International Journal of Research in Pharmacy and Pharmaceutical Sciences
www.pharmacyjournal.in
ISSN: 2455-698X
Received: 02-12-2025, Accepted: 01-01-2026, Published: 15-01-2026
Volume 11, Issue 1, 2026, Page No. 7-15

Emerging pyrazole and quinazoline derivatives as bioactive scaffold: Synthesis and pharmacological evaluation

Pallavi K M*, Rashmi T
Department of Pharmaceutical Chemistry, Bharathi College of Pharmacy, Bharathinagara, Maddur Taluk, Mandya, Karnataka, India

Abstract
Pyrazole and quinazoline heterocycles have emerged as privileged scaffolds in medicinal chemistry due to their remarkable structural versatility and broad spectrum of biological activities. These frameworks possess favorable electronic and steric properties that enable effective interactions with a variety of therapeutic targets. This review presents a comprehensive overview of recent progress in the synthesis and pharmacological evaluation of pyrazole and quinazoline derivatives. Emphasis is placed on modern synthetic methodologies, including microwave-assisted, multicomponent, one-pot and green chemistry approaches, which facilitate the efficient construction of structurally diverse analogues. Structure activity relationship (SAR) studies are critically discussed to highlight the impact of substitution patterns on biological potency and selectivity. Pyrazole and quinazoline derivatives have demonstrated significant pharmacological activities such as anticancer, antimicrobial, anti-inflammatory, antiviral, antidiabetic and kinase inhibitory effects, with particular relevance to targets like epidermal growth factor receptor (EGFR), cyclooxygenase (COX) and microbial enzymes. Overall, this review underscores the continued importance of pyrazole and quinazoline derivatives as key scaffolds in the rational design of next-generation bioactive agents.

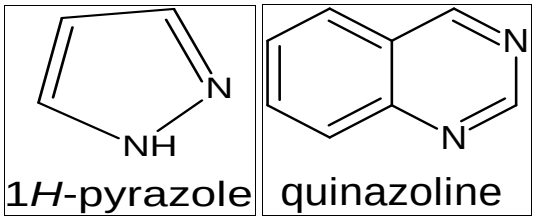
Keywords: Pyrazole derivatives, quinazoline derivatives, structure activity relationship, molecular docking, pharmacological evaluation

Introduction

Heterocyclic compounds constitute a significant portion of biologically active molecules in medicinal chemistry. Their structural diversity and ability to interact with biological targets through hydrogen bonding, π-stacking and hydrophobic interactions make them valuable cores in drug development [1, 2]. Among them, nitrogen-containing heterocycles, especially five- and six-membered rings, exhibit a wide spectrum of pharmacological activities including anticancer, antimicrobial, antiviral and anti-inflammatory properties. Their incorporation into drug-like molecules enhances bioavailability, selectivity and pharmacokinetic profiles [3].

Pyrazole, a five-membered aromatic heterocyclic ring with two adjacent nitrogen atoms at 1st and 2nd position and it is planar, aromatic and electron-rich structure contribute to chemical stability and biological reactivity. Chemically, pyrazole ($C_3H_4N_2$) undergoes electrophilic substitution at the C-4 position and allows N-alkylation or acylation at the N-1 position, offering flexibility for structural modifications [4]. These properties enable the formation of strong hydrogen bonds and π–π interactions with biological targets. Its versatile reactivity and proven therapeutic relevance form the basis for selecting pyrazole as a scaffold [5].

On the other hand, Quinazoline is a bicyclic aromatic compound composed of a benzene ring fused with a pyrimidine ring, containing nitrogen atoms at 1st and 3rd positions [6]. Quinazoline ($C_8H_6N_2$) is chemically reactive, particularly in electrophilic substitution on the benzene ring allowing for diverse structural modifications [7]. Its planar, rigid structure and electron-rich nature make it favourable for strong binding to enzyme targets. Continued research into novel synthetic stratergies and SAR is a crucial for developing next-generation therapeutics based on quinazoline scaffold [8].



Synthetic approach of pyrazole and quinazoline derivatives

1. Mohit Kotnala [9] *et., al* have synthesized pyrazole derivatives by cyclization reaction of 1,3-diketones with hydrazines yield dimethyl pyrazole. The process proceeds through hydrazine's nucleophilic attack on the carbonyl group, followed by ring closure and dehydration to form the pyrazole. [Fig. 1: (a)]
2. Hamada S A [10] *et., al* (2024) have synthesized pyrazole-based Schiff bases (1-phenyl-3-p-tolyl-1H pyrazole-4-carbaldehyde) by condensation reaction between pyrazole aldehyde and aromatic amine in methylene chloride were stirred until a clear solution. Then triethylamine was added, and the reaction was refluxed and solvent was removed under reduced pressure. Recrystallized from ethanol. [Fig. 1: (b)]
3. A E Khairulah [11] *et., al* (2024) have synthesized novel pyrazole derivatives by the Claisen–Schmidt reaction by cyclization reaction of chalcones with hydrazine hydrate in ethanol in the presence of a 10% sodium hydroxide solution. [Fig. 2: (c)]
4. Norhan Yasser [12] *et., al* (2024) have synthesized pyrazolyl-chalcone (1-(3-(Thiophen-2-yl)-1H-pyrazol-4-yl) ethan-1-one) by Claisen-Schmidt condensation by chlorination of thiophene 2-carbohydrazide gave thiophene-2 carbohydrazonoyl chloride. The treatment

of acetyl acetone in an ethanolic sodium ethoxide solution, is produced via the intermediary of nitrilimine. [Fig. 2: (d)]

5. Salma Mortada [13] *et., al* have synthesized 2-pyrazole derivatives by condensation reaction of pyrazole hydrazine and phenyl iso-cyanate under reflux of methanol to form (pyz-1). Pyz-2 is treated with CS_2 in ethanol in presence of KOH to form intermediate the carbodithioate salt. This intermediate was then converted to the triazole–thiol derivative through reaction with hydrazine hydrate under reflux of ethanol give pure Pyz-2. [Fig. 2: (e)]
6. Monika Sihag [14] *et., al* (2024) have reported the synthesis of pyrazole derivatives of β-ionone and phenyl hydrazine through oxidative C–H amination reaction by intramolecular cyclization of hydrazone derivatives mediated by hypervalent iodine reagent in HFIP solvent. The reaction completes within 5min at room temperature. pyrazoline synthesis is also achieved using hydrochloride salt of hydrazines undergo oxidative dehydrogenation using PIDA in dichloromethane yielded corresponding pyrazoles. [Fig. 2: (f)]
7. Rabindra Nath Das [15] *et., al* (2024) have synthesized bis-quinazoline derivatives. Initially, two moles of anthranilic acid were condensed with pyridine-2,6-dicarboxylic acid using methane sulfonyl chloride and pyridine to form bis-benzoxazin. Amination of bis-quinazolinone was refluxed with thionyl chloride to give bis-chloro-quinazoline. Coupling with substituted amines provided the final bis-quinazoline derivatives. [Fig. 3: (g)]
8. Maryam Moghtader Mansouri [16] *et., al* (2025) have synthesized 3-substituted phenyl quinazoline derivatives reaction between anthranilic acid with phenyl isocyanates to form 3(2-mercapto-3-phenyl quinazolin-4(3H)-one which was then methylated to form 2-methylthio-3-phenyl quinazolin-4(3H)-one. This intermediate coupled with hydrazine hydrate and urea derivatives in DMF. [Fig. 3: (h)]
9. Leila Emami [17] *et., al* (2022) have synthesized series of quinazoline derivatives by reacting with anthranilic acid and chloroacetyl chloride in dichloromethane and di-isopropyl ethylamine (DIPEA) to form benzoxazine intermediate. The resulting intermediate was coupled with 4-benzyl piperidine in acetonitrile using base DIPEA. [Fig. 3: (i)]
10. Citldi Vazues [18] *et., al* (2024) have synthesized quinazoline-2,4,6-triamine by cyclization reaction of 2-amino-5-nitro benzonitrile with guanidine carbonate to form 6-nitro quinazoline-2,4-diamine followed by hydrogenation over palladium/carbon. [Fig. 3: (j)]
11. M S Raghu [19] *et., al* (2023) have synthesized quinazoline based thiazole derivatives by condensation reaction between 1-(4-hydroxyquinazolin-7yl) thiourea and 7-aminoquinazolin-4-ol and ammonium thiocyanate under acidic condition. [Fig. 3: (k)]
12. Reda R. Mabrouk [20] *et., al* (2025) have synthesized quinazoline based derivatives by cyclization reaction of 4-chloro (or 4-nitro)-2-aminobenzoic acid with formamide to give the substituted quinazolin-4(3H)-ones, then converted into their potassium salts using potassium hydroxide. Meanwhile, unsubstituted or substituted anilines were reacted with chloroacetyl chloride in cold DMF to form the corresponding 2-chloro-N-phenylacetamide intermediates. Finally, each potassium salt was heated with its respective phenylacetamide intermediate in DMF. [Fig. 4: (l)]

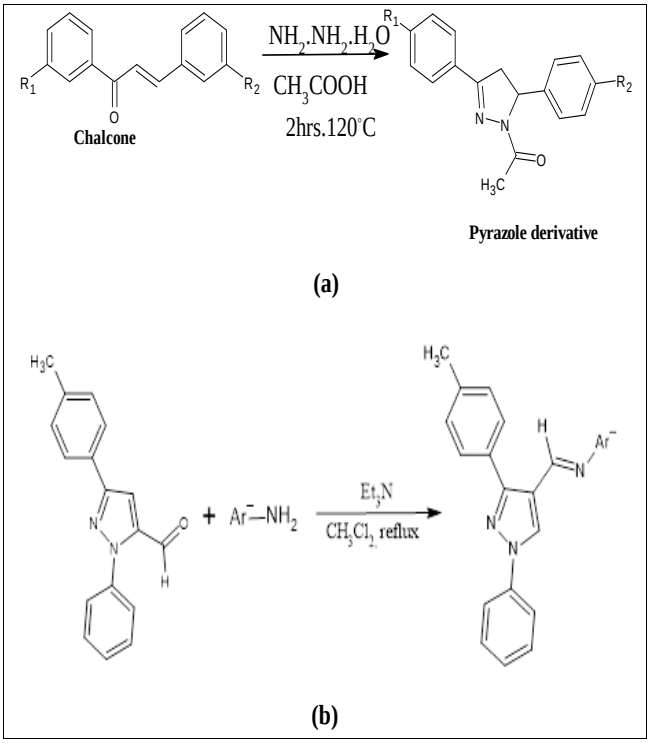


Fig 1: synthesis of pyrazole derivatives

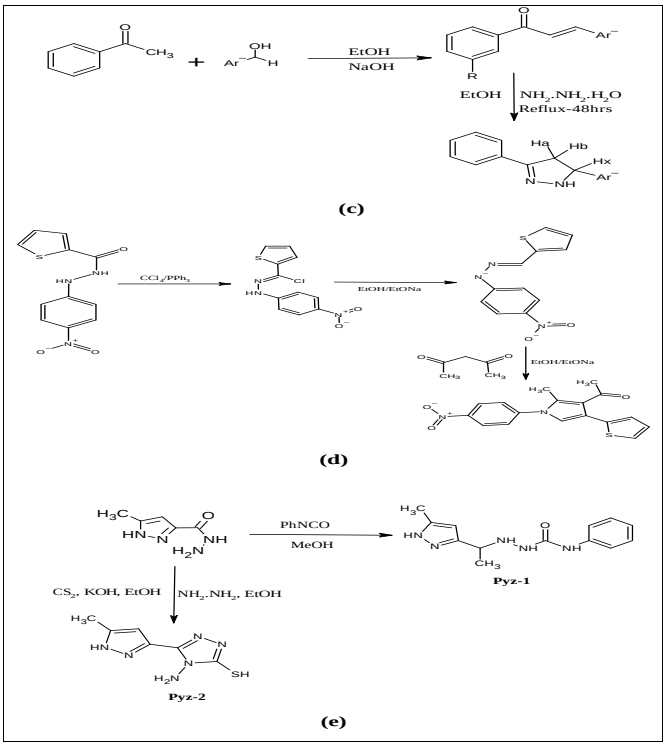


Fig 2: synthesis of pyrazole derivatives

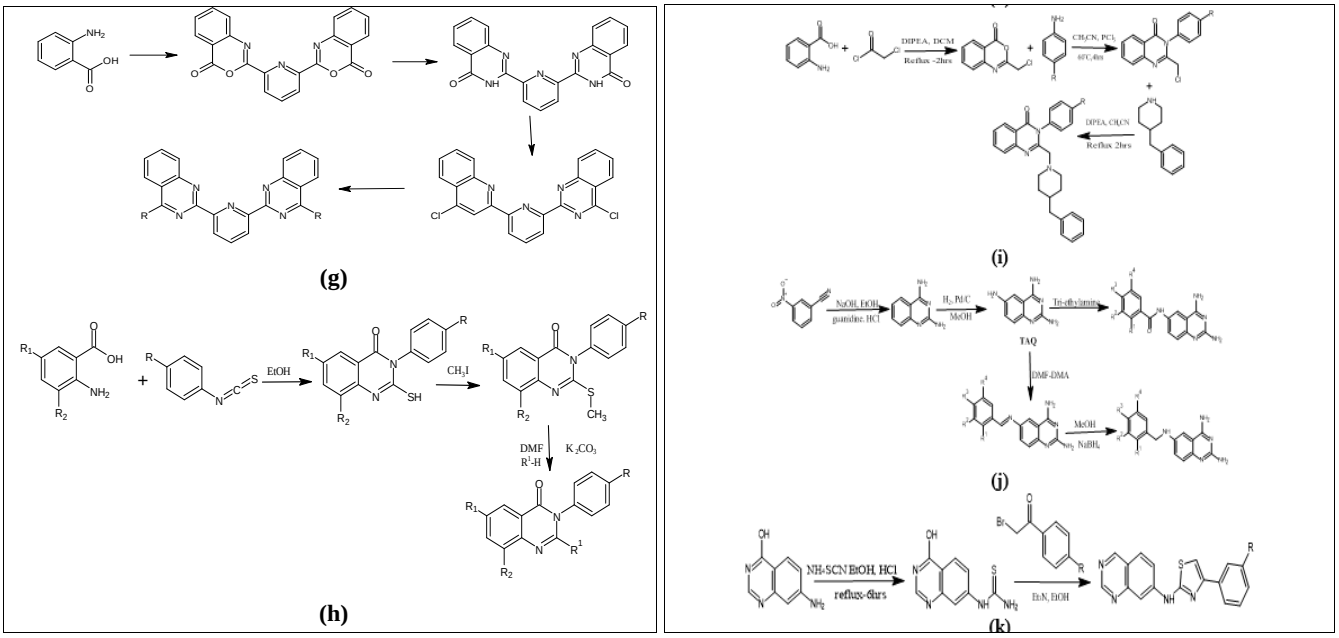


Fig 3: synthesis of quinazoline derivatives

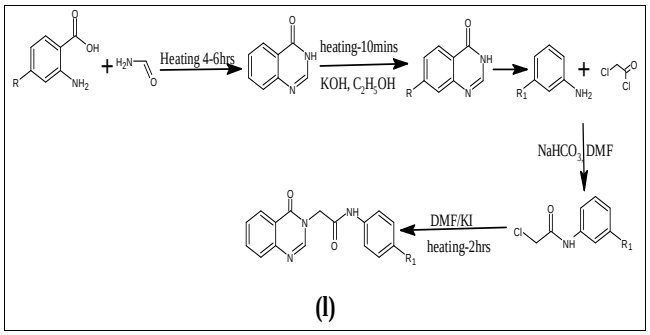


Fig 4: synthesis of quinazoline derivatives

Pharmacological significance of pyrazole and quinazoline derivatives

Pyrazole and quinazoline based compounds are significant in pharmaceutical chemistry because of their broad range of medicinal and therapeutic activities such as, anti-cancer, anti-viral, anti-inflammatory, anti-diabetic, anti-tuberculosis, antibacterial, anti-fungal and other activities. Certain synthesized compounds having pyrazole and quinazoline moieties exhibited anti-cancer activity such as epidermal growth factor receptor (EGFR) inhibitory activity with half maximal inhibitory concentration (IC_{50}) values equal to known drugs.

Table 1: Pyrazole based marketed drugs

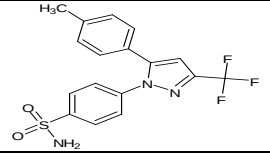
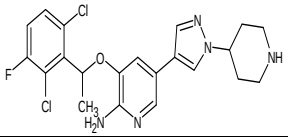
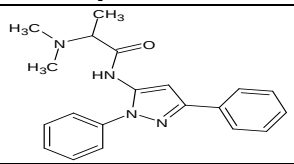
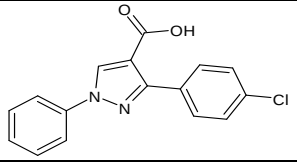
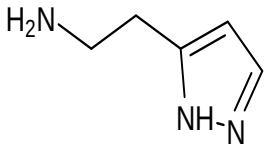
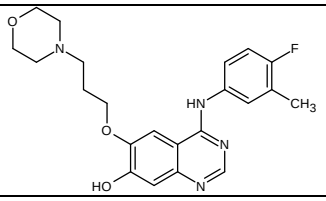
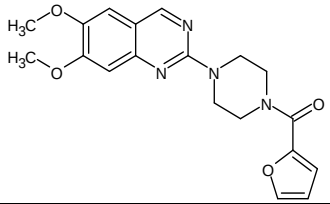
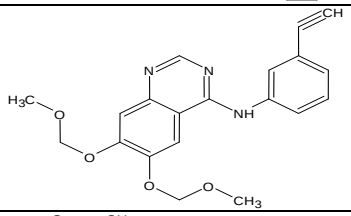
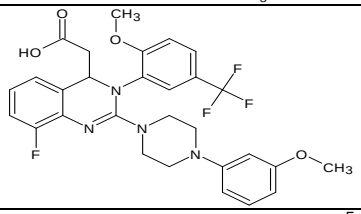
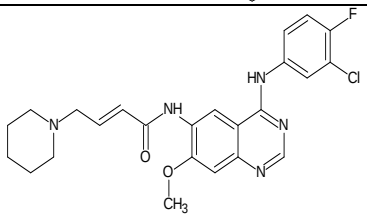
Sl. No	Commercial name	Structure	Uses	Ref.
1.	Celecoxib		Anti-inflammatory	21
2.	Crizotinib		Anti-cancer	22
3.	Diphenamizole		Analgesic	23
4.	Lonazolac		Anti-inflammatory	24
5.	Betazole		H_2-receptor agonist	25

Table 2: Quinazoline based marketed drugs

Sl. No	Commercial name	Structure	Uses	Ref.
1.	Gefitinib		For treatment of non-small cell lung cancer.	26
2.	Prazosin		For high blood pressure	27
3.	Erlotinib		For treatment of non-small cell lung cancer, pancreatic cancer and several other type of cancer.	28
4.	Letermovir		Antiviral drug	29
5.	Vandetanib		Antagonist of the vascular endothelial growth factor receptor	30

Biological activities of pyrazole and quinazoline derivatives

1. Nargisbano A [31] *et., al* (2024) reported a series of methoxy substituted pyrazole based pyrazoline derivatives were synthesized and evaluated for their *in-vitro* anti-inflammatory, antioxidant, antidiabetic, and antibacterial activities. Among the series, the compound-1a (72.22%) and compound-1b (66.22%) showed better anti-inflammatory activity as compared to diclofenac sodium (90.21%) as a standard drug by using protein denaturation assay and also better anti-bacterial activity against *E. coli* (15.78mm) and *S. aureus*(16.75mm) as compared to *streptomycin* (19.15mm) was a standard by using agar-well diffusion method and also shows good anti-diabetic activity (51.16 and 60.46%inhibition) as compared to acarbose (81.39% inhibition) as a standard by using assay of alpha-amylase inhibition. In DPPH free radical scavenging assay, the compound 1c (90.78%) shows a potent anti-oxidant activity as compared to standard ascorbic acid (90.78%). (Fig. 5)
2. Jiao Meng [32] *et., al* (2024) reported a series of quinazoline derivatives were synthesized and evaluated for their *in-vitro* anti-bacterial activity. The compound-2 exhibited more potent anti-bacterial activity against Xanthomonas oryzae, PV. oryzae with an EC_{50}:13.20 µM by using bis-merthiazol (BT) and thiodiazole copper (30.72 µM) as a reference compound by using ABPP technology and shows more cytotoxicity against lung cancer (A549) cell line (23.05 µM) as compared to 5-Fluorouracil as a positive control (1.42 µM) by using cell viability assay. (Fig. 5)
3. Priya Deivasigamani [33] *et al.*, (2024) reported a series of novel 1,5-diaryl pyrazole derivatives were synthesized and evaluated for *in-vitro* anticancer activity against (A549) lung cancer and (HepG2) liver cancer cell lines with concentration of 6.25, 12.5, 25, 50 and 100µg/ml using MTT growth inhibition assay with IC_{50} of 31.49, 40.14, 60.95, >100 and 3.97µM using cisplatin as a reference drug. The compound-3a and 3b showed moderate anti-cancer activity against lung cancer (A549) 25ug/mL and liver 50µg/mL (HepG2) cancer cell lines and compound-3c showed potent anticancer activity against the HepG2 cell line. (Fig. 6)
4. Wesam S. Shehab [34] *et., al* (2025) reported the synthesis of new heterocyclic derivatives generated from pyrazole by condensation and oxidative cyclization and evaluated for their anti-bacterial, anti-oxidant and anti-fungal activities. The compound-4a furopyrazole shows a strong anti-oxidant activity

(87.6%) as compared to ascorbic acid (88.40%) as a reference compound by using ABTS inhibition assay and also shows remarkable anti-fungal activity against *candida albicans* (15.6mm/mg) and *aspergillus fluvus* (7.8mm/mg) as compared to clotrimazole (5.8 & 3.9mm/mg) was a reference compound. The compound-4b showed strong anti-bacterial activity against *E. coli*(187.5mm/mg), *P. aeruginosa* (125mm/mg), *S. aureus* (187.5mm/mg), *Bacillus subtilis* (93.7mm/mg) as compared to standard drug Ampicillin (125, 187.5, 125mm/mg) by using Kirby-Bauer diffusion technique. (Fig. 6)

5. Arora P K [35] *et al.,* (2023) reported a synthesis of some 2-methoxyphenylquinazolin-4-one were synthesized and evaluated for their *in-vitro* cytotoxicity against lung cancer cells, colorectal cancer and normal cell lines using MTT assay at IC50 of 9.74µg/ml and 27.88µg/ml using erlotinib as a reference drug. The compound-5 (IC50:9.74µg/ml) exhibited more cytotoxicity against lung cancer cells (16.88µg/ml), colorectal cancer cells (IC50: 16.13 µg/ml). (Fig. 6)
6. Ahmed M. Naglah [36] *et., al* (2024) reported the synthesis of pyrazole-based Schiff bases and evaluated for their *in-vitro* anti-diabetic, anti-Alzheimer's, anti-inflammatory and cytotoxic activity. The compound-6 active against lung cancer (A549) cell line (IC_{50};49.40µM) and highest cytotoxicity towards colon(caco-2) cells (IC_{50}42.42µM) as well as normal Caucasian fibroblast like foetal lung cancer (WI-38) cell lines (IC_{50}736.26 µM) as compared to Doxorubicin was reference compound (IC_{50}36.45, 54.94, 304.94 µM). The compound-6 (52.34 mg &34.33µg/ml) showed potent anti-oxidant activity and iron-reducing power as compared to ascorbic acid was reference drug (71.85µg/ml, IC_{50}:41.25µM by using DPPH assay and ABTS inhibition assay and also possess a higher inhibitory effect on alpha-amylase (31.30%) and alpha-glucosidase (26.91%) as compared to acarbose was standard drug (76.58, 53.94%) and shows a potent anti-inflammatory activity as compared to diclofenac sodium(49.08%) by using protein denaturation assay. (Fig. 6)
7. Gonul Bukulmez [37] *et., al* (2024) reported the synthesis of novel quinazoline-sulfonamide derivatives and evaluated for their Alzheimer's disease. The compound-7a and compound-7b more effective against AchE (Ki values of 4.84, 6.32 µM) and BchE (Ki values of 4.74, 5.67 µM) as compared to tacrine (7.76, 6.78 µM) was reference compound. (Fig. 6)
8. Youssef M [38] *et al.,* (2023) reported the synthesis of pyrazole-based derivatives by Perkin condensation of 5-chloro-4-formyl-3-methyl-1-phenylpyrazole with 3-(4-methylbenzoyl) propionic acid in presence of cyclo-dehydrating agent and evaluated for antiviral replication in specific pathogen-free chicken embryos against Avaian influenza (HPAI-H5N1) with CC_{50} values from 300 to 500µL/egg using curcuminol and hypericin as a reference. The Compound-8 shows good anti-viral activity against AIV 500µL/egg. (Fig. 7)
9. Yi Deng [39] *et., al* (2024) reported a series of novel quinazoline derivatives containing sulfonamide moiety were synthesized and evaluated for their anti-viral activity. The compound-9a and compound-9b shows better inhibitory activity towards TMV (tobacco mosaic virus) with an EC_{50} values of curative, protective and inactivating activities (132.1, 152.8, 57.4mg/L and 278.0, 165.3, 94.5mg/L) as compare to ribavirin (318.2, 201.5, 128.6mg/L) as a reference drug by using bioassay. (Fig. 7)
10. Thomas Dipuma, Jr [40] *et., al* (2024) reported a synthesis of pyrazole-based derivatives and evaluated for their potential antibiotics. The inhibition of pyrazole-based inhibitors of N-succinyl-L, L-2,6-diaminopimelic acid desuccinylase (DapE) from Haemophilus influenzae (HiDapE). The most potent pyrazole analogue compound-10 bears an aminopyrimidine amide with an IC_{50}:17.9µm as Potential Antibiotics. (Fig. 7)
11. Aseel Jassim Mohammed [41] *et., al* (2023) reported a synthesis of novel quinazoline derivatives and evaluated for their anti-bacterial activity. The compound-11a (8mm,10mm) and compound-11b (8mm,13mm) most effective against *E. coli* and less effective against *Staphylococcus aureus* as compared to reference drug amikacin (15, 32mm) by using agar-well diffusion method. (Fig. 7)
12. Citlali Vázquez [42] *et., al* (2025) reported a series of quinazoline 2,4,6-triamine derivatives were synthesized and evaluated for their anti-chagasic activity. The compound-12a and compound-12b shows potent anti-protozoal activity against T. cruzi (epimastigotes and trypomastigotes) and low toxicity against HFF1 (human foreskin fibroblast) by using bioassay. (Fig. 7)
13. Ahmed M. Naglah [43] *et., al* (2025) reported a series of pyrazole-indole and pyrazole-isatin were synthesized and evaluated for their anti-diabetic, anti-arthritic and anti-inflammatory activity. The compound-13 exhibit potent anti-diabetic activity against alpha-amylase (65.74%, IC_{50}:4.21µg/ml) and alpha-glucosidase enzymes (55.49%, IC_{50}:2.7µg/ml) as compared to standard drug acarbose (72.58%, IC_{50}:3.8 µg/ml & 62.33%, IC_{50}:2.4 µg/ml) and potent anti-arthritic activity against proteinase enzyme (46.55%, IC_{50}:6.77µg/ml) as compared to reference drug diclofenac sodium (46%, IC_{50}:6.85µg/ml). The compound-13 also shows potent anti-inflammatory activity against COX-1 (69.83%, IC_{50}:5.44µg/ml) and COX-2 enzyme (72.08%, IC_{50}:5.37µg/ml) as compared to indomethacin (80.51,82.76%, IC_{50}:5.50, 4.68µg/ml) and 5-LOX as compare to zileuton (72.6%, IC_{50}:6.83µg/ml) was reference compound. (Fig. 8)
14. Ladan Baziar [44] *et., al* (2024) reported a series of 4-aminopiperidin-3,4-dihyroquinazoline-2-uracil derivatives were synthesized and evaluated for their anti-diabetic activity. The compound-14 shows a promising activity with an IC_{50}:9.25 µM against DPP4 as compared to sitagliptin (0.021 µM) was reference compound by using DPP4 inhibition assay and more cytotoxic activity against NIH/3T3 (embryonic mouse fibroblast cell line) (IC_{50}:76.93 µM) as compared to sitagliptin (IC_{50}:111.25 µM) as a standard drug by using MTT assay. (Fig. 8)

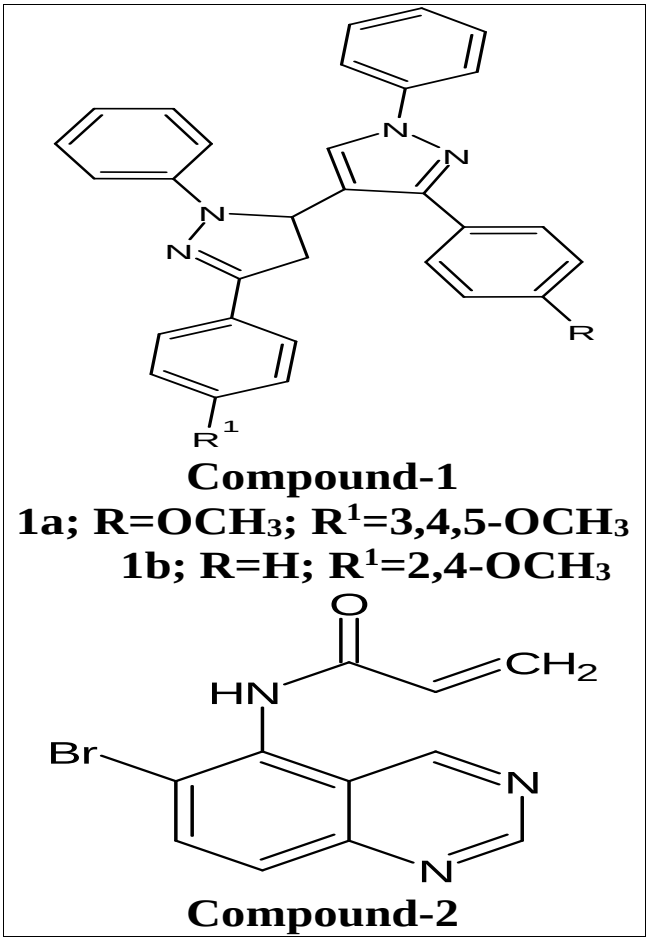


Fig 5: Biological activities of pyrazole and quinazoline derivatives

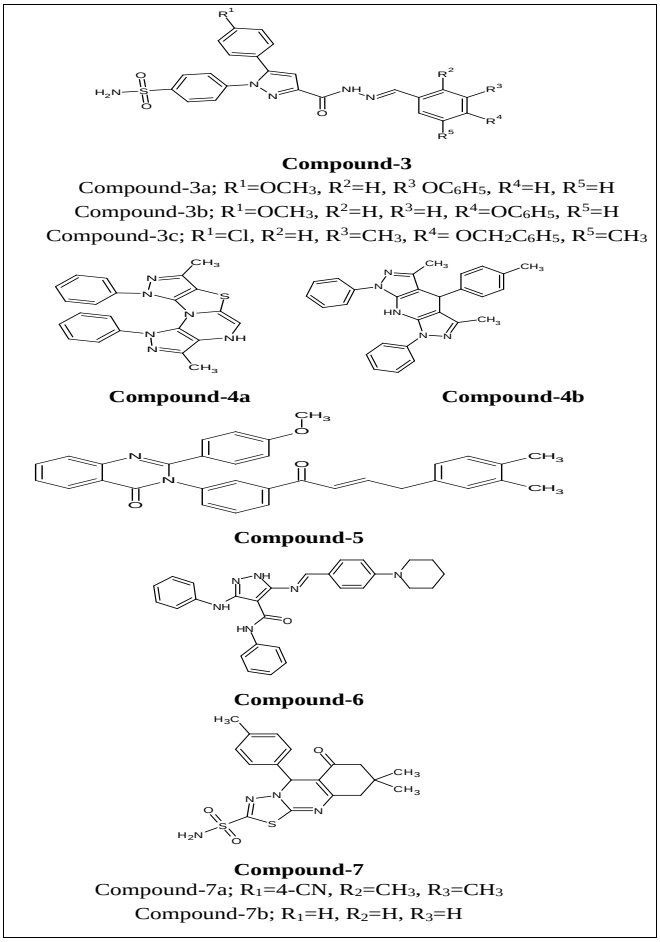
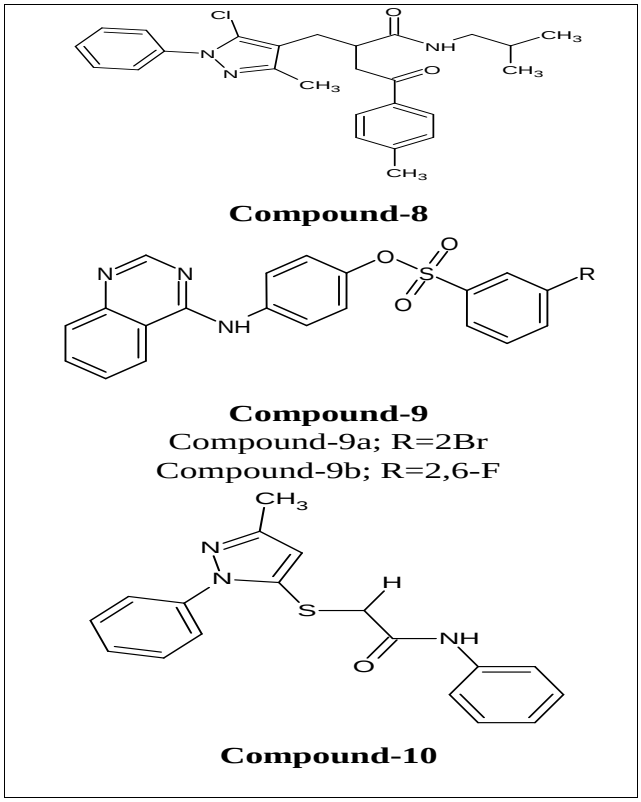


Fig 6: Biological activities of pyrazole and quinazoline derivatives



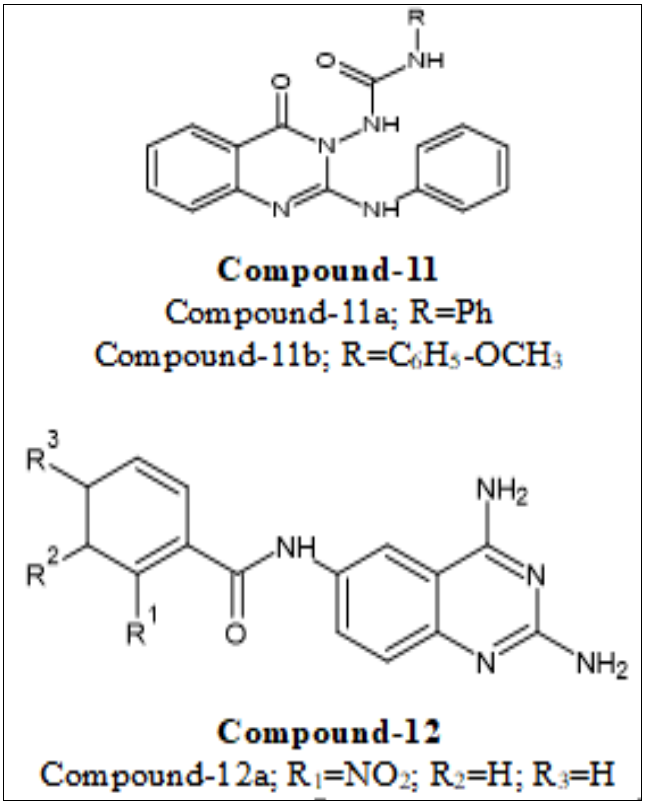


Fig 7: Biological activities of pyrazole and quinazoline derivatives

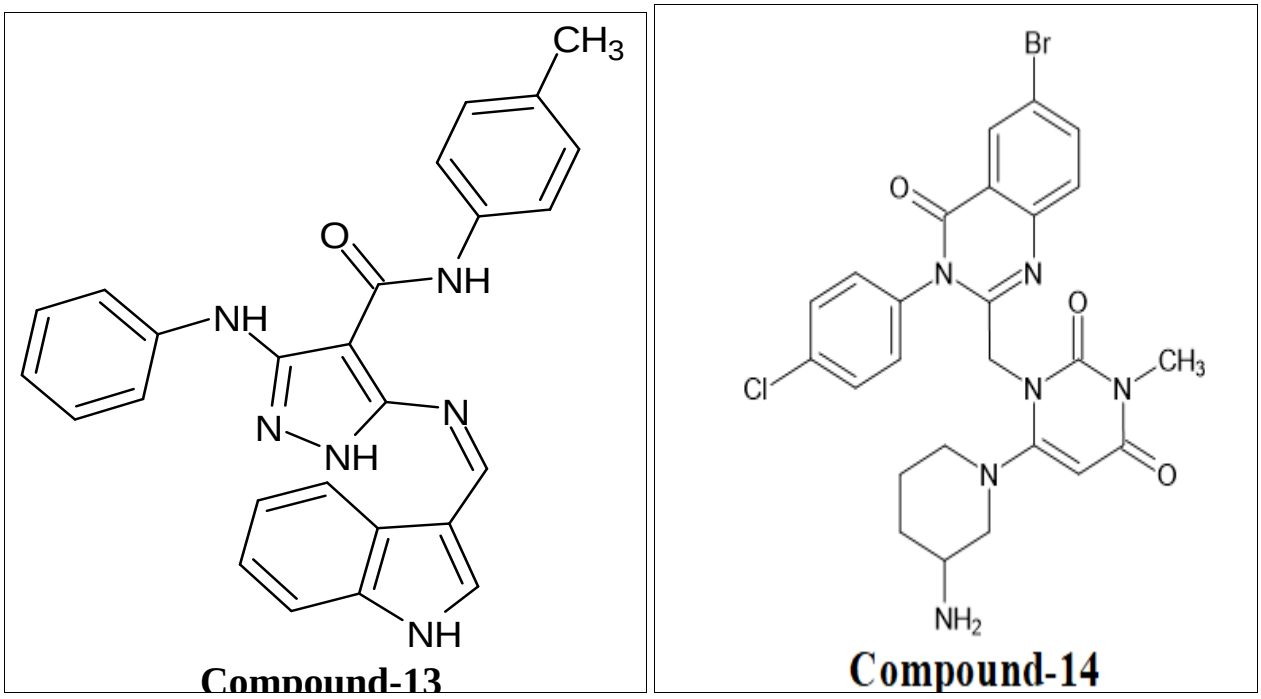


Fig 8: Biological activities of pyrazole and quinazoline derivatives

Conclusions

Pyrazole and quinazoline derivatives have emerged as important scaffolds in medicinal chemistry due to their diverse biological activities, structural versatility, and favorable pharmacokinetic properties. Enhanced synthetic approaches have increased their chemical diversity, leading to potent compounds with anticancer, anti-inflammatory, antimicrobial, and antiviral effects. These frameworks thus remain promising candidates for the design of future therapeutic agents. Overall, pyrazole and quinazoline derivatives continue to serve as promising platforms for the development of next-generation drugs.

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