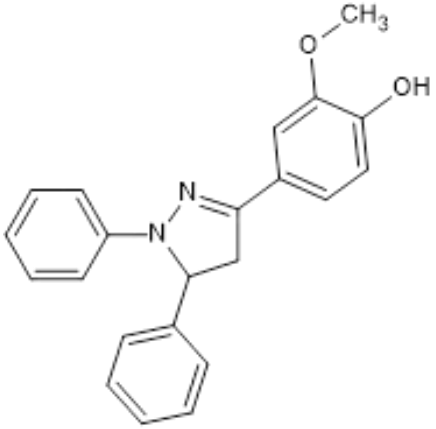
Compound 24



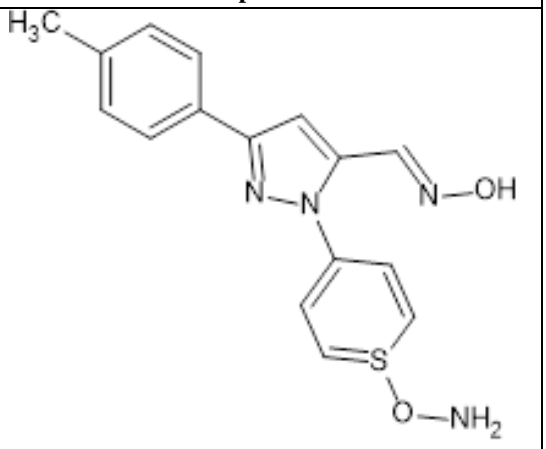
Compound 25



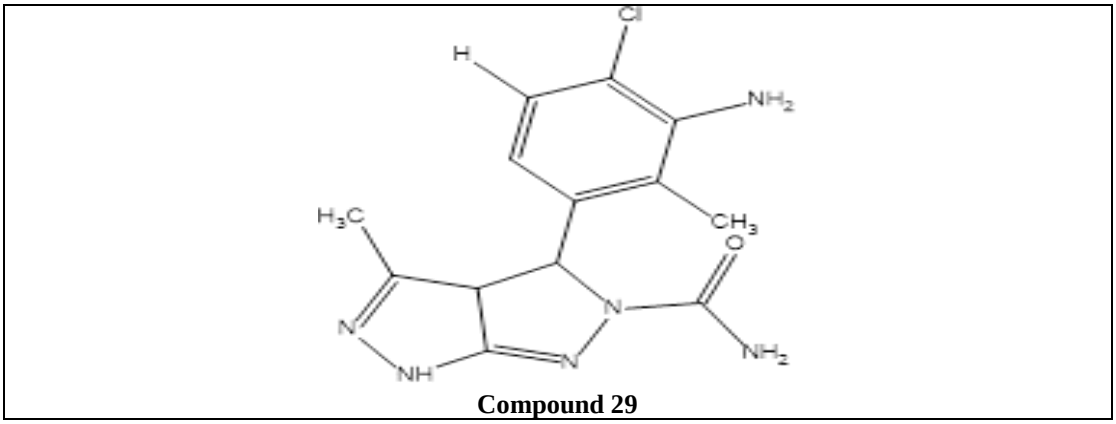
Compound 26



Compound 27



Compound 28



Compound 29

Conclusion

Pyrazoline derivatives have emerged as highly promising heterocyclic scaffolds in medicinal chemistry owing to their broad spectrum of pharmacological activities and favorable structural versatility. Extensive research has demonstrated their potential as anticancer, antimicrobial, anti-inflammatory, antioxidant, antiviral, antidiabetic, anticonvulsant, and analgesic agents. Advances in synthetic methodologies, structure–activity relationship studies, and computational drug design have significantly accelerated the identification and optimization of potent pyrazoline-based lead compounds. Nevertheless, further preclinical and clinical investigations are essential to establish their safety, efficacy, and pharmacokinetic profiles. Overall, pyrazoline derivatives remain valuable candidates for the development of innovative and effective therapeutic agents for diverse human diseases.

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