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Quinazolinone-based compounds in modern drug discovery: Pharmacological activities and future prospects

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Abstract
Quinazolinone derivatives constitute an important class of nitrogen-containing heterocyclic compounds that have attracted considerable attention in medicinal chemistry owing to their broad spectrum of pharmacological activities and favorable structural versatility. The quinazolinone scaffold serves as a privileged pharmacophore for the development of novel therapeutic agents through structural modifications that enhance biological efficacy and target selectivity. Over the past decade, extensive research has demonstrated the potential of quinazolinone-based compounds as anticancer, antimicrobial, anti-inflammatory, antiviral, antitubercular, antimalarial, anticonvulsant, antioxidant, antidiabetic, and analgesic agents. Several derivatives have exhibited promising activity against clinically relevant molecular targets, including kinases, microbial enzymes, and inflammatory mediators, highlighting their significance in contemporary drug discovery. Advances in synthetic methodologies, computational drug design, molecular docking, and structure–activity relationship (SAR) studies have further accelerated the optimization of quinazolinone analogues with improved pharmacokinetic and pharmacodynamic profiles. This review comprehensively summarizes the recent progress in the chemistry, synthesis, pharmacological activities, molecular mechanisms, and therapeutic applications of quinazolinone derivatives. Furthermore, it discusses the influence of structural modifications on biological activity and outlines emerging trends, current challenges, and future research directions for the rational design of quinazolinone-based therapeutics. Collectively, the available evidence emphasizes the continued importance of the quinazolinone scaffold as a valuable platform for the development of innovative and clinically relevant drug candidates.

Keywords: Quinazolinone derivatives, Medicinal chemistry, Pharmacological activities, Drug discovery, Structure–activity relationship, Molecular targets, Therapeutic applications

Introduction

Quinazolinone derivatives represent a prominent class of fused nitrogen-containing heterocyclic compounds that have gained considerable importance in medicinal chemistry because of their remarkable structural diversity and extensive pharmacological potential [1]. The quinazolinone nucleus consists of a benzene ring fused with a pyrimidinone moiety, providing a versatile scaffold for structural modification and the development of biologically active molecules. Owing to its favorable physicochemical properties and ability to interact with diverse biological targets, this scaffold has emerged as a privileged pharmacophore in modern drug discovery [2-3].

Over the past several decades, extensive research has demonstrated that quinazolinone derivatives exhibit a wide range of biological activities, including anticancer, antimicrobial, antiviral, anti-inflammatory, antitubercular, antimalarial, anticonvulsant, antioxidant, analgesic, and antidiabetic effects. These compounds exert their therapeutic actions through modulation of multiple molecular targets, such as protein kinases, microbial enzymes, inflammatory mediators, and various cellular signaling pathways. Continuous advances in synthetic chemistry, computational drug design, molecular docking, and structure–activity relationship (SAR) studies have facilitated the discovery of quinazolinone analogues with enhanced potency, selectivity, and pharmacokinetic characteristics [4-5].

This review provides a comprehensive overview of the chemistry, synthetic strategies, pharmacological activities, molecular mechanisms, and therapeutic applications of quinazolinone derivatives. It also highlights recent developments, discusses current challenges, and outlines future perspectives to support the rational design of novel quinazolinone-based therapeutic agents.

Chemistry of Quinazolinone

Quinazolinone is a bicyclic nitrogen-containing heterocyclic compound comprising a benzene ring fused to a pyrimidinone nucleus. Depending on the position of the carbonyl group, quinazolinones are mainly classified into 2(1H)-quinazolinone, 4(3H)-quinazolinone, and the less common 2,4(1H,3H)-quinazolinedione derivatives, with 4(3H)-quinazolinone being the most extensively investigated because of its broad pharmacological significance. The quinazolinone scaffold possesses a rigid, planar aromatic structure that facilitates interactions with a variety of biological targets through hydrogen bonding, π–π stacking, and hydrophobic interactions [6-8]. Structural modifications at the C-2, C-4, C-6, C-7, and N-3 positions markedly influence the physicochemical properties and biological activities of these compounds, enabling the development of derivatives with enhanced potency and selectivity. Quinazolinones can be synthesized through several well-established methods, including cyclization of anthranilic acid or anthranilamide derivatives with amides, aldehydes, nitriles, or carboxylic acid derivatives under

conventional or microwave-assisted conditions [9-10]. Their synthetic flexibility and favorable pharmacological profile have established quinazolinones as privileged scaffolds in modern medicinal chemistry and drug discovery.

Review of literature

David Hansen SA [11] *et al*., (2025) they reported that novel quinazolinone derivatives were designed, performed molecular docking studies against the selected targets included Topoisomerase II (PDB ID: 5ZAD), Vascular Endothelial Growth Factor Receptor 2 (VEGFR2, PDB ID: 3WZE), Hepatocyte Growth Factor Receptor (c-Met, PDB ID: 3U6I), Epidermal Growth Factor Receptor (EGFR, PDB ID: 1M17), and Estrogen Receptor Alpha (ERα, PDB ID: 3ERT),were synthesized using conventional method and screened for in-*vitro* anticancer activity against cancer cell lines Topoisomerase II, VEGFR2, c-Met, EGFR, and Estrogen Receptor Alpha. Compound 1 shows potent activity for all the cell lines with IC_{50} value of 52.06µg/ml, when compound1 with standard drug Doxorubicin, sorafenib, crizotinib, gefitinib, and 4-hydroxytamoxifen.

Ameen Ali Abu-Hashem [12] *et al., (*2024) reported that new Quinazolinone based heterocyclic compounds such as pyrido [2,3-d] pyrimidinones 1,2,4triazolopyrimidines, pyrimidoquinazolines, and quinoline derivatives were designed, performed molecular docking studies against (MCF-7) breast carcinoma cell line and human normal Retina pigment epithelium cells (RPE-1) synthesized using conventional methods and screened for *in-vitro* anticancer activity against quinoline2-thioxopyrido [2,3-d] pyrimidinone (1) and methylthioquinoline-pyrido[2,3-d] pyrimidinones (2) were used as starting materials among those compound 2 shows potent activity for all the starting material with The IC_{50} values of these Compound 2 ranged from 6.2 to 15.1 µM and 17.5–26.4 µM for MCF-7 and RPE-1 cell lines when compared with standard drug Doxorubicin.

Fadhil Lafta Faraj [13] *et al*., (2014) they reported that new Quinazolinone Derivatives were designed, performed molecular docking studies against MCF-7 Cells synthesized using conventional methods and screened for *in-vitro* anticancer activity against MCF7 human breast cancer cell line. Among that Compound 3 show potent activity for all the cell lines with the IC50 value of 6.246 × 10−6 mol/L and 5.910 × 10−6 mol/L with standard drug Doxorubicin.

Feyzi Sinan Tokali [14] *et al*., (2023) they reported that Novel Quinazolinone Derivatives were designed, performed molecular docking studies against some metabolic enzymes, were synthesized using conventional method and screened for in-*vitro* anti diabetes activity against important metabolic enzymes AChE, BChE, α-Glu and hCA I–II. Among that Compound 4 shows potent activity for all the cell lines when compared with standard drug Acarbose.

5. Mohamed Ayman El-Zahabi [15] *et al.,* (2022) they reported that new Anti-Hyperglycemic Evaluation of Quinazolinone-Sulfonylurea Hybrids were designed, performed molecular docking studies against peroxisome proliferator-activated receptor gamma (PPARγ), synthesized using conventional methods and screened for *in-vivo* antidiabetic activity against peroxisome proliferator-activated receptor gamma (PPARγ). Among those Compound 5 shows potent activity for all the cell lines when compared with the standard drug Glibenclamide.

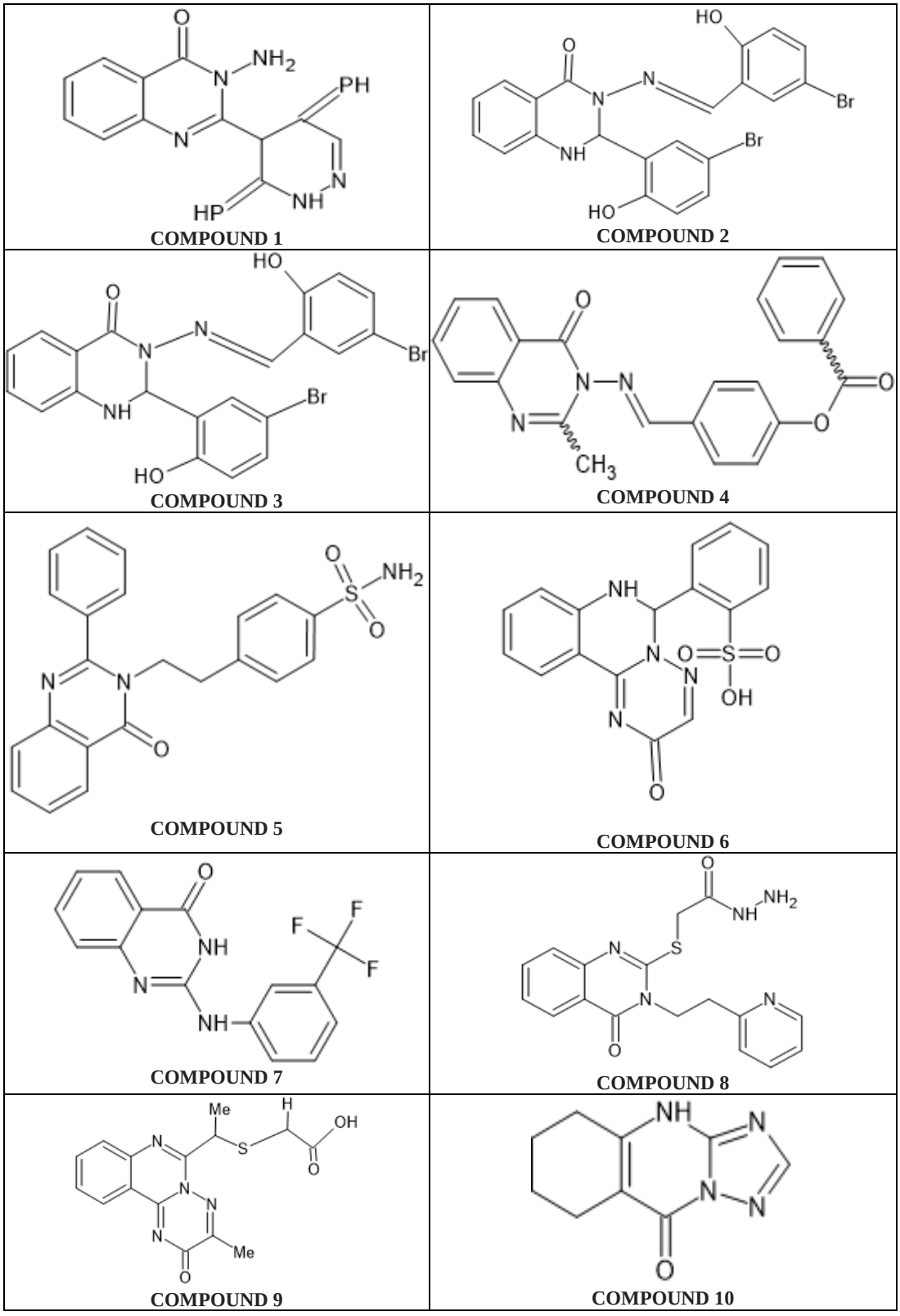
Serhii Trzhetsynskyi [16] *et al.,* (2025) they reported that new hypoglycemic activity of [1,2,4] triazino [2,3-*c*]quinazoline derivatives were designed, performed molecular docking against hypoglycaemic activity synthesized using conventional methods and screened for *in-vivo* antidiabetic activity against amylase (PDBID: 1HNY), glucokinase (PDB ID: 1V4S), 11b-hydroxysteroid dehydrogenase (PDB ID: 2BEL), a-glucosidase (PDB ID:3WY1), maltase-glucoamylase (PDB ID3TOP), fructose-1,6-bisphosphatase (PDB ID: 2JJK), and PPAR-g (PDB ID: 2PRG).Among those Compound 6 shows potent activity for all the cell lines when compared with the standard drug Metformin.

Le Than Hang Nguyen [17] *et al.,* (2025) they reported that new Quinazolinone were designed, performed molecular docking studies against a role in stimulating the production of inflammatory mediators and is recognized by toll-like receptor 4 (TLR4),synthesized using conventional methods and screened for in*vitro* anti-inflammatory activity against toll-like receptor 4 (TLR4).among those Compound 7 shows potent activity for all the cell lines with IC50 100 mM when compared with the standard drug Dexamethasone.

Alaa Abdel-Aziz AM [18] *et al*., (2016) they reported that 2,3-disubstitued 4(3H)-quinazolinone derivatives were designed, performed molecular docking studies against both COX-1 and COX-2 isoenzymes, synthesized using conventional method and screened for *in-vivo* anti-inflammatory activity against Many Compounds exhibited potent anti-inflammatory activity. Among that Compound 8 shows potent activity for all the cell lines with IC 50 value of 0.30 µM. when compound with standard drug

Aleksandra Gripsack [19] *et al.,* (2024) they reported that new Quinazolinone derivatives were designed, performed molecular docking studies against compounds inhibited carragenan-induced rat paw edema by affecting inflammatory mediators (ins activation, decreasing levels of nitro tyrosine, COX-2 and IL-1β synthesized using conventional methods and screened for *in-vitro* anti-inflammatory activity against inhibited carrageenan-induced rat paw edema. Among those Compound 9 shows potent activity for all the cell lines when compared with the standard drug Ibuprofen.

Walid Ettahiri [20] *et al*., (2023) they reported that 1,2,4-Triazolo[1,5-a]quinazolinone derivatives were designed, performed molecular docking studies against four bacterial and four fungal strains were evaluated for their susceptibility to the antifungal properties,synthesized using diffusion method and screened for *in-vivo* anti-fungal activity against four bacterial strains, namely *Escherichia coli*, *Staphylococcus aureus*, *Proteus mirabilis*, and *Bacillus subtilis* and four fungal strains, namely *Aspergillus niger*, *Candida albicans*, *Fusarium oxysporum* and *Aspergillus flavus*. Among that Compound 10 shows potent activity for all the cell lines with IC_{50} value of 23.56µM. when compound with standard drug Fluconazole.



Ran Zhou [21] *et al*., (2023) they reported that new antifungal activity of Novel 1,4-Pentadiene-3-one Containing Quinazolinone were designed, performed molecular docking studies against *Sclerotinia Sclerotiorum*, synthesized using conventional methods and screened for *in-vitro* antifungal activity against tobacco mosaic virus. Among those Compound 11 shows potent activity for all the cell lines with IC_{50} value of 5.4 µg/M when compared with standard drug Azoxystrobin.

Rong Zeng [22] *et al*., (2023) they are reported that studies against Quinazolinone Derivatives were designed, performed molecular docking studies effect against *Fusarium oxysporum*, *Niveum fungus*, synthesized using conventional methods and screened for *in-vitro* antifungal activity against seven plant fungi, including *Rhizoctonia Solani* AG1, *Phytophthora parasitica* var. *Nicotianae*, *Fusarium verticillioides*, *Sphaeropsis Sapinea*, *Fusarium Oxysporum*, *Niveum*, *Colletotrichum Fructicola* and *Colletotrichum Acutatum*. Among those Compounds 12

shows potent activity for all the cell lines compared with standard drug Azoxystrobin.

Walid Ettahiri [23] *et al*., (2023) they reported that 1,2,4-Triazolo[1,5-a]quinazolinone derivatives were designed, performed molecular docking studies against Four bacterial and four fungal strains were evaluated for their susceptibility to the antifungal properties, synthesized using diffusion method and screened for *in-vivo* anti-fungal activity against four bacterial strains, namely *Escherichia coli*, *Staphylococcus aureus*, *Proteus mirabilis*, and *Bacillus subtilis* and four fungal strains, namely *Aspergillus Niger*, *Candida Albicans*, *Fusarium Oxysporum* and *Aspergillus flavus*. Among that Compound 13 shows potent activity for all the cell lines with IC_{50} value of 15.75µM. when compound with standard drug Ketoconazole.

Hatem Abuelizz A [24] *et al*., (2023) they are reported that studies Quinazolinone derivatives were designed, performed molecular docking studies effect against showed good activity against Human Rotavirus Wa Strain synthesized using conventional methods and screened for *in-vivo* antiviral activity against herpes simplex, coxsackievirus B4and hepatitis A and C. Among those the Compound 14 shows potent activity for all the cell lines when compared with standard drug Ribavirin.

Krishnan Suresh Kumar [25] *et al*., (2021) they reported that 2-phenyl quinazoline-4(3) H-ones derivatives were designed, performed molecular docking studies against unexplored drug targets synthesized using conventional methods and screened for *in-vivo* antiviral activity against viruses representative of herpes simplex virus-1 (KOS),herpes simplex virus-2 (G), vaccinia virus, vesicular stomatitis virus, herpes simplex virus-1 TK- KOS ACVr, para influenza-3 virus, reovirus-1, Sindbis virus, Coxsackie virus B4, Punta Toro virus, feline corona virus (FIPV), feline herpes virus, respiratory syncytial virus, influenza A H1N1 subtype, influenza A H3N2 subtype, influenza B and vesicular stomatitis virus. Among those compound 3 shows potent activity for all the cell lines When compared with standard drug Acyclovir.

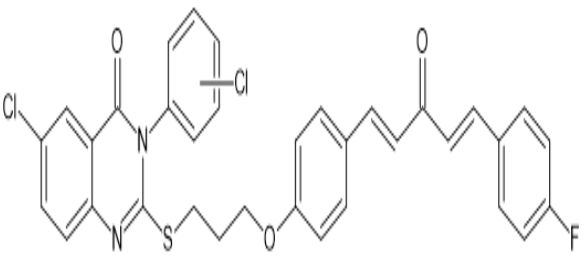
Igor Jose Dos Santos Nascimento [26] *et al*., (2026) they reported that quinazolinone derivatives are synthesized by using conventional method and screened for the *in-vitro* antimalarial activity against *P. Falciparum*. Among those the Compound 16 shows the potent activity with IC_{50} value of 4.10uM. When compared with the standard drug Artemisia.

Girma Worku Seifu [27] *et al*., (2022) they reported that 3-aryl-2-styryl substituted-4(3H)-quinazolinone derivatives were designed, performed molecular docking studies against *Plasmodium Berghi* ANKA and *Leishmania Donovani* strain, respectively. synthesized using diffusion method and screened for *in-vivo* anti malarial activity the Compounds showed better antimalarial activities with percent suppression of 70.01 and 74.18, respectively. Among that Compound 17 shows potent activity for all the cell lines with IC 50 value. when compound with standard drug Chloroquine Phosphate.

Benoit Laleu [28] *et al*., (2021) they reported that Quinazolinone-2- carboxamide derivatives were designed, performed molecular docking studies against laboratory-resistant strains of malaria. synthesized using diffusion method and screened for *in-vivo* anti-malarial activity against Profiling suggested a fast *in-vitro* killing profile. *In-vivo* activity in a murine model of human malaria in a dose-dependent manner constitutes a concomitant benefit. Among that Compound 18 shows potent activity for all the cell lines. when compound with standard drug Pyrimethamine.

Katharigatta Venugopala N [29] *et al*., (2022) they reported that Dihydroquinazolinone derivatives were designed, performed molecular docking studies against the tubercular strain H37Rv and multidrug-resistant (MDR) Mycobacterium tuberculosis (MTB) strains. synthesized using diffusion method and screened for *in-vitro* anti tubercular activity against Compound 3k with an imidazole ring at the 2-position of the dihydroquinazolin-4(1H)-one also showed significant inhibitory action against both the susceptible strain H37Rv and MDR strains with MIC values of 4 and 16 µg/mL, respectively. Among that Compound 19 shows potent activity for all the cell lines with IC_{50} value of 9.56µM. when compound with standard drug Isoniazid.

Bhavya Patel [30] *et al*., (2024) they reported that Quinazoline-2,4(1H,3H)-Dione Derivatives were designed, performed molecular docking studies against *M. Tuberculosis*, synthesized using conventional methods and screened for *in-vitro* antitubarcular activity against Enoyl-acyl carrier protein reductase (InhA, PDB: 4TZK) and Dihydrofolate reductase (DHFR, PDB: 4KM2) revealed excellent binding affinities. Among those Compound 20 shows potent activity for all the cell lines When compared with standard drug Isoniazid.



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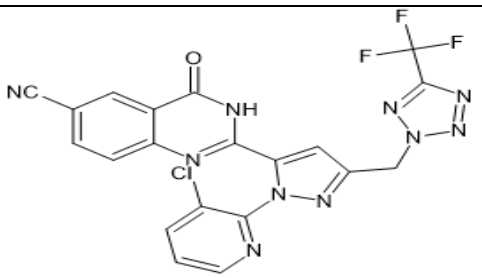

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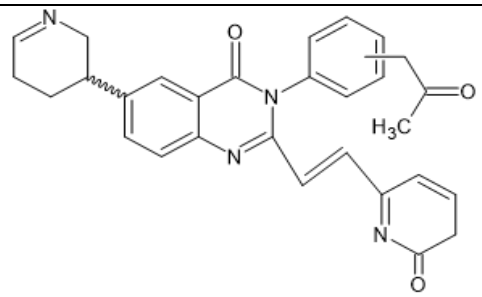
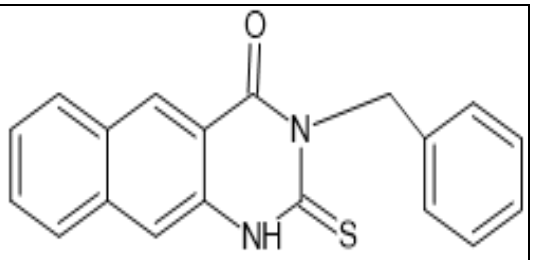
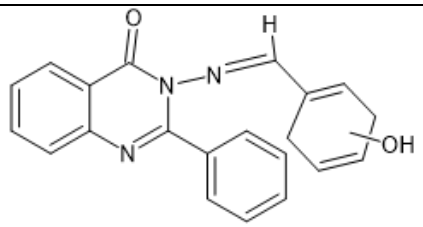
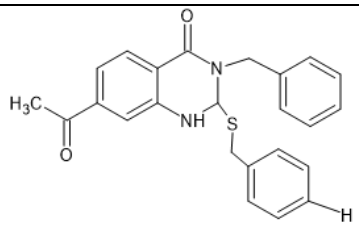
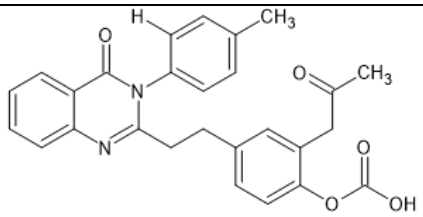
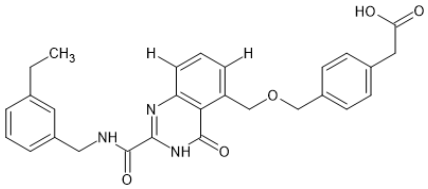
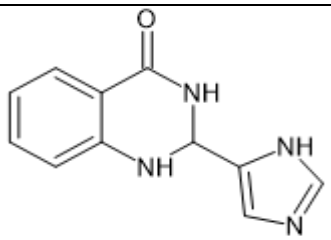
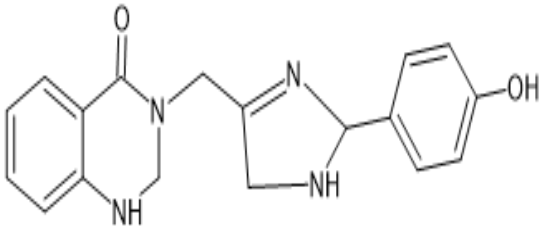
 **COMPOUND 13**	 **COMPOUND 14**
 **COMPOUND 15**	 **COMPOUND 16**
 **COMPOUND 17**	 **COMPOUND 18**
 **COMPOUND 19**	 **COMPOUND 20**

Rajasekhar KK [31] *et al*., (2024) they reported that 2,3-disubstituted quinazolinone derivatives were designed, performed molecular docking studies against Mycobacterium tuberculosis, synthesized using conventional method and screened for *in-vitro* anti tubercular activity against Many Compounds showed a minimum inhibitory concentration value between 6.25 and 100 µg/mL against Mycobacterium tuberculosis. Among that Compound 21 shows potent activity for all the cell lines, when compound with standard drug Ciprofloxacin.

Rasha Mohamed Hassan [32] *et al*., (2025) they reported that new quinazolinone derivatives were designed, performed molecular docking studies against *Pseudomonas Aeruginosa*, synthesized using diffusion method and screened for *in-vitro* anti microbial activity against Many Compounds showed the most broad spectrum antimicrobial agents in this study with safe profile on human cell lines. Among that Compound 22 shows potent activity for all the cell lines with IC_{50} value of 3.55 and 6.86µg/ml. when compound with standard drug Ciprofloxacin.

Maria Coanda [33] *et al*., (2025) they reported that N-Acyl-Hydrazone-Linked Quinazolinone derivatives were designed, performed molecular docking studies against *C. albicans* and *S. aureus* synthesized using diffusion method and screened for *in-vitro* anti-microbial activity against synthesized compounds. Among that Compound 23 shows potent activity for all the cell lines with IC_{50} value of 15.36µg/ml. when compound with standard drug Ketoconazole.

Redha Al-Bayati I [34] *et al*., (2010) they reported that Novel quinazolinone derivatives were designed performed molecular docking studies and synthesized using conventional methods and screened for *in-vivo* antimicrobial against *Staphylococcus aurous*, *E.coli*, *Proteus vulgaris*, *Pseudomonas* and *Klebsiella*) and two fungal *Aspergillus Niger* and *Candida Albicans* in order to assess their antimicrobial properties. Among those Compound 24 shows potent activity for all the cell lines. When compared with standard drug Fluconazole.

Huda Al-Salem AS [35] *et al*., (2015) they are reported that molecular modeling study of some new hydrazine carbothioamide, benzene sulfonohydrazide and phenacylacetohydrazide analogues of 4(3H)-quinazolinone derivatives were designed, performed molecular docking studies effect against PTZ induced convulsions. synthesized using conventional methods and screened for *in-vitro* anti-convulsant activity. Among those, Compound 25 shows potent activity for all the cell lines when compared with standard drug Sodium valproate.

Neelam Sharma [36] *et al*., (2026) reported that 3-Substituted Quinazoline-2,4-dione derivatives were designed, performed molecular docking studies against anti-microbial

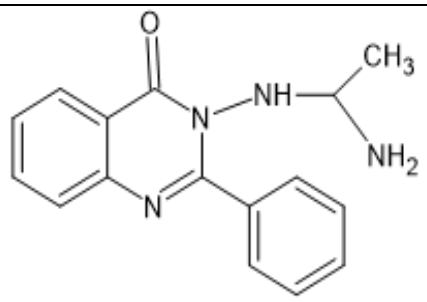
receptors and synthesized using conventional methods and screened for in-*vitro* antimicrobial activity against Gram-positive bacteria (*Bacillus subtilis*, *Staphylococcus aureus*) and Gram-negative bacteria (*Escherichia coli*, *Pseudomonas aeruginosa*) Among those Compound 26 shows potent activity for all the cell lines with IC_{50} value of 50µg/ml when compared with phenytoin sodium as a standard drug.

Ghanda Hassan [37] *et al*., (2012) reported that Novel 4(3H)-quinazolinone analogs derivatives were designed, performed molecular docking studies against GABA receptor agonists, synthesized using conventional method and screened for *in-vitro* anti-convulsant activity against PTZ-induced seizures acting as GABA A receptor agonists among that the Compound 27 shows potent activity for all the cell lines when compound with standard drug Sodium valproate.

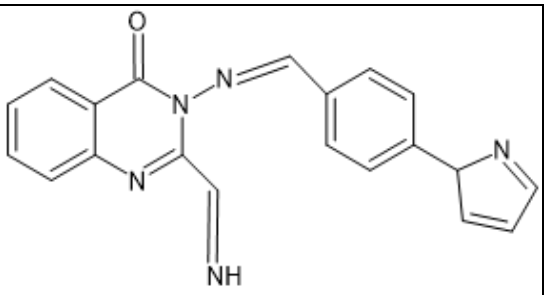
Hassanzadeh F [38] *et al*., (2012) they reported that new quinazolinone derivatives were designed, performed molecular docking studies, synthesized using diffusion method and screened for *in-vitro* anti-bacterial activity against *C. albicans* and *A. niger* (*Staphylococcus aureus* PTCC 1337, *Bacillus subtilis* PTCC 1023 and *Listeria monocitogenes* PTCC 1165) and three Gram-negative bacteria (*Escherichia coli* PTCC 1338, *Pseudomonas aeruginosa* PTCC 1074 and *Salmonella Entritidis* PTCC 1091) by agar diffusion method among that the Compounds 28 exhibited acceptable cytotoxicity approximately 50% at 10 µM concentration when compound with standard drug Ciprofloxacin.

Renee Bouley [39] *et al*., (2016) they reported that 4(3H)-Quinazolinone derivatives were designed, performed molecular docking studies against MRSA strains. synthesized using diffusion method and screened for *in-vitro* anti-bacterial activity against gram positive and gram-negative bacteria by agar diffusion method Among that the Compound 29 shows potent activity for all the cell lines with IC_{50} value of 25.36µg/ml. when compound with standard drug Linezolid.

Eleni Ioanna Tzaferi [40] *et al*., (2025) reported that Redox-Active Quinazolinone derivatives were designed, performed molecular docking studies, synthesized using conventional method and screened for *in-vitro* anti-bacterial activity against *Escherichia coli* (*E. coli*) and *Staphylococcus aureus* (*S. aureus*) bacterial strains using agar diffusion method. Among that the Compound 30 shows potent activity for all the cell lines with IC_{50} value of 4.2 ± 1.4 µg mL^{-1}. when compound with standard drug Ampicillin.



COMPOUND 21



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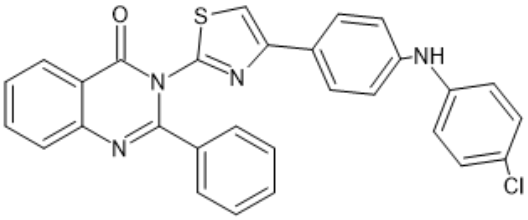

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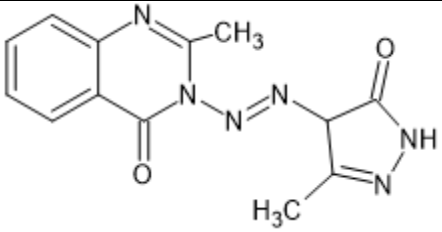

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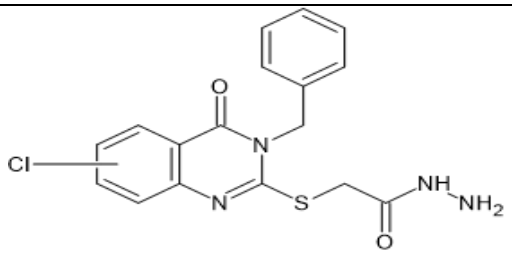

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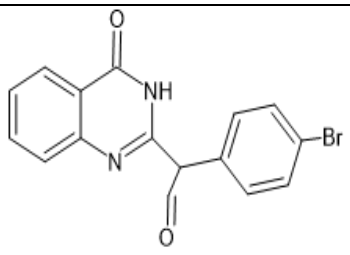

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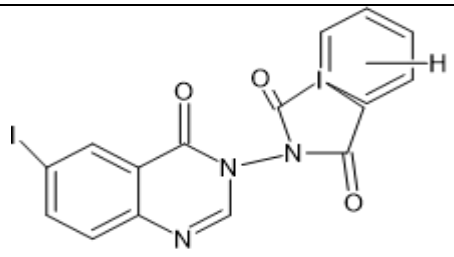

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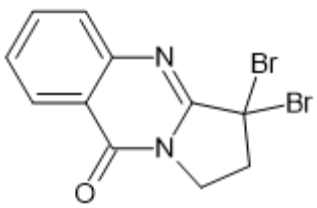

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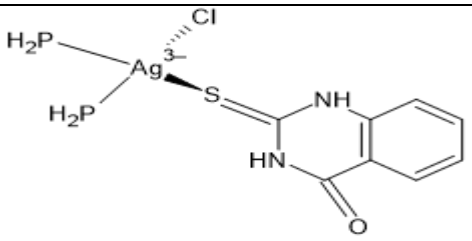
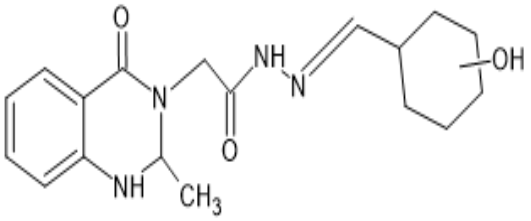


COMPOUND 29



COMPOUND 30

Conclusion

Quinazolinone derivatives continue to attract significant interest in medicinal chemistry owing to their structural versatility and broad spectrum of pharmacological activities. Extensive research has demonstrated their potential as promising therapeutic agents with anticancer, antimicrobial, antiviral, anti-inflammatory, antidiabetic, anticonvulsant, and other clinically relevant properties. Advances in synthetic methodologies, structure–activity relationship studies, and computational drug design have facilitated the development of quinazolinone analogues with improved potency, selectivity, and pharmacokinetic profiles. Future research focusing on molecular target validation, optimization of drug-like properties, and comprehensive preclinical and clinical evaluations will further establish quinazolinone-based compounds as valuable candidates for the development of safe and effective therapeutic agents.

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