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Review on Design and Development of Pyridyl Triazole Derivatives

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Abstract: *Triazole-based compounds, which combine pyridine and triazole rings, are studied in the paper. Design and development of pyridyl triazole derivatives, along with their synthesis and biological activities. The study emphasizes how important these derivatives are to Pharmacology and agro chemistry. For coordination chemistry to advance, heterocyclic legends especially five-membered triazoles are essential. Because of their wide range of biological activities, triazoles Named for their three nitrogen atoms are significant. Pyridyl Triazoles are being researched for a number of therapeutic applications, and the addition of Pyridine improves these compounds therapeutic qualities.*

Keywords: Design, Pyridyl Triazole, Synthesis, Biological Application

I. INTRODUCTION

Heterocyclic ligands are crucial to the growth of coordination chemistry. Amid the accessible Five-membered triazoles, ring systems, offer an intriguing class of substances as a result of the Existence of three nitrogens.[1-3] Numerous triazole-related compounds are widely recognizedTo have a significant impact on the synthesis of agrochemicals such as insecticides, Nematocides, acaricides, and regulators of plant growth [(4-8).] When pyridine is added to parent Compounds in the study of medicines and agrochemicals, the compounds' characteristics and Biological activities may be enhanced of the substances, and numerous substances containingPyridyl are known to exhibit a variety of pharmacological and biological properties.[8-11] Pyridyl Triazole derivatives are chemical compounds that combine the pyridine and triazole rings, and Are used to explore new chemical moieties. The name triazole was first coined by Bladin in 1885 to assign the five-membered three Nitrogen containing heterocyclic aromatic ring system having molecular formula C2H3N3 (Bladin, 1885).[12] Triazoles are a significant category of heterocyclic compounds that displayAn extensive array of pharmacological properties. It is also referred to as pyrrodiazoles. It is aFive-membered, diunsaturated ring system with two potential isomeric forms, 1,2,3 triazoles and1,2,4 triazoles, and three nitrogen atoms in a heterocyclic core. Triazoles are soluble in alcohol and water, crystallizing white to pale yellow at a melting point of 120 °C.[13] Pyridine is a mononitrogen containing a six-membered heteroaromatic molecule with the Chemical formula C5H5N that is structurally similar to benzene. It is the parent compound of the Class pyridines and goes by several names, including monoazabenzene, azaarene, azine, etc. This most basic and widespread compound has a bp of 115.5°C and mp of -41.6°C, is Combustible, and is a colorless to yellow liquid. Water miscibility makes it useful for dissolving other materials. Nevertheless, pyridine has certain dangerous qualities as well as an offensive Odor. [14]

Design of Pyridyl Triazole Derivatives:

The core structure of the aforementioned hit (compound 1) contains pharmacophoric groups Such as a hydrophilic spacer followed by a lipophilic tail at C3 and a heterocyclic nucleus Attached directly with aryl rings at N4 and C5. Compound 1 is made up of a 1,2,4-triazole ring System that is joined at N4 and C5 by pyridyl and phenyl substituents, respectively. Additionally, there is a lipophilic tail that follows a hydrophilic linker in the form of an N-arylacetamide moiety at C-3. Three key interactions are involved in compound 1s proposed mode of binding to the A2BReceptors active site. Asn254 and Thr89 residues engage in hydrogen bonding interactions with Thetriazoles N1 and the pyridyl nitrogen, respectively. H is 280 and Se r 279 displayed stacking with the pyridyl ring at C-5.

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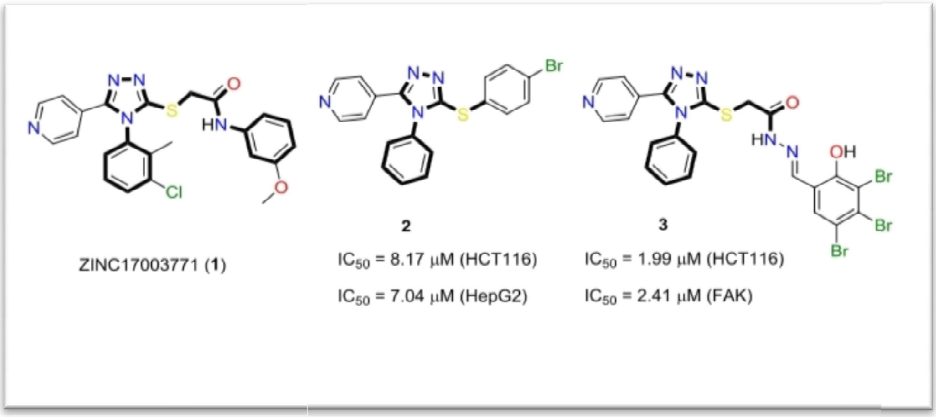

Fig no.1 .hydrophobic bucket containing amino acid residuesVal253 and Met179 was occupied by the terminal N-aryl moiety

The hydrophobic bucket containing amino acid residues Val 253 and Met 179 was occupied by the terminal N-aryl moiety (Figure 1). Compound 1Demonstrated a good affinity toward the human adenosine A2B receptor as a result of these Favorable interactions.[15-18]

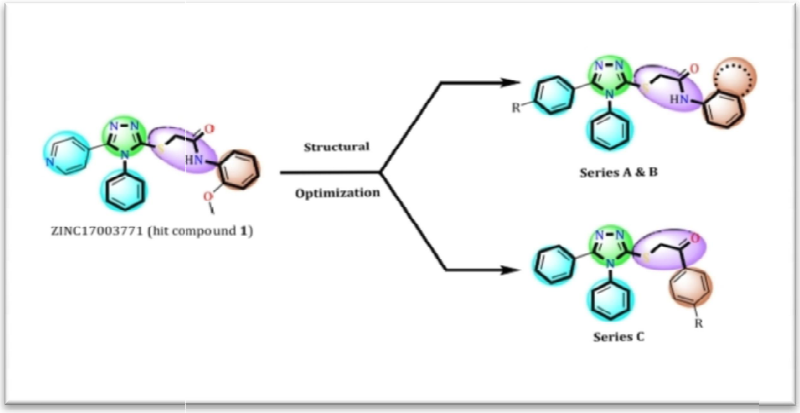

Fig no. 2 -The predicted binding mode for compound 1 with the homology model of the humanAdenosine A2B receptor.

In view of the aforementioned information and in keeping with our earlier research on theIdentification of novel anticancer agents, the primary goal of this work is to design andSynthesize a new set of 1,2,4-triazole derivatives that have the same structural characteristics as compound 1 and nearly the same binding mode with the A2B receptor. Here, motivated by the adaptability of the 1,2,4-triazole ring, three novel series of analogous structures were Designed and synthesized (Figure 2) in order to assess their anticancer activity. Only threeBioisosteric modifications were accomplished in the designed new triazole derivatives: (a) Replacement of the pyridyl group at C-5 with the isosteric phenyl ring, which is eitherUnsubstituted or attached with an electron-donating group at the paraposition; (b) replacement.[19]

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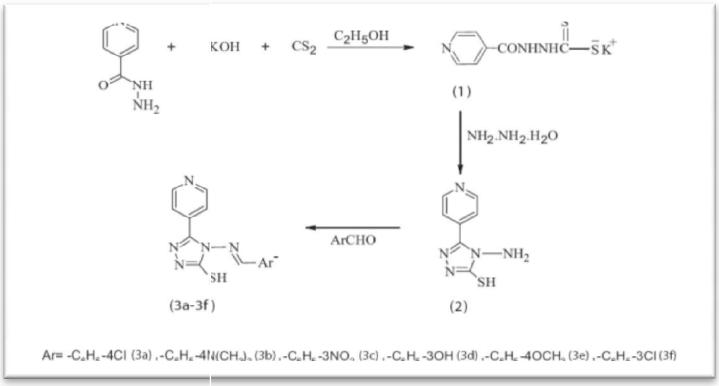

Fig no. 3 -The hit compound and structure based design of newly designed derivatives.

1. Synthesis:

E. Merck (Germany) and S.D. Fine Chemicals (India) provided the chemicals. The open tubeCapillary method was used to calculate the melting points, and it was not corrected. On thinLayer chromatography (TLC) plates (silica gel G), the compounds Purity was examined using the solvent systems toluene-ethyl formate-formic acid (5:4:1) and benzene-methanol (8:2); the Spots were seen under UV light and iodine vapors. Using Perkin-Elmer 1720 FT-IRSpectrometers (KBr pellets), the infrared (IR) spectra were acquired. With TMS serving as the internal standard in DMSO-d6/CDCl3, 1H NMR spectra were captured on a Bruker AC 400 MHz Spectrometer. A VG Prospec instrument was used to record mass spectra under fast atom Bombardment conditions (FAB) at an ionizing voltage of 70 eV. The resulting spectra were shown as m/z. A UV-Visible Spectrophotometer Pharma Spec-1700 (SHIMADZU) was used to Record UV spectra. Using tungsten (VI) oxide as a combusting agent and sulfanilic acid as a Standard, elemental analysis was performed on CHNS Elementar (Vario EL III). Results for C,H, and N were within ± 0.4% of the theoretical values.

2. Synthesis- of 4-amino-3-(4-pyridyl)-5-mercapto-4H-1,2,4-triazole –13.7 g (0.1 mol) of isonicotinic acid hydrazide was transferred to a 1000 mL round-bottom flask And dissolved in 200 mL of absolute ethanol containing 11.2 g (0.1 mol) of potassium hydroxideAt room temperature. Partially added to this was 12.5 mL of carbon disulfide, and the reactionMixture was stirred at room temperature for 16 hours. Following the completion of the reaction, 100 ml of diethyl ether was added, and the reaction mixture was stirred for an additional threeHours. The potassium dithiocarbazinate salt was then gradually mixed with 10.3 g (0.1 mol, 99%) of hydrazine hydrate, which was dissolved in 100 mL of water while being stirred. The Mixture was then refluxed for eight hours, during which time hydrogen sulfide gas evolved and the reaction mixture color turned deep green. After cooling, it was acidified to pH 1 with Hydrochloric acid. The yellow-colored solid that separated from the ethanol was filtered, purified, and then recrystallized to yield compound. Standard protocol for 4-[{1-(aryl) methylidene}-amino] synthesis3-(4-pyridyl)3-a3f) -5-Mercapto4H-1,2,4-triazolesA solution of compound 2 (4-amino-3-(4-pyridyl)-5-mercapto-4H-1,2,4-triazole) dimethylformamide (20 mL) was mixed with a few drops of glacial acetic acid, 0.01 mol of Different benzaldehyde derivatives, and refluxed for nine hours. To obtain the final compound, the reaction mixture was cooled, and the precipitate was filtered, vacuum-dried, and recrystallized from ethanol.[20]

3. Synthesis -of 5-benzyl-N-(heterocylclicnucleus-2-yl) methyl-1 (pyridin-3-yl)-1H1, 2, 4triazole-3-carboxamide 5-benzyl-N-(heterocylclic nucleus-2-yl) methyl-1-stirred for two hours at room temperature. ViaVacuum removal of the solvent, the residue was dissolved in 50 milliliters of dry chloroform andFiltered to yield (pyridin-3-yl).NH4Cl is removed by -1H-1,2,4-triazole-3-carboxamide. Acetate Was obtained by evaporating the filtrate and triturating it with 25g of 3-aminopyridine (0.265mol) Dissolved in 250mL of 6N HCl diethylether (197). Drop by drop, phenolacetyl (250 mL), sodium Nitrite (18.2 g, 0.265 mol), chloride (4.4 g, 0.0288 mol), and water (50 mL) were added to aStirred solution. The mixture was then stirred for 30 minutes. Later, at 0°C, ethyl-2-of 197 (5g, 0.024mol) in 25 ml of toluene

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was heated to room temperature. After adding 43g of 0.265 mol Chloroacetoacetate to 100mL of ethanol, the mixture refluxed for 12 hours, the solvent Evaporated, and the residue dissolved drop-wise for an hour at 0°C. Following 30 minutes, 1NHCl, 10% NaHCO3, and sodium acetate 65g, 0.CH2Cl2 (120mL) were used for washing. [21]

4. Synthesis –4. Synthesis of targeted N-phenyl-5-(pyridin-3-yl)-4H-1,2,4-triazol-3-aminesCompounds 4.112 by condensation of nicotinohydrazide with phenyl-S-Methylisothioure as a result, a different synthetic route for fornicotinamide derivatives was created, utilizing this Weak amide bond (Scheme 3). N-(phe-nylcarbamothioyl) benzamide precursors 1.1132 couldBe hydrolyzed under harsh reaction conditions in a hot alkaline solution (aq. 2 M NaOH, 85 °C),Resulting in substituted 1-phenylthioureas 3.112. S-methylation of these compounds enabled Effective triazole cyclization, which in turn produced the desired N-phenyl-5-(pyridin-3-yl)-4H1,2,4-triazol-3-amines 4.112.[22]

5. Synthesis: Synthetic route of 1H- [1,2,3] triazolo [4,5-b] pyridineDiazinyl ?-3-2-(4-chlorophenyl) 2,6-diamine -4-(benzyloxy) pyridine 4-(benzyloxy) pyridine-2,6diamine 1 and 4-chlorobenzene Diazonium chloride 2, which was created by theDiazotization of 4-chloroaniline at 0 °C, interacted to form Diazene 3. Wurtz et al. observed thatLate-stage diversification was enabled by cleavage of the zinc-diazene bond, resulting in the Production of 7-(benzyloxy)-1H-[1,2,3] triazolo[4,5-b]pyridin-5-amine 4 (Fig. 2) (Wurtz et al.,2018). The diamine is cyclized with isoamyl nitrite. [23]

6. Synthesis Synthetic route of 3H? [1,2,3] triazolo[4,5-c] pyridineUsing 2-Bromo-5-fluoropyridine 5 N-oxidized utilizing trifluoroacetic anhydride, hydrogenPeroxide, and urea with constant stirring at room temperature for 15 hours, Matsuda andColleagues successfully created synthetic 3H-[1,2,3] triazolo[4,5-c]pyridine derivatives. This wasFollowed by quenching with a saturated solution of sodium sulfite in an ice-cold environment. ToObtain compound 7, the resulting compound 6 was nitrated using fuming nitric acid and strongSulfuric acid while being stirred at 100 °C for four hours. Furthermore, compound 8 was createdBy reacting compound 7 with the proper amine to generate compound 9, which was cyclizedUsing trifluoroacetic acid and NaNO2 to create derivatives of the 3H-[1,2,3] triazolo[4,5-c]Pyridine 10 by continuously stirring at room temperature for one hour, followed by stirringContinuously for one hour at room temperature before the reaction mixture is concentrated in aVacuum. Chloroform was used to extract the residue after it had been diluted with an aqueousSodium bicarbonate solution.[24]

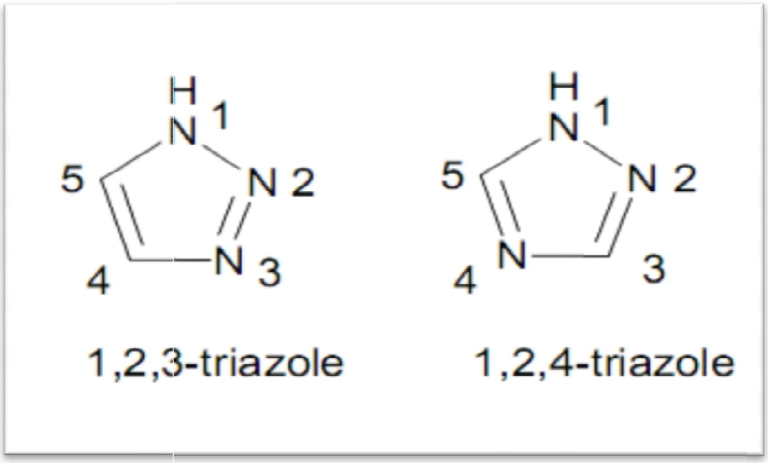

Fig no. 4. Structure Activity Relationship of Triazole derivatives

The structure–activity relationship (SAR) of triazole derivatives has been thoroughly investigated over the last three decades. These investigations have shown that while substitutents on the Triazole nucleus at positions 1, 3, and 5 can be changed, the groups bonded to the nitrogen Atom at position 1 exert the biggest influence on structure and properties. For instance, the Addition of a biaryloxy side chain at the N-1 of the triazole nucleus allowed for the synthesis of a Series of 1-(substituted biaryloxy)-2-(2,4-difluorophenyl)-3-(1H-1,2,4-triazol-1-yl) propan-2-ol Derivatives, which demonstrated superior antifungal activity against candida albicans compared To voriconazole.[25]

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Fig no. 5. Biological activity of pyridyl triazole derivatives :

Anticonvulsant Activity:

Since current antiepileptic medications have not been able to control every type of seizure, there is an ongoing need for novel anticonvulsant agents.Approximately one-third of patients do not react well to the current multidrug regimen. Current Medications like mephobarbital and phenobarbital are highly effective at controlling seizures, But they have significant adverse effects like hypnosis and sedation[26] It has been reported that derivatives of triazolefs exhibit strong anticonvulsant properties. Numerous Schiff bases, including N-4-(4?-chlorophenyl-thiazol-2-yl) semicarbazides and 3-(4pyridyl)-4-amino-5-mercapto-4(H)-1,2,4-triazoles (30), were synthesized by Pandeya et al. The compounds Neurotoxic and anticonvulsant qualities were assessed. These substancesBecame the most potent.[27]

Antimyco bacterial Activity:

Not the same After being created and tested for antitubercular activity against Mycobacterium Tuberculosis H37Rv, 1,4-disubstituted -1,2,3-triazoles show antitubercular activity with MICs Ranging from 12.5 to 3.12 ug/ml. Recently, analogs of 1,2,4 triazoles were synthesized and Demonstrated antitubercular activity against the Mycobacterium tuberculosis H37Rv strain in Vitro. 3-(3-pyridyl)-5-(4-methylphenyl) compound-4-(N-4-amino thiazol-2-amino-1,3-benzo)-4HCompared to rifampicin, -1,2,4 triazole demonstrated superior antitubercular activities.[27]

Antibacterial Activity:

A new series of 1,2,4-triazole-indole hybrids was created by Fabrice et al., who also ole Assessed the compounds' antifungal properties. Mass and elemental spectroscopy, NMR, and infrared spectroscopy were used to characterize each of the produced hybrids. The chemical 3(1H-indol-1-yl)-2-(2,4-Dichlorophenyl) Excellent action against Candida was demonstrated by 1-(1,2,4-1H-triazol-1-yl) propan-2-ol 1a, especially against species that are vulnerable to low Fluconazole. According to the results, this chemical had strong efficacy against Candida Glabrata, Candida krusei, and Candida albicans when compared to fluconazole and comparableTo voriconazol.[28] The ten compounds that contain the manic base 1,2,4 triazole were Synthesized by Wujec et al. The antibacterial activity of these compounds was assessed using the broth microdilution technique against both Gram-positive and Gram-negative bacteria. It Seems that the phenyl ring in piperazine's 4-position is necessary for its antibacterial properties. With MIC values of 30 µg/mL against M. luteus and 60epidermidis), compound 2a demonstrated Strong action.[29]

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Anti-cancer properties :

A panel of human tumor cell lines was used to test the in vitro synthesis of a number of Heterocycle-fused 1,2,3 triazoles using 1, 3-dipolar cycloaddition of heterocyclic ketene aminals Or N, O-acetals with sodium azide and polyhalo isopthalonitriles. Compound 4: The mostEffective derivative against A 431 was discovered to be methyl-phenyl substituted1,3, oxazoheterocycle fused 1,2,3 triazoles. And human carcinoma cell lines K 562. Using the? Click chemistry? Method, pregnenolone acetate, the starting material, has been transformed to create 21-triazolyl derivatives of pregnenolone. When tested against seven human cancer cell Lines, the compound exhibited the strongest anticancer efficacy.[30-31]

Antifungal Activity:

Antifungal activity: A class of medications used to treat fungal infections in humans is known as Antifungals. Heterotropic microorganisms, fungi are identified from algae by their incapacity for Photosynthetic activity. Molds and yeast are examples of fungi. The former are elongated cells that typically reproduce by budding and forming branches of cells, while the latter are spherical, oval, and mucosid colonies in agar medium. Synthesized 5-(N-substituted carbamidomethylthio)-3-(3'-pyridyl) – 1, 2, 4-triazole Derivatives were produced by R.K. Mali et al. (52). Using fluconazole as the standard, antifungal Activity was tested against Candida albicans and Candida Niger at concentrations of 50 and 100 Mg/mg.[32]

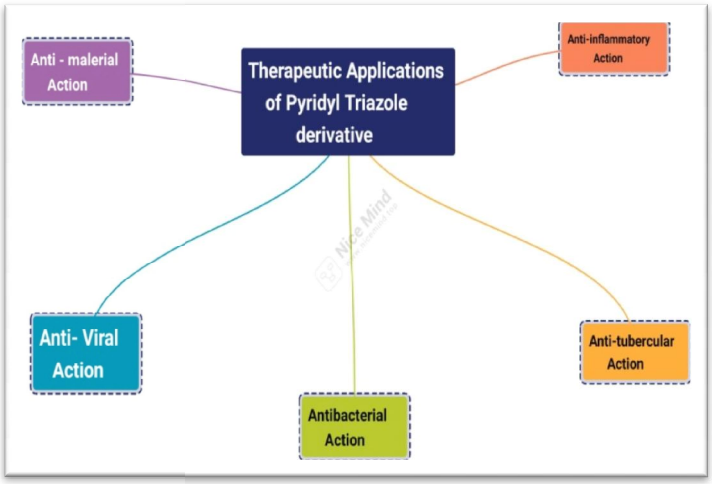

Fig no. 6. Therapeutic Applications of Pyridyl Triazole derivatives

Anti-inflammatory activity:

Non-steroidal anti-inflammatory medicines (NSAIDs), which are used to treat a variety of Arthritis conditions, have limited therapeutic use due to adverse effects such as ulceration and Gastrointestinal bleeding. Thus, novel medications with minimal adverse effects and potentAntiinflammatory properties have been created. The ability of 4-(substituted benzylidene) to reduce inflammation Derivatives of -5-(pyridin-4-yl)-4H-1,2-triazole-3-thiol.[33]

Antitubercular Action:

Anti-tubercular activity Mycobacterial tuberculosis is the primary cause of tuberculosis. TheEmergence of drug-resistant TB (DR-TB), multidrug-resistant TB (MDR-TB), extensively Drugresistant TB (XDR-TB), and fully drug-resistant TB (TDR-TB) has complicated efforts to eradicate tuberculosis (TB) worldwide. INH-resistant bacterial strains are unfortunately becoming more prevalent, despite the fact that the chemicals employed in frontline anti-TB Medications are pyridine-derived. Because of this, INH compounds with higher lipophilicity appear to be among the most promising anti-TB drugs. Dandawate et al. synthesized thePlumbagin -isoniazid analog (Fig. 13) and its inclusion complex with -cyclodextrin. [34]The synthesized plumbagin-isoniazid analog seems promising, especially considering

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it's MICValues under both high and low iron conditions, which are significantly better than those of theStandard isoniazid drug. The fact that its inclusion complex with -cyclodextrin enhances yourThermal stability and aqueous solubility further strengthens its potential as an effectiveAntitubercular agent. Your exploring an exciting area of research keep up the great work this could lead to breakthroughs in tuberculosis treatment.[35] Lipophilic adaptations of pyridine-derived isonicotinic acid hydrazide: A frontline drug (likely Referring to isoniazid) was structurally modified by N2-acetylation of its hydrazine moiety using N-arylaminoacetyl transferases. These modifications aimed to improve its lipophilicity, resulting in excellent activity against both M. tuberculosis and tuberculosis-infected macrophages. Amino Azetidinones: A series of these compounds were designed via in silico methods, derived from Azetidin-2-ones. The synthesis involved reacting isoniazid Schiff bases with chloroacetyl Chloride. The Alamar blue assay was used to test the activity of these compounds, revealingSignificant antitubercular activity. [36-37]

Antibacterial Action:

By combining 1,2,3-triazole with pyridine or pyrimidine, Marepu et al. synthesized a novelMoiety and investigated its antimycobacterial properties. Buchwald's strategy was used toSynthesize the targeted compounds in a regioselective manner. When compared toStreptomycin, two of the triazolopyridines demonstrated promising antibacterial activity.Although triazolopyrimidines did not perform as expected, there is still room for research intoThem because these compounds can be improved to become more potentantimycobacterialAgents. [38]

Antiviral Action:

A family of substances known as antiviral medicines is used to treat a variety of viral illnesses.Since most antiviral medications aim to stop the development of certain viruses, pyridine Derivatives are a great class of chemical molecules to work with for creating new and potentAntiviral medications. Given the wide range of physiological actions exhibited by pyridinederivedCompounds, they are essential in the field of medicinal chemistry. Viral infections are one of theMost dangerous illnesses, and the antiviral chemotherapy drugs currently on the market areInsufficiently effective in the clinic, which causes fatalities and other severe illnesses in people. As a result, it is imperative to discover novel antiviral candidates.[39]synthetic pyridine NoxideDerivatives a, b, and c, and their efficacy against the feline coronavirus and SARS wasAssessed. Remarkably, compounds a and b were discovered to possess promising actionAgainst the feline coronavirus strain and SARS-CoV. Ghosh and associates. Assessed theAntiviral efficacy of 5-chloro-4-methylpyridin-3-yl-1H-indole-4 carboxylate. Compound DProduced an intriguing result; it exhibited strong antiviral efficacy against SAS-CoV-2 3CLproAnd was on par with Remdesivir. The compounds antiviral effect? Is what causes its damagingProperties rather than its cytotoxic ones. The chemical bound to SARS-CoV 3CLpro andSARS-CoV-2 3CLpro enzymes through a covalent bond between the indole carbonyl andCys145, as seen by the high-resolution X-ray. Furthermore, there exist stacking interactions between the indole ring of compound and the imidazole of His41. Star Structures of compounds a, b, c and 5-chloro-4-methylpyridin-3-yl-1H-indole- 4-Carboxylate. [40]

Antimalerial Activity:

Xue et al. developed pyridine scaffolds with a fosmidomycin moiety, which effectively inhibitedThe growth of Plasmodium falciparum, the parasite responsible for malaria. The most potentCompound they synthesized was eleven times more effective than fosmidomycin alone. TheEnhanced antimalarial activity is believed to stem from a hydrogen bond formed between the Nitrogen atom of the pyridine ring and cysteine residues in a P. falciparum protein. Additionally, These compounds have shown efficacy against chloroquine-resistant bacteria. This innovativeApproach opens up new avenues for combating both malaria and drug-resistant infections.[41]

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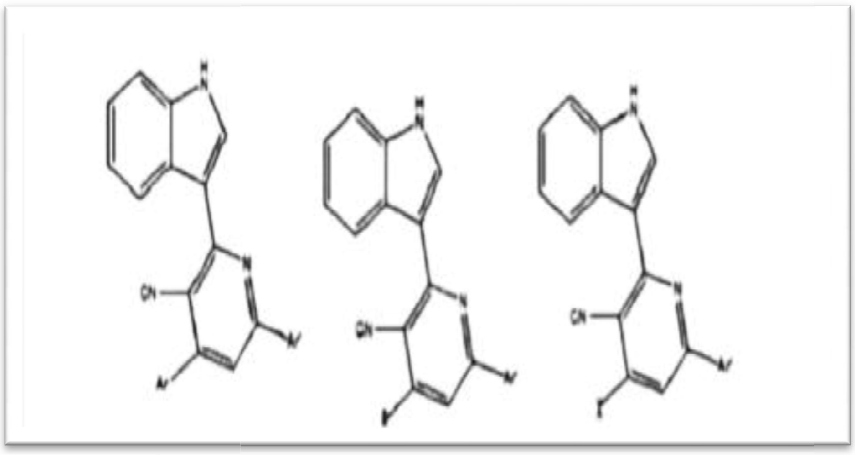

Fig. no. 7 Pyridyl derivative as an Anti- malerial agent

Colleagues synthesized multiple series of pyridine derivatives and evaluated theirAntimalarial efficacy in vivo using chloroquine-sensitive mice infected with P. berghei. At aDosage of 50 mol/kg, compounds 2a, 2g, and 2h significantly inhibited parasite growth. AmongThese, compound 2g demonstrated particularly strong activity, with an IC50 of 0.040 µM againstChloroquine-resistant P. falciparum RKL9 strains, making it a promising candidate for furtherAntimalarial research. [42]

II. CONCLUSION

The design, synthesis, and biological properties of pyridyl triazole derivatives Which combine pyridine and triazole rings Are covered in the paper. Because of their many Biological characteristics, these derivatives are important in pharmacology and agrochemistry. With an emphasis on their potential as anticancer agents, the study aims to improve these Compounds core structures in order to increase their binding affinity with the human adenosineA2B receptor. Using methods like mass spectrometry, IR, and NMR, the synthesis of these Compounds was confirmed. Anticonvulsant, antimycobacterial, antibacterial, antifungal, Anticancer, and anti-inflammatory qualities are among the biological activities investigated. According to the findings, pyridyl triazole derivatives have potential as medicinal agents for the Treatment of conditions like inflammation, cancer, TB, and epilepsy.

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