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DESIGN, SYNTHESIS, AND DOCKING STUDIES OF PYRIDINE-SULFONAMIDE THIAZOLE INDOLE DERIVATIVES FOR POTENTIAL BIOLOGICAL APPICATION

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1. ABSTRACT

This study presents an in silico molecular docking analysis of heterocyclic compounds 35a–35l and their modular derivatives targeting tubulin proteins from two pathogens: Pseudomonas sp. ADP (PDB ID: 6C6G, for antimicrobial activity) and Candida albicans SC53114 (PDB ID: 7RJC, for antifungal activity). The goal was to evaluate binding affinities and conformational stability of nitrogen-containing compounds using predicted binding energies and RMSD values relative to both unbound and lowest-energy bound conformations. Among all compounds, Compound 35a Module 1 showed the strongest binding affinity (−16.6 kcal/mol) with no deviation (RMSD = 0), indicating high binding stability. Compound 35b also demonstrated promising results, with several modules exhibiting affinities below −14.0 kcal/mol; however, high RMSD values in some modules suggested less stable or alternative binding modes. In contrast, Compounds 35c, 35k, and 35l had lower binding affinities (−6.6 to −8.0 kcal/mol), indicating weaker interaction with the target protein. Docking results against 7RJC highlighted Compound 35f Module 1 and Compound 35k Module 1 as potential antifungal leads, showing binding affinities of −14.1 and −15.9 kcal/mol, respectively, with minimal RMSD values. Overall, structural modifications among the modules were found to significantly influence binding strength and pose stability. These findings provide valuable insight for optimizing the physicochemical properties and biological activity of nitrogen-containing heterocycles in the development of antimicrobial and antifungal agents.

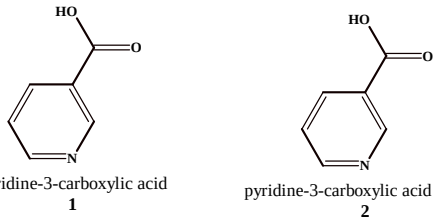
KEYWORDS: Heterocyclic compounds, In silico, Nitrogen-containing compounds, Binding affinity, RMSD, Physicochemical properties.

2. INTRODUCTION

Pyridine is a basic heterocyclic organic matter with the chemical formula C_5H_5N. In many respects, it is similar to the popular and simple aromatic chemical benzene, which has a nitrogen atom in place of one C-H group. Pyridine contains a conjugated system of six π-electrons that are delocalized over the heterocyclic ring, similar to how benzene has. The molecule matches the Huckel guidelines for aromaticity and is planar in nature.[5]

The Greek term "pyridine" is a mixture of the words "pyr," which shows fire, and "idine," which means aromatic bases. The first pyridine base, picoline (Compound 1), was identified by Anderson in 1846.Its organization was ultimately set up independently by Wilhelm Korner in 1869 and James Dewar in 1871. It is suggested that pyridine's structure might resemble that of naphthalene and quinoline. It has been shown that pyridine is formed from benzene and that substituting a nitrogen atom for a CH moiety can produce its structure.

Niacin and picoline is a derivative from pyridine, as shown in **Figure 1, Compound 1, 2.**[5]



pyridine-3-carboxylic acid
1

pyridine-3-carboxylic acid
2

***Figure* 1. Niacin and picoline pyridine derivatives.**

Given their synthetic and useful biological significance, 1,2,4-triazole-pyridine hybrids and their fused heterocyclic derivatives have drawn significant attention among a broad range of heterocyclic compounds being investigated for the expansion of fresh compounds for healthcare chemistry.[1] Our previous investigations show the **antibacterial, anti-inflammatory, and anticancer**

effects of multiple substituted pyridine and Schiff base derivatives.[2]

We recently demonstrated the value of 2,6-di substituted pyridine derivatives as congeners with biological properties.[3] Considering these results and as a continuation of our previous work in peptido-heterocyclic chemistry, we developed a few new substances with hetero-organic and amino acid moieties and investigated their potential biological consequences.[4] Some of our recently substituted heterocyclic compounds displayed **antiparkinsonian, cancer prevention. antimicrobial, and anti-inflammatory** effects in a prior study. Many different compounds in the interesting class of pyrazoles have wide pharmacological effects, including antipyretic, **antirheumatic, and analgesic properties**.**[6]** To evaluate their **antimicrobial efficacy**, we have synthesized several novel derivatives putting a heterocyclic ring fused with a substituted benzosuberone structure in light of these reports and in continuation of our earlier work in heterocyclic chemistry.[7] It was developed to produce a new series of pyrazole derivatives, structure 5 and 6, that would have a high safety margin and function as **dual antimicrobial, non-acidic, anti-inflammatory drugs** with little adverse reactions in the gut. To correspond with the diaryl heterocycle template of drugs known to work selectively as inhibiting **COX-2**, such celecoxib and pyrazofurin the substitution pattern of the pyridine ring was rationalized.[8]

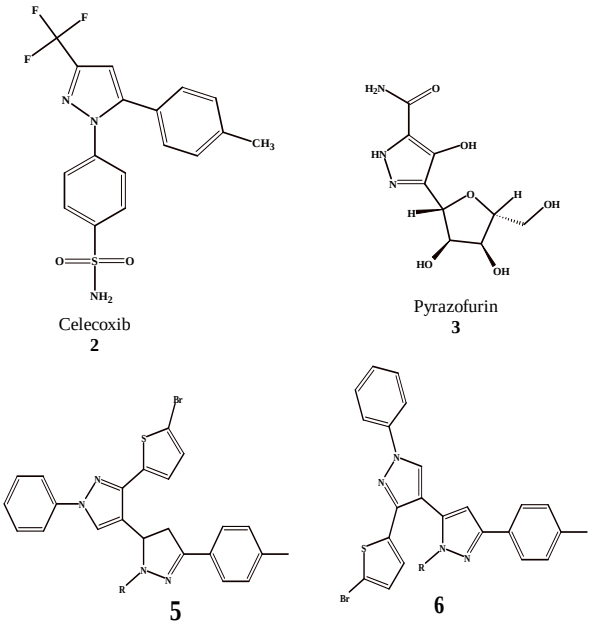


***Figure* 2. Compounds of pyrazofurin, celecoxib, and the recently.**

introduced pyrazole 5 and 6 series[8]

Here, we report the synthesis and antimicrobial analysis of a few new structural hybrids that combine the ring systems of **piperidine, pyridine, and benzimidazole**. In a bid to give the target molecules some synergistic biological significance, this combination was offered for studying the effect of such hybridization and structure variation on predicted biological activities and Benzimidazole and pyridine ring substitution sequences have been carefully selected to give the molecules different electrical power environs.[9] Important pharmacologically active chemical molecules present in medicinally beneficial compounds are the pyrazole moieties. Many pharmaceutical benefits, including **anti-cancer, anti-viral, anti-oxidant, anti-microbial, anti-pyretic, anti-diabetic, anti-inflammatory, anti-convulsant, anti-psychotic, anti-obesity,** an H2-receptor agonist, anti-depressant, or analgesic properties, have gained widespread attention for it.[10] Additionally, heterocyclic compounds containing nitrogen, such **quinoline, indoles, pyrroles, and pyrrolidines** (as likewise as their alkylated homologues), have become highly desirable in the manufacturing industry for use as intermediates in the production of **medicines, dyes, fungicides, herbicides,** as well as other compounds.**[12]** due to the broad spectrum of possible biological functions, pyrazole derivatives are the focus of many research efforts. Bernardino et al. developed and evaluated different kinds of pyrazolonaphthyridine that might possess **anti-HSV-1** effects.[14] In medicinal chemistry, nitrogen-containing heterocyclic substances like pyrimidines, quinoline, pyrrole, indole, triazole, imidazole, pyrazole, and pyrazine play an essential part. Because of their pharmacological and biological properties, pyrazole, indole, and triazole are seen as the most important hetero moieties among them.[15] Since it directly contributes to high mortality and morbidity, antimicrobial resistance in bacterial pathogens is an important obstacle of the 21st century. Commercial antibiotics made readily available encourage bacteria to acquire resistance. In an effort to remedy this deficiency, there is a severe lack of effective interventions and preventative measures. This led several research teams worldwide to create novel medications and substitute antibacterial agents. We concentrated on the growth of molecules by combining various active pharmacophores, such as pyrazole, pyrazoline, and pyridine, into a single common structure in order to find the structure with exceptional biological activity. Numerous biological actions are shown by these tiny particles. Pyrazole substances have interesting biological activities, including **antiviral, antitubercular, antimicrobial, anti-consultant, even anticancer activities.** Drugs that contain pyrazoline and pyridine are crucial to pharmaceutical chemistry and have a number of therapeutic benefits. As seen in Fig. (3), Perampanel, Epirizole, and Edaravone showed distinct biological activities.[16]

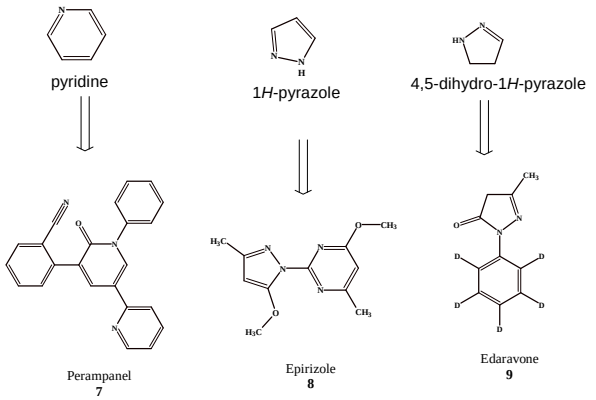
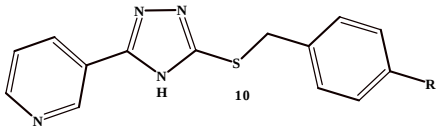


***Figure* 3. Marketed available drugs of Parampanel, Epirizole and Edaravone.[16]**

3. REVIEW OF LITERATURE

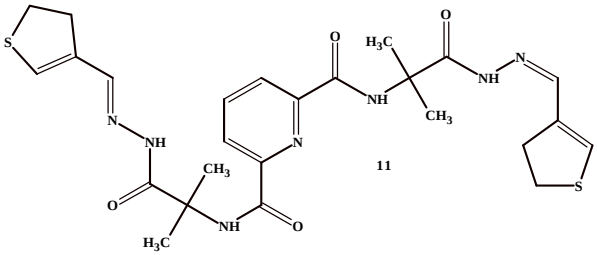
- Ahirwar J., *et al.* (2018). reported by Synthesis, Characterization, Molecular Modeling, and Biological Evaluation of 1,2,4-Triazole-pyridine Hybrids as Potential Antimicrobial Agents. Journal of Heterocyclic Chemistry.[1]

As methotrexate and fluconazole are used as reference drugs, the cup plate is used. In addition, **compounds 3g** and **3h** shown potent antibacterial properties over Acinebactoer baumanni and Staphylococcus aureus, whereas **compounds 3h** and **3i** demonstrated good antibacterial activity against E. coli and gram-negative bacteria. Out of all the compounds produced in this work utilizing a procedure with adjusting reagents, compounds **3c** exhibited a good binding affinity (-11.83) with bond lengths of 2.825 and 2.467, according to docking in the Argus lab investigation.



- Al-Omar MA., *et al.* (2010). reported by Synthesis of some new pyridine-2,6-carboxamide-derived schiff bases as potential antimicrobial agents. Molecules.[2]

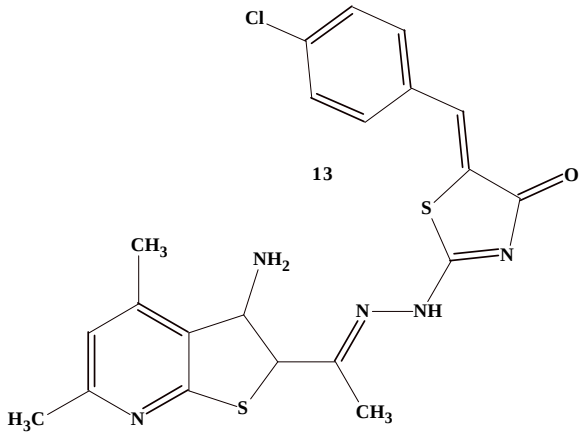
Starting from 2,6-pyridinedicarbonyl dichloride (1) and L-alanine or 2-methylalanine methyl ester, a series of pyridine-bridged 2,6-bis-carboxamide Schiff's bases was constructed. The newly discovered compounds' structural assignments have been confirmed by spectroscopic and chemical data. The bactericidal and fungicidal effects of the newly synthesized compounds 2–5 have been assessed, and the Schiff's bases **4b–f** and **5b–f** exhibit notable antimicrobial properties in relation to streptomycin and fusidic acid, which were used as reference drugs for antifungal and antibacterial properties, respectively. Two thienyl-derivatives, 4-chloro-4d, **5d**, 3-4,5-trimethoxy-**4c**, **5c**, 2-chloro-6-flouro-**4e**, **5e**, and substituted 4-methoxy-**4b**, **5b** When compared with **4a,5a,** which contain an unsubstituted phenyl group, 4f,5f have stronger antimicrobial effects.



- Al-Salahi RA., *et al.* (2010) reported by Synthesis of chiral macrocyclic or linear pyridine carboxamides from pyridine-2,6-dicarbonyl dichloride as antimicrobial agents. Molecules.[3] We may conclude that pyridine and amide moieties are crucial based on the presented comprehensive synthesis, spectroscopic data, and antimicrobial screening for the obtained compounds for antibacterial benefits. We may infer from present findings that the antibacterial activity results from: The existence of heterocyclic rings of nitrogen. In general, the activity is increased by the presence of the amide linkage groups. The stated substances in the molecule's used reagents are the cause of any differences in activity between the compounds. The antibacterial capabilities of compounds 5, 6, 7, 9, 10, and 11 are higher compared to that of the other produced compounds.

- Alenazi NA., *et al.*(2023). reported by New thieno[2,3-b]pyridine-based compounds: Synthesis, molecular modelling, antibacterial and antifungal activities. Arabian Journal of Chemistry.[4]

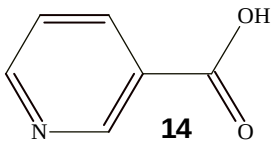
Strong antibacterial activity was demonstrated by compounds 8–10 against Gram-positive S. aureus, Gram-negative E. coli bacteria, and C. albicans (antifungal).



13

- Ali Altaf A., *et al.* (2015). reported by Review on the Medicinal Importance of Pyridine Derivatives. Journal of Drug Design and Medicinal Chemistry [Internet].[5]

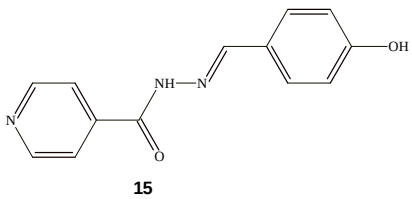
Many substances have clinical use, and pyridine derivatives have been shown to exhibit a range of biological functions. Additionally, pyridine derivatives become more and more significant in current medical applications.



14

- Amr AGE., *et al.* (2006). reported by Anticancer activities of some newly synthesized pyridine, pyrane, and pyrimidine derivatives. Bioorganic and Medicinal Chemistry.[6]

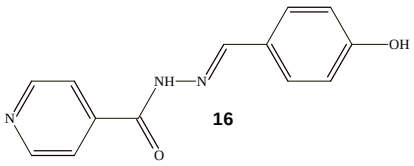
59 different human tumor cell lines—representing leukemia, melanoma, lung, colon, brain, ovary, breast, prostate, and the kidney—were used to evaluate the therapeutic properties of the synthesized compounds. Especially 2, 3, 4c, 6, 7, 9b, 10a, and 11, some of the compounds that were looked at had better in in vitro anticancer effects at low doses.



15

- Bekhit A., *et al.* (2012). reported by 70 A.[7]

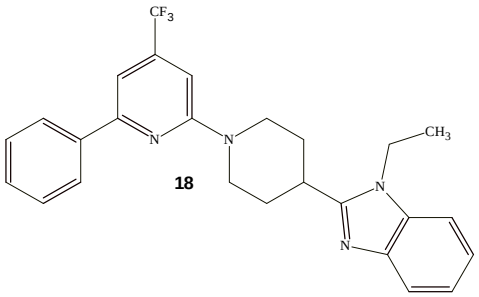
Compounds 2a, 2g, and 2h showed 90, 91, and 80% prevention of the parasite growth at the therapy level of 50 µmol/kg, respectively. likewise, compounds 2a, 2g, and 2h showed promising effects with an IC50 of 0.0402 µM were evaluated in vitro against strains of Plasmodium falciparum RKL9 which were resistant with CQ. At 300 and 100 mg/kg, respectively, the compounds were non-toxic were administered orally and via ingestion. Docking the most active chemicals (2a, 2g, and 2h) in the active region of the dihydrofolate reductase enzyme revealed a number of hydrogen and hydrophobic bonds that support the observed anti-malarial activities.



16

- Bekhit AA., *et al.* (2004). reported by Design, synthesis and biological evaluation of some pyrazole derivatives as anti-inflammatory-antimicrobial agents. Bioorganic and Medicinal Chemistry.[8]

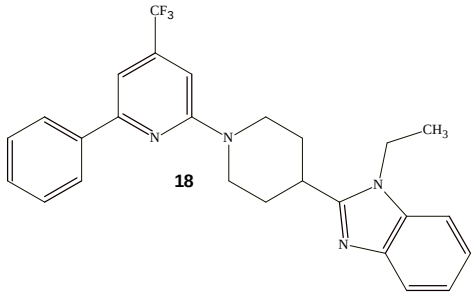
Because of their strong antibacterial properties similar to ampicillin against Gram-positive bacteria and their remarkable anti-inflammatory efficacy both in vivo and in vitro, compounds 4 and 12a are the most remarkable derivatives identified in the present study. Yet, compound 12a exhibited strong selective inhibition of the COX-2 enzyme. Therefore, the substance could act as a beneficial matrix for the creation of anti-inflammatory and antimicrobial candidates.



18

- Beulah K., *et al.* (2023). reported by Design, Synthesis and Biological Evaluation of Benzimidazole-pyridine-Piperidine Hybrids as a New Class of Potent Antimicrobial Agents.[9]

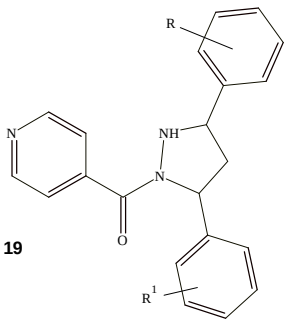
Compounds 4a-h and 5a-c were evaluated for their in vitro antibacterial activity against gram-positive (Bacillus subtilis, Staphylococcus aureus, and Staphylococcus epidermidis) and gram-negative (Escherichia coli, Pseudomonas aeruginosa, and Klebsiella pneumonia) organisms and fungal (Candida albicans, Saccharomyces cervisiae of yeasts, Aspergillus flavus, and Aspergillus niger) strains were evaluated according to with the CLSI Standard Protocol. Compound 5a was favorable advantages against all tested bacteria, with the exception of Bacillus subtilis, as opposed with currently available medications.



18

- Bhirud JD., *et al.* (2020). reported by Sulfamic acid catalyzed synthesis of new 3,5-[(sub)phenyl]-1H-pyrazole bearing N1-isonicotinoyl: And their pharmacological activity evaluation. Bioorganic and Medicinal Chemistry Letters.[10]

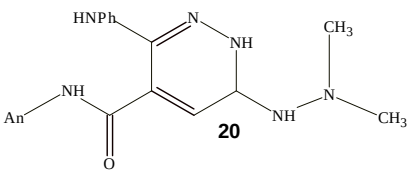
While antibacterial screening of compounds bringing 3e, 3k, and 3j found major inhibition (27 mm) against Staphylococcus aureus, in vitro anti-mycobacterial activity of compounds bearing 3e and 3k showed total inactivation (99%) at the MIC of 31 and 34 μM, respectively.



19

- Bondock S., *et al.* (2008). reported by Synthesis and antimicrobial activity of some new heterocycles incorporating antipyrine moiety. European Journal of Medicinal Chemistry.[11]

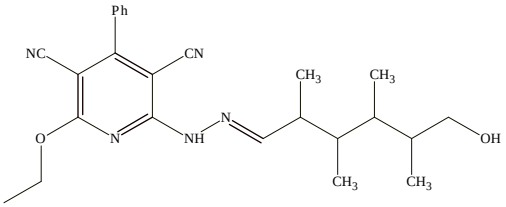
according to the antibacterial activity results, compounds 2, 13, and 14 showed beneficial effects. However, most of the produced compounds 2, 10, and 14 displayed oddly potent antifungal activity in contrast to the reference chemotherapeutics.



20

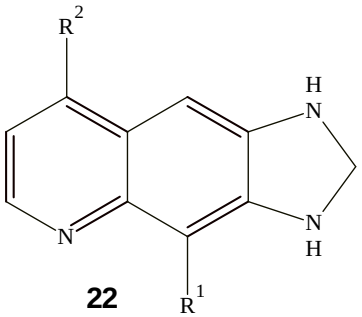
- Campanati M., *et al.* (2000). reported by Environment-friendly synthesis of nitrogen-containing heterocyclic compounds.[12]

The vapour phase synthesis of quinolines or alkylquinolines can be performed using solid acid catalysts such as acid-treated clays or zeolites. The hypothesized chemical route uses solid acid catalysts to create 2-methyl-8-ethylquinoline (MEQUI).



- Carta A., *et al.*. reported by Quinoline tricyclic derivatives. Design, synthesis and evaluation of the antiviral activity of three new classes of RNA-dependent RNA polymerase inhibitors. Bioorganic and Medicinal Chemistry.[13]

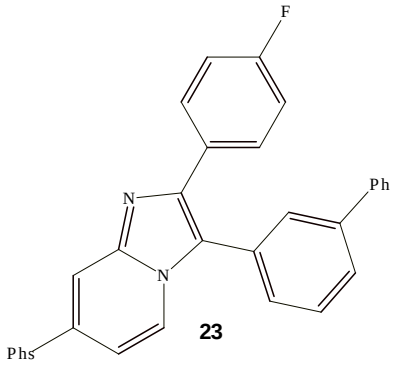
In the present study, the quinoline nucleus fused with 1,2,3-triazole with imidazole generated three novel families of linear N-tricyclic molecule. The cytotoxicity and antiviral activity of title compounds have been tested in cell-based assays against RNA viruses that are representative of the three genera of the Flaviviridae family: BVDV (pest virus), YFV (flavivirus), and HCV (hepacivirus). The imidazoquinolines 2e and 2h, the pyridoquinoxalines 4h, 4j, and 5n (EC50 range 1–5 lM), and the bis-triazoloquinoline 1m were among the most efficient. Compound 2h was the first derivative to exhibit anti-HCV activity in a replicon assay (EC50 = 3.1 lM). In enzyme tests, the BVDV RNA-dependent RNA polymerase (RdRp) were severely inhibited by 1m, 2h, 5m, and 5n, while only 2h also inhibited the recombinant HCV enzyme.



22

- De A., *et al.* (2021). reported by Recent advances on heterocyclic compounds with antiviral properties. Chemistry of Heterocyclic Compounds.[14]

Because of the wide variety of physiological effects, heterocyclic compounds are becoming more and more crucial in medicinal chemistry. Derivatives of indole, imidazole, thiazole, pyridine, and quinaxoline are the most promising among heterocycles of N and S. The antiviral effects of these heterocyclic compounds are noted in this review.

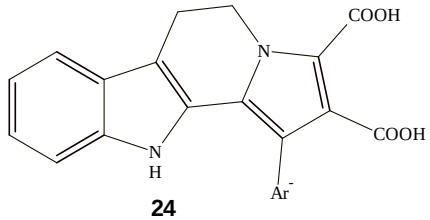


23

- Depa N., *et al.* (2022). reported by Synthesis and biological active compounds of nitrogen-containing heterocyclic compounds: a review. Rasayan Journal of Chemistry.[15]

Many heterocyclic substances containing nitrogen as a heteroatom have significant biological properties and significant applications in medicine.

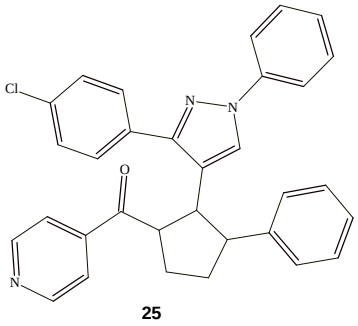
This review article focuses on novel moieties of indole, pyrazole, and triazole compounds and their medical value. Nitrogen-containing heterocyclic compounds are regarded as an important category given their wide range of therapeutic applications, like antibacterial, antimalarial, anticancer, antifungal, anti-HIV, and anti-inflammatory properties.



24

- Desai NC., *et al.* (2019). reported by Synthesis, Biological Evaluation and Molecular Docking Study of Pyrazole, Pyrazoline Clubbed Pyridine as Potential Antimicrobial Agents. Anti-Infective Agents.[16]

We report the synthesis of several pyrazole, pyrazoline, and pyridine-based novel bioactive heterocycles (3a-t) as a part of our ongoing look for new antimicrobials. A review of newly synthesized compounds' antibacterial properties was conducted. The antibacterial effect of pounds 3c, 3h, 3i, 3k, 3n, and 3q was noteworthy.



25

- Ebenezer O., *et al.* (2022). reported by An Overview of the Biological Evaluation of Selected Nitrogen-Containing Heterocycle Medicinal Chemistry Compounds. Vol. 23, International Journal of Molecular Sciences.[17]

Since heterocyclic compounds are a class of chemicals that occur naturally with useful properties, they provide significant advantages for health. They also have major medical importance. This review discusses recent new research on the biological study of nitrogen-containing compounds, including pyrimidines, quinolines, imidazole/benzimidazoles, triazoles, and tetrazoles. It focuses at papers published from April 2020 to February 2022 and will be useful to researchers in medicinal chemistry and pharmacology. The structure of the current work is determined by the size of the heterocyclic ring.

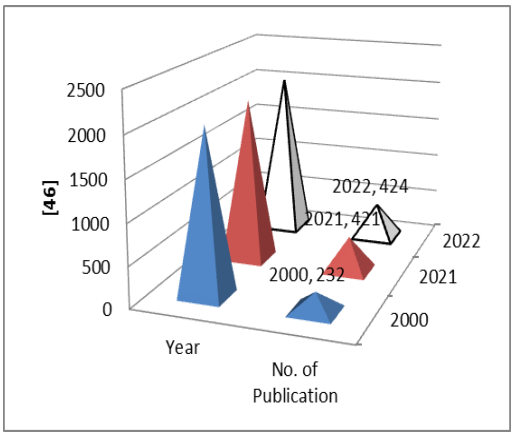
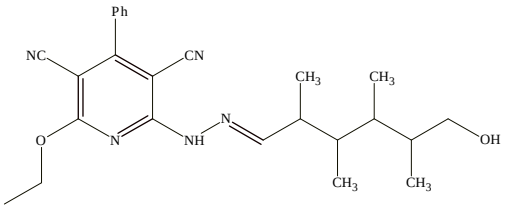


Figure 1: The number of publications with the term"nitrogen-containing compounds" in the titles is based on the calendar year of publishing (July 1068 articles).

- El-Sayed HA., *et al.* (2017). reported by A series of pyridines and pyridine based sulfa-drugs as antimicrobial agents: Design, synthesis and antimicrobial activity. Russian Journal of General Chemistry.[18]

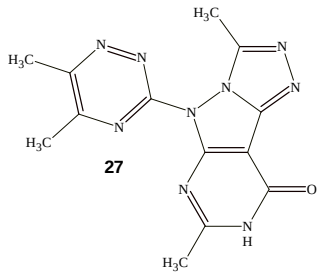
The antibacterial abilities of a variety of pyridines and their sulfa drug derivatives are discussed here. High activity was demonstrated by compounds 8–11 and 17–

19 in the antimicrobial testing of the freshly produced compounds.



- El-Sayed Ali T., *et al.* (2009). reported by Synthesis of some novel pyrazolo[3,4-b]pyridine and pyrazolo[3,4-d]pyrimidine derivatives bearing 5,6-diphenyl-1,2,4-triazine moiety as potential antimicrobial agents. European Journal of Medicinal Chemistry.[19]

Each substance has undergone evaluation for antifungal and antibacterial properties. The highest activity of compounds 9, 10, 13, 19, and 21 were equal to that of the standard drugs, with compounds 9 and 10 showing lower toxicity.



- Elsayed MA., *et al.* (2024). reported by Novel biologically active pyridine derivatives: Synthesis, structure characterization, in vitro antimicrobial evaluation and structure-activity relationship. Medicinal Chemistry Research.[20]

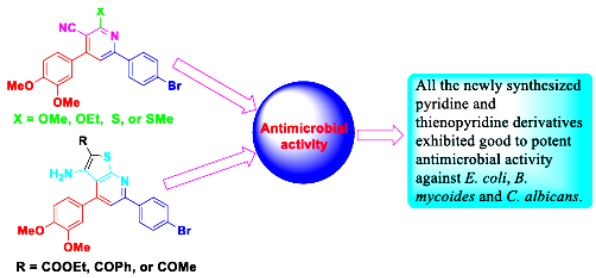


Figure 2: Nitrogen containing derivatives compounds with potential antimiocrobial activity.

- Vitaku E., *et al.* (2014). Analysis of the structural diversity, substitution patterns, and frequency of nitrogen heterocycles among U.S. FDA approved pharmaceuticals. Journal of Medicinal Chemistry. 2014 Dec 26;57(24):10257–74.[22]

Among U.S. FDA-approved drug, nitrogen-containing heterocycles such as pyridine, pyrimidine, pyrazole, indole, imidazole, quinoline, and triazole are among the frequently encountered ring system.

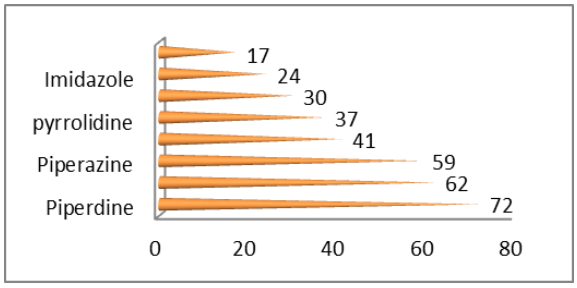


Figure 3: U.S. FDA-approved drug, nitrogen-containing heterocycles such as pyridine, pyrimidine, pyrazole, indole, imidazole, quinoline, and triazole are among the frequently encountered ring system.

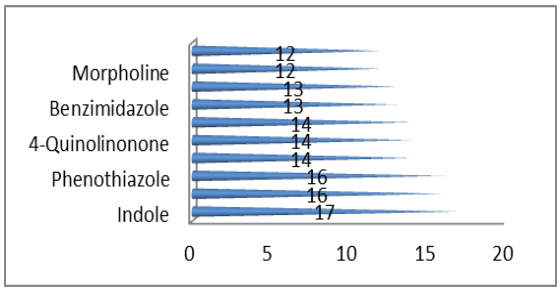


Figure 4: U.S. FDA-approved drug, nitrogen-containing heterocycles such as pyridine, pyrimidine, pyrazole, indole, imidazole, quinoline, and triazole are among the frequently encountered ring system.

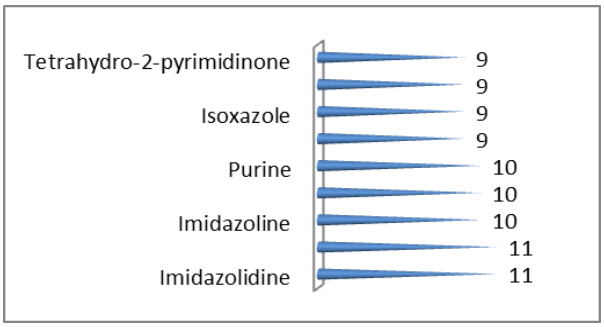
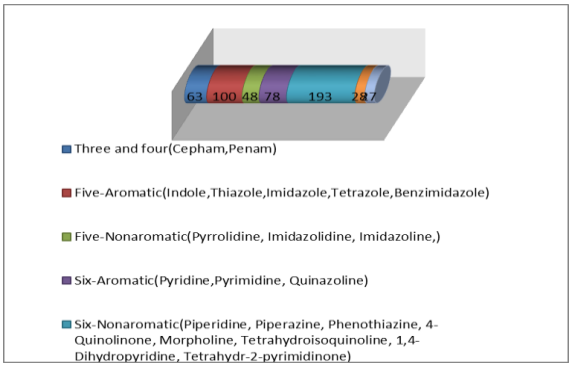


Figure 5: U.S. FDA-approved drug, nitrogen-containing heterocycles such as pyridine, pyrimidine, pyrazole, indole, imidazole, quinoline, and triazole are among the frequently encountered ring system.



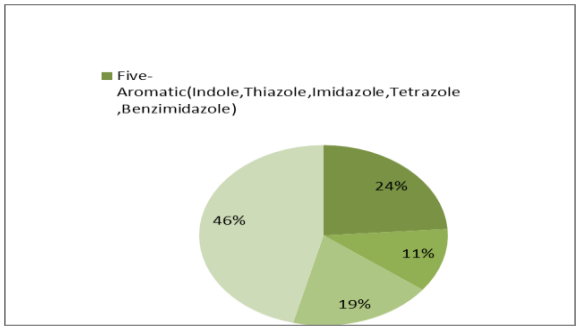


Figure 5: U.S. FDA-approved drug, nitrogen-containing heterocycles such as pyridine, pyrimidine, pyrazole, indole, imidazole, quinoline, and triazole are among the frequently encountered ring system.

SYNTHETIC SCHEME

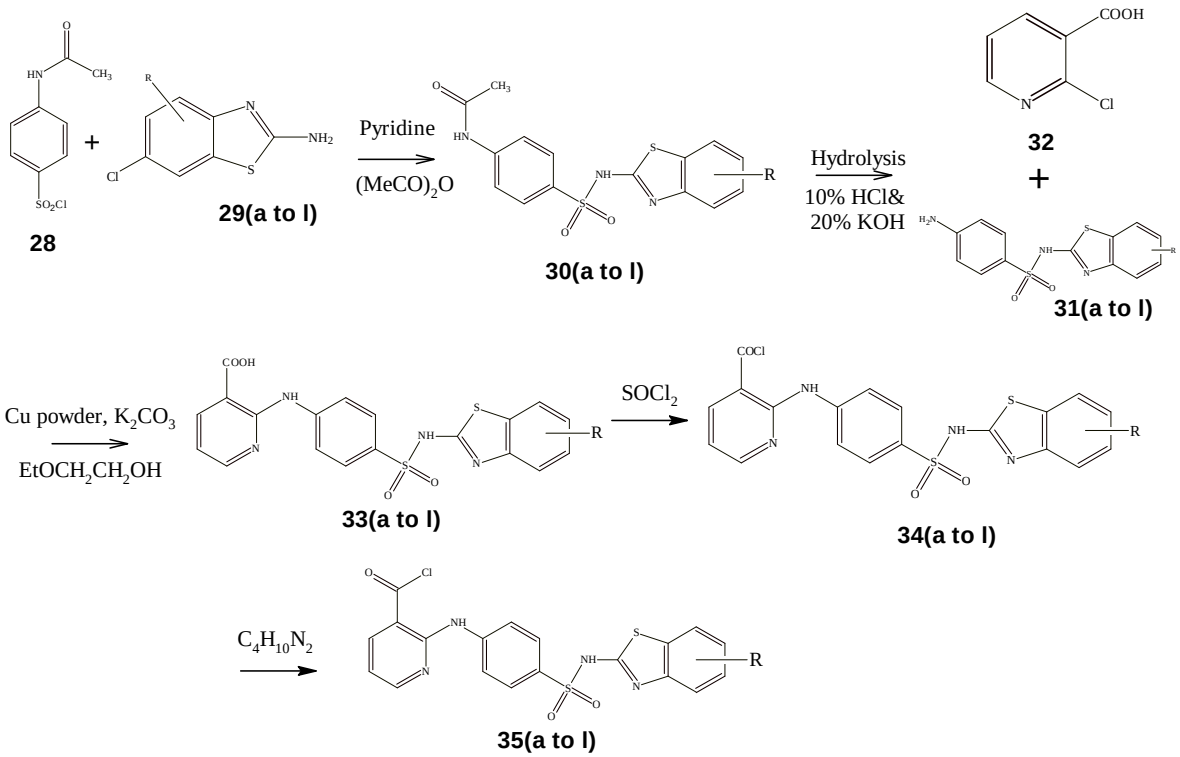


Figure 6: Synthetic scheme for compounds 35(a-l).

Sl. No	29	R	30	R	31	R	33	R	34	R	35	R
1.	a	H	a	H	a	H	a	H	a	H	a	H
2.	b	4-NO_2	b	4-NO_2	b	4-NO_2	b	4-NO_2	b	4-NO_2	b	4-NO_2
3.	c	5-NO_2	c	5-NO_2	c	5-NO_2	c	5-NO_2	c	5-NO_2	c	5-NO_2
4.	d	6-NO_2	d	6-NO_2	d	6-NO_2	d	6-NO_2	d	6-NO_2	d	6-NO_2
5.	e	4-Cl	e	4-Cl	e	4-Cl	e	4-Cl	e	4-Cl	e	4-Cl
6.	f	5-Cl	f	5-Cl	f	5-Cl	f	5-Cl	f	5-Cl	f	5-Cl
7.	g	6-Cl	g	6-Cl	g	6-Cl	g	6-Cl	g	6-Cl	g	6-Cl
8.	h	4-Me	h	4- Me	h	4- Me	h	4- Me	h	4- Me	h	4- Me
9.	i	5- Me	i	5- Me	i	5- Me	i	5- Me	i	5- Me	i	5- Me
10.	j	6- Me	j	6- Me	j	6- Me	j	6- Me	j	6- Me	j	6- Me
11.	k	4-OMe	k	4- OMe	k	4- OMe	k	4- OMe	k	4- OMe	k	4- OMe
12.	l	6- OMe	l	6- OMe	l	6- OMe	l	6- OMe	l	6- OMe	l	6- OMe

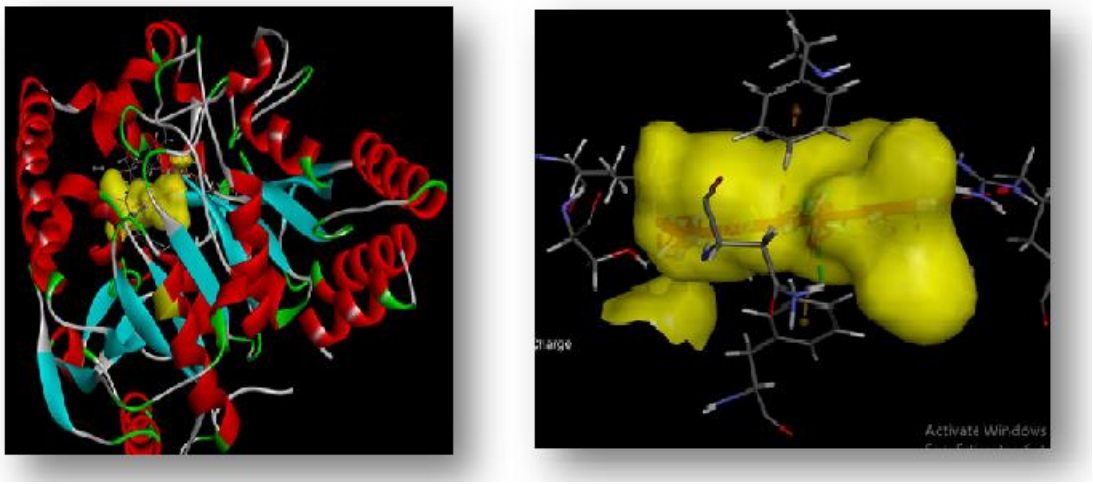


Figure 7: Docking poses of Compound 35a modules in the binding site.

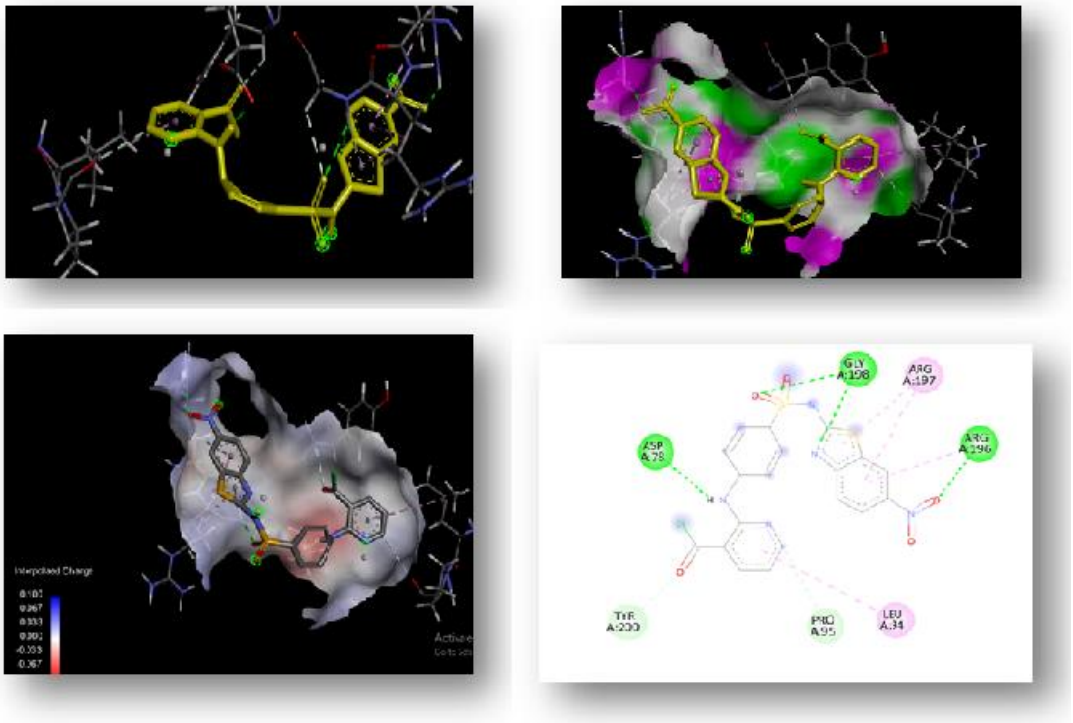


Figure 8: Docking poses of Compound *35c* modules in the binding site.

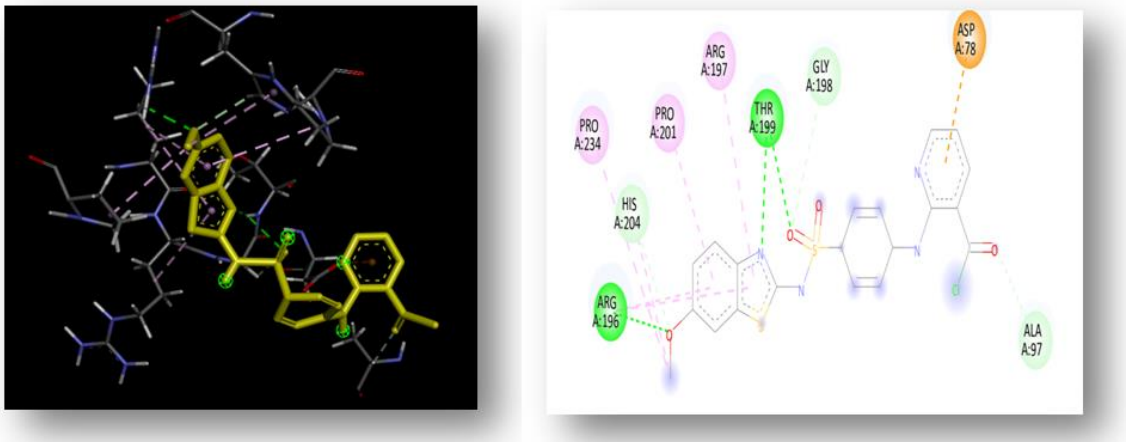


Figure 9: Docking poses of Compound *35k* modules in the binding site.

Compound 35a				
PDB ID:	**Ligand**	**Binding Affinity**	**rmsd/ub**	**rmsd/lb**
6C6G	Compounds 35a Module 1	-16.6	0	0
6C6G	Compounds 35a Module 2	-14.4	14.047	11.126
6C6G	Compounds 35a Module 3	-13.7	14.16	11.631
Compound 35b				
6C6G	Compound 35b Module 1	-14.8	0	0
6C6G	Compound 35b Module 2	-14.2	33.845	29.898
6C6G	Compound 35b Module 3	-14	2.142	2.111
6C6G	Compound 35b Module 4	-14	27.829	26.369
6C6G	Compound 35b Module 5	-13.8	15.45	14.188
6C6G	Compound 35b Module 6	-13.5	34.571	30.313
6C6G	Compound 35b Module 7	-13.5	15.885	14.793
6C6G	Compound 35b Module 8	-13.3	26.282	25.931
6C6G	Compound 35b Module 9	-13.3	16.355	16.283
Compound 35c				
6C6G	Compound 35c Module 1	-7.9	0	0
6C6G	Compound 35c Module 1	-7.9	9.317	3.284
6C6G	Compound 35c Module 1	-7.8	7.559	4.573
6C6G	Compound 35c Module 1	-7.6	2.83	2.336
6C6G	Compound 35c Module 1	-7.4	2.74	2.005
6C6G	Compound 35c Module 1	-7.4	7.291	4.19
Compound 35g				
6C6G	Compound 35g Module 1	-14.5	0	0
6C6G	Compound 35g Module 2	-14	3.181	1.599
6C6G	Compound 35g Module 3	-13.8	5.374	3.601
6C6G	Compound 35g Module 4	-13.5	44.914	43.909
6C6G	Compound 35g Module 5	-13	44.974	44.015
6C6G	Compound 35g Module 6	-12.9	3.478	2.52
6C6G	Compound 35g Module 7	-12.8	29.134	28.387
6C6G	Compound 35g Module 8	-12.5	29.243	28.464
6C6G	Compound 35g Module 9	-12.4	30.96	30.282
Compound 35k				
6C6G	Compound 35k Module 1	-7.7	0	0
6C6G	Compound 35k Module 2	-7.6	2.226	1.806
6C6G	Compound 35k Module 3	-7.3	9.217	5.44
6C6G	Compound 35k Module 4	-7.2	9.836	4.541
6C6G	Compound 35k Module 5	-7.2	2.805	2.099
6C6G	Compound 35k Module 6	-7.2	2.983	2.219
6C6G	Compound 35k Module 7	-7.1	7.728	6.062
6C6G	Compound 35k Module 8	-7	9.471	3.543
6C6G	Compound 35k Module 9	-6.9	9.882	5.66
Compound 35l				
6C6G	Compound 35l Module 1	-8	0	0
6C6G	Compound 35l Module 2	-7.7	9.002	3.538
6C6G	Compound 35l Module 3	-7.3	10.073	4.698
6C6G	Compound 35l Module 4	-7.2	2.535	1.856
6C6G	Compound 35l Module 5	-7	9.584	3.787
6C6G	Compound 35l Module 6	-6.8	9.206	4.382
6C6G	Compound 35l Module 7	-6.7	10.025	6.373
6C6G	Compound 35l Module 8	-6.7	2.223	2.005
6C6G	Compound 35l Module 9	-6.6	28.234	26.413
Compound 35f				
7RJC	Compound 35f Module 1	-14.1	0	0
7RJC	Compound 35f Module 2	-13.4	29.837	26.288
7RJC	Compound 35f Module 3	-12.3	31.667	28.443
7RJC	Compound 35f Module 4	-11.9	19.178	17.7
7RJC	Compound 35f Module 5	-11.3	16.311	14.652

7RJC	Compound 35f Module 6	-11.2	18.013	17.574
7RJC	Compound 35f Module 7	-11.2	15.753	11.735
7RJC	Compound 35f Module 8	-11.2	26.586	23.667
Compound 35f				
7RJC	Compound 35k Module 1	-15.9	0	0
7RJC	Compound 35k Module 2	-13.9	31.258	27.465
7RJC	Compound 35k Module 3	-13.3	31.509	28.047
7RJC	Compound 35k Module 4	-13.3	30.215	26.959
7RJC	Compound 35k Module 5	-13.1	30.082	25.994

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