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"A Design and Synthesis of Some New 1, 3, 4-Oxadiazole Analogues for Using Anticancer Agents"

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ABSTRACT
The abstract of the design and synthesis of 1,3,4-oxadiazole analogues as anticancer agents discusses the creation of new compounds with potential anticancer properties. The study focused on developing 1, 3, 4-oxadiazole derivatives as promising agents against cancer. These derivatives were designed and synthesized, aiming to enhance their cytotoxicity against various cancer cell lines. The development of novel anticancer agents with improved efficacy and reduced toxicity is a pressing need in cancer research. In this study, we report the design, synthesis, of a series of 1,3,4-Oxadiazole analogues as potential anticancer agents.

Keywords: ODZ- Oxadiazole, TDZ- Thiadiazole, Anticancer

I. INTRODUCTION

Among the various heterocyclic frameworks explored in recent years, **1,3,4-oxadiazoles** have gained significant attention in medicinal chemistry due to their broad spectrum of biological activities, including antimicrobial, anti-inflammatory, antiviral, and notably, anticancer properties. The 1,3,4-oxadiazole ring system serves as a versatile bio-isostere of esters, amides, and carboxylic acid groups, and is known to improve metabolic stability and pharmacokinetics of drug candidates.

Structurally, the oxadiazole nucleus offers opportunities for functionalization at multiple positions, which can be exploited to fine-tune interactions with biological targets, particularly enzymes and receptors involved in cancer proliferation such as tubulin, tyrosine kinases, and topoisomerases. Recent studies have reported that **1,3,4-oxadiazole derivatives exhibit cytotoxic effects against various cancer cell lines, including breast (MCF-7), lung (A549), colon (HT-29), and cervical (HeLa) cancers**.

In light of these findings, the current study focuses on the rational design, synthesis, and preliminary biological evaluation of **novel 1,3,4-oxadiazole analogues** as potential anticancer agents. The structural modifications are guided by structure-activity relationship (SAR) data and molecular modeling studies to enhance the anticancer efficacy while maintaining drug-likeness. This work aims to contribute to the growing body of literature on oxadiazole-based anticancer agents and identify promising lead compounds for further development.

The cancer is these cod leading cause of death globally, accounting for an estimated and 9.6 million deaths, or one in six deaths, in 2018. Cancer is a leading cause of death worldwide, accounting for 11 million deaths in 2024.

OXADIAZOLE:- 1,3,4-Oxadiazole is a five-membered heterocyclic ring consisting of two nitrogen atoms at positions 3 and 4 and one oxygen atom at position 1, along with two carbon atoms. It exists as one of the three isomeric forms of oxadiazole (1,2,4-, 1,3,4-, and 1,2,3-), with the **1,3,4-isomer being the most biologically active and widely studied** in medicinal chemistry.

The 1,3,4-oxadiazole ring has garnered significant attention due to its **unique physicochemical properties** such as planarity, aromaticity, high dipole moment, and the ability to form hydrogen bonds. These characteristics contribute to its **excellent binding affinity with biological targets**, making it a privileged structure in drug design.

From a pharmacokinetic perspective, the 1,3,4-oxadiazole moiety often acts as a **bioisostere of esters, amides, and carboxylic acids**, improving metabolic stability and enhancing lipophilicity. It has been used in various FDA-approved drugs and investigational compounds, which underlines its **drug-like nature** and **favorable ADME profile** (absorption, distribution, metabolism, and excretion).

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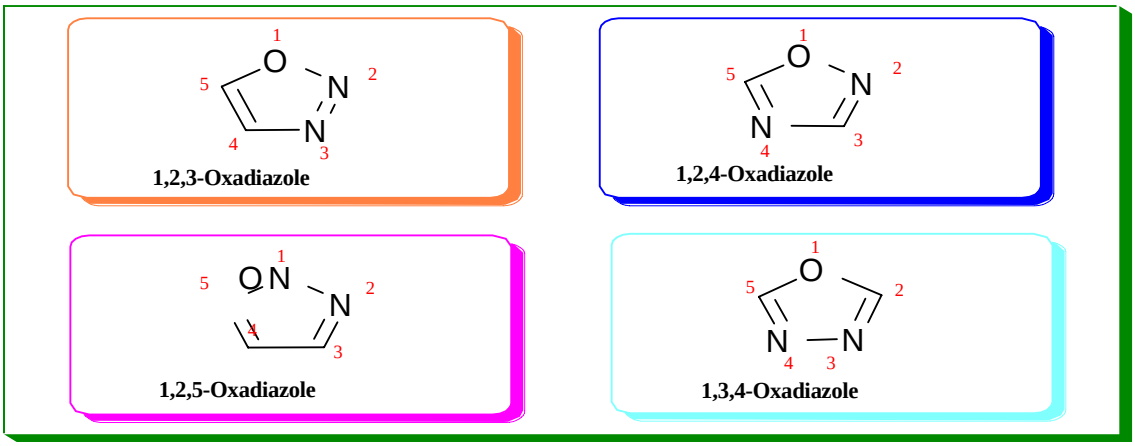


Fig:- Different isomers of Oxadiazoles

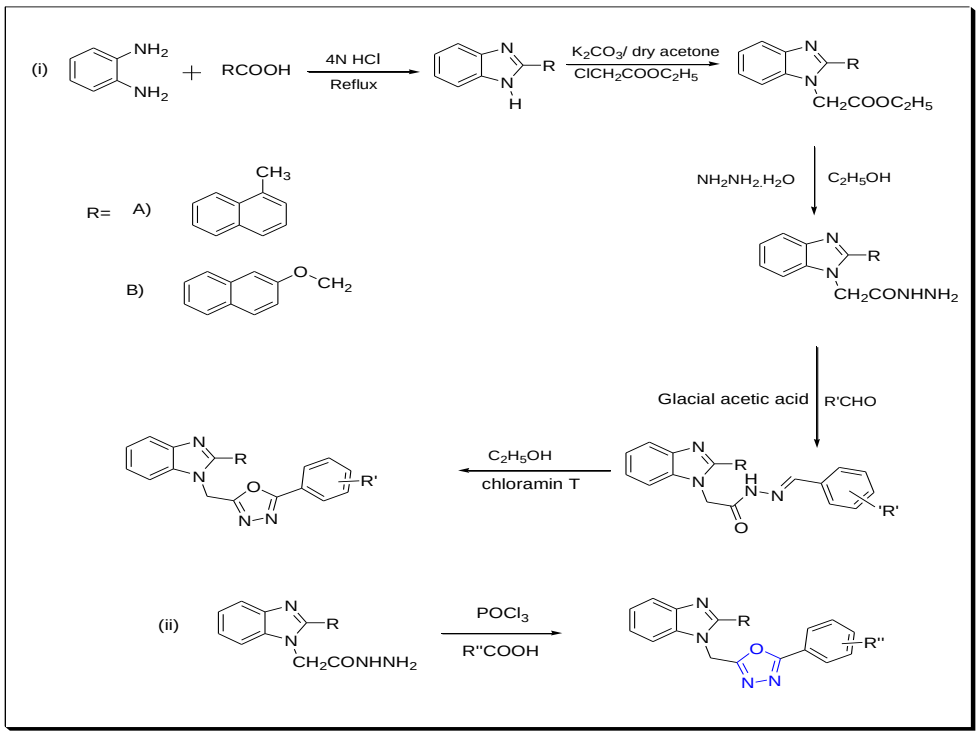
Searching and synthesis of novel compounds: It is an important, challenging task for medicinal chemists to develop new anticancer, anti-microbial, anti-inflammatory, analgesic, antitumor, anticonvulsant, anti-mycobacterial and anti-oxidant agents. There are two basic approaches for the development of new drugs:

a) Synthesis of analogous and their modifications as well as derivation gives novel substituted compounds for better and improved treatment

b) Searching and synthesis of novel compounds, that the bacteria and diseases has never been presented before. For this purpose, substituted 1,3,4-oxadiazoles are already being used as potent antimicrobial, anti-inflammatory, analgesic, anti-tumor and anticonvulsant documented as well as patented.

Salahuddin et al. (2014), were synthesized and characterizes a series of 1,3,4- oxadiazole derivatives **[Scheme-1]** and evaluated for anticancer activity.

R'=H,4-Cl,4-NO_2,4-OCH_3,4-dimethylamino,2-OH:R"-Cl,=H,24-NH_3,4-NO_2, 3,5-diNO_2



[Scheme-1]

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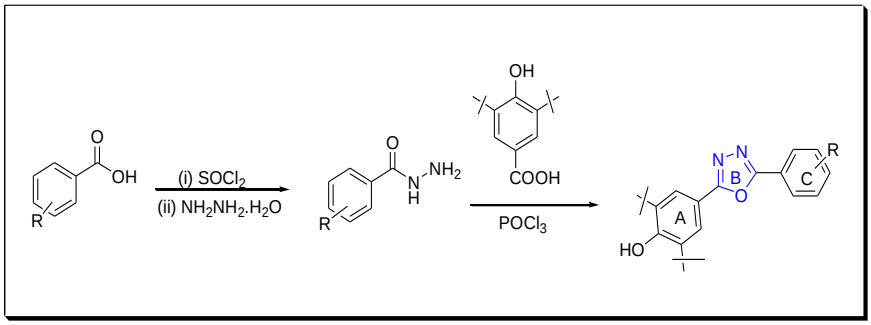
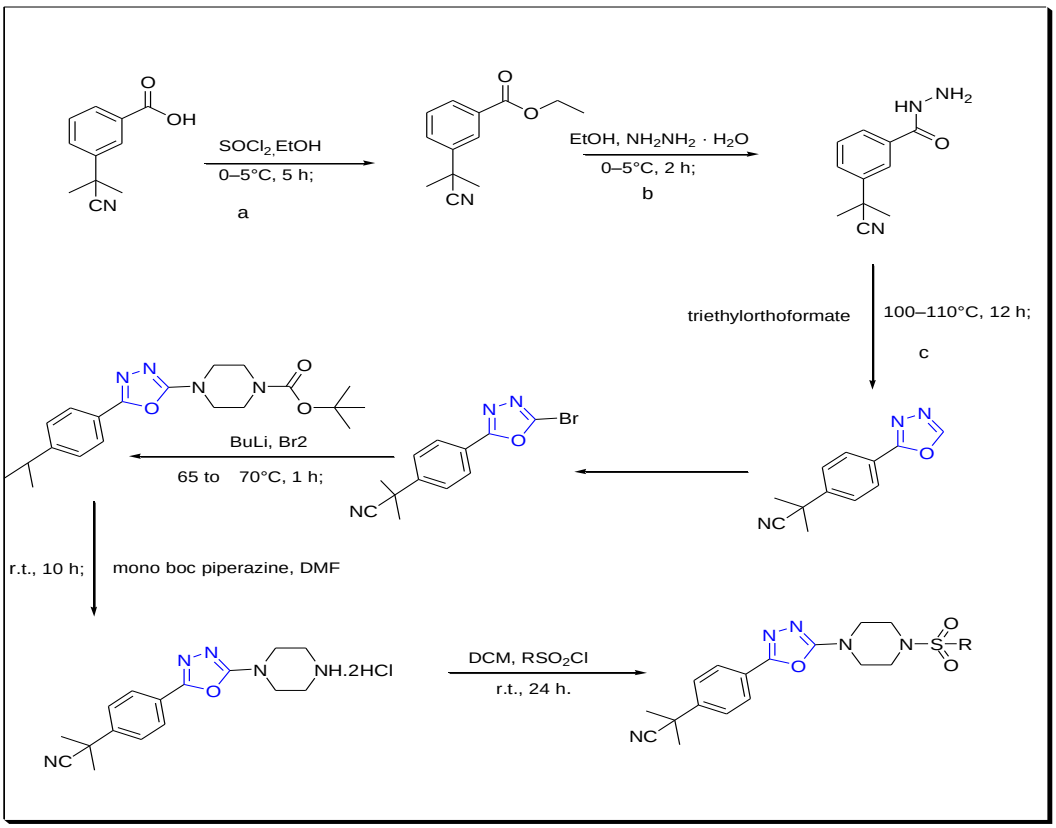
Shakir, et.al. (2014) were synthesized of new 2,6-di-tert-butyl-4-(5-aryl-1,3,4-oxadiazol-2-yl) phenols **[Scheme-2**s**]** reacting aryl hydrazides with 3,5-di-tert butyl 4-hydroxybenzoic acid in the presence of phosphorus oxychloride and screened against antioxidant activity using Molecules 2014, 19 3447 the FRAP and DPPH assays.



[Scheme-2]

Kikkeri, et al., (2014) were synthesized a new series of novel 2-methyl-2-[3-(5-piperazin-1-yl-[1,3,4]oxadiazol-2-yl)-phenyl]-propionitrile derivatives **[Scheme-3]**.and evaluated them for their anticonvulsant activity.



[Scheme-3]

Qiao, Fang. Etal, (2015) were synthesized a novel series of 4-alkoxy quinazoline derivatives containing 1,3,4-oxadiazole derivatives [**Scheme-4**] and designed a novel inhibitor of VEGFR2. Were evaluated their anti-proliferative activities against A549, MCF-7 and Hela cell lines.

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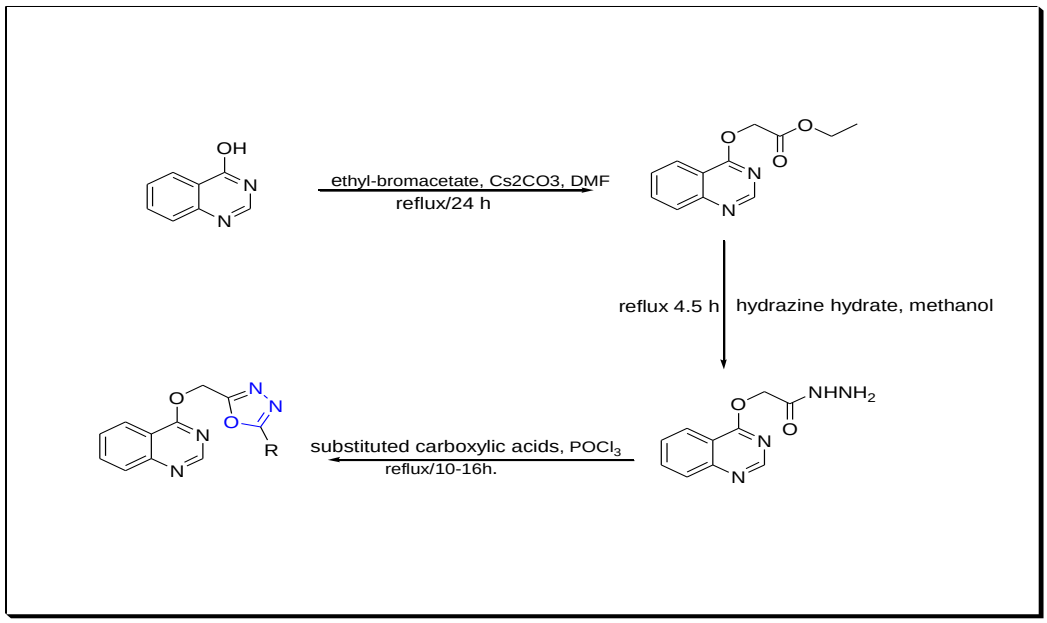
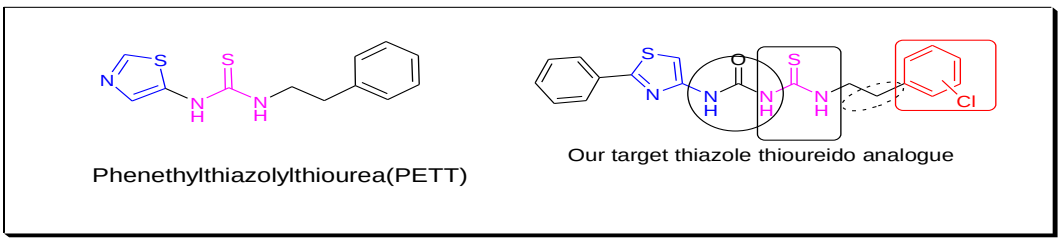
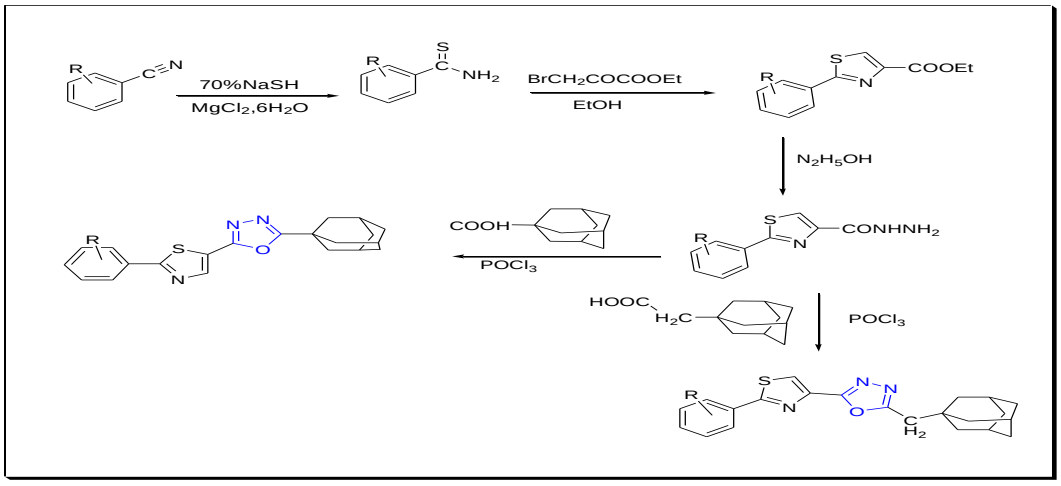


[**Scheme-4**]

Khan et al. (2015) was synthesized of new series of 2-adamantyl-5-arylthiazolyl-1,3,4-oxadiazoles derivatives and 2-phenylthiazole-4-carboxamide analogs A and B**. [Scheme-5]** were evaluated in vitro toxicity and anti proliferative activity against human immunodeficiency virus type-1 and human immunodeficiency virus type-2 activity in MT-4 cells.



(A)



(B)

[Scheme-5]

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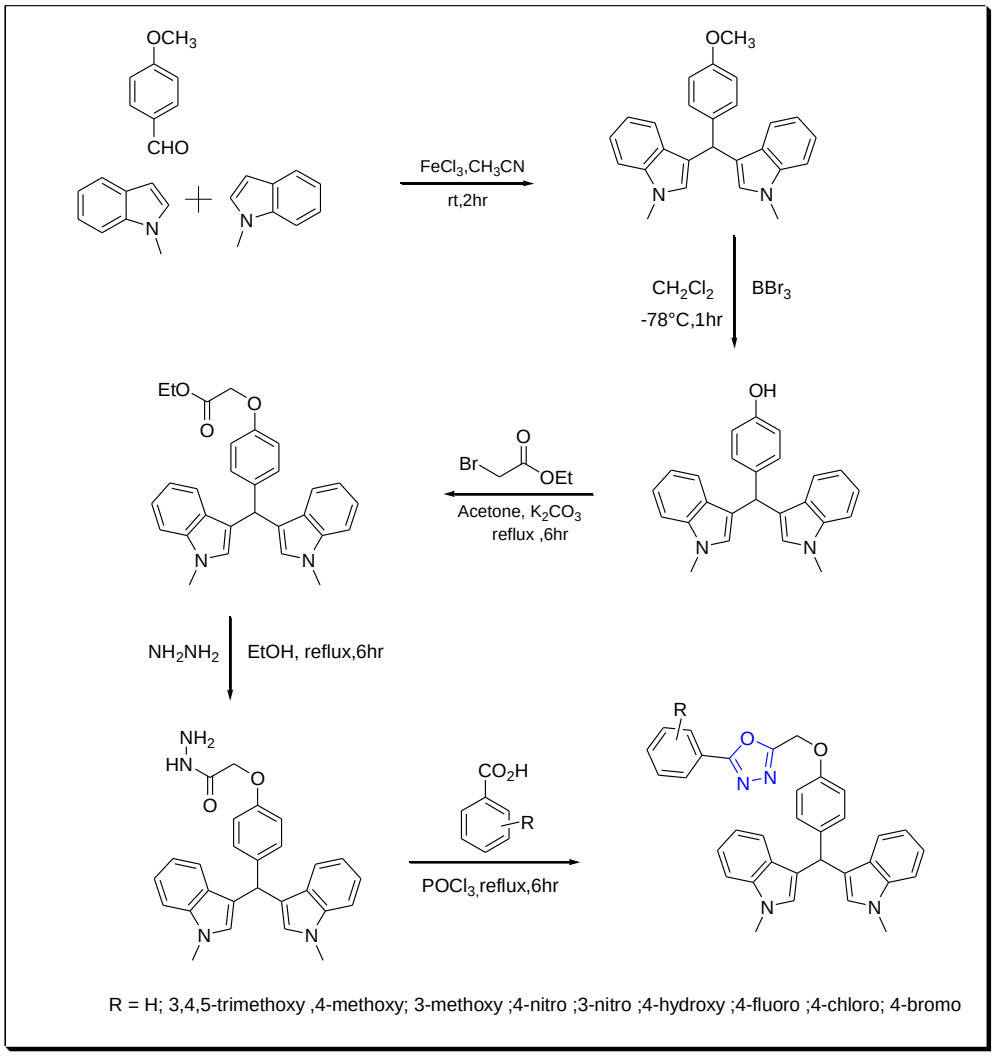
Hatti et al. (2015) synthesized. A newer novel series of ten 1,3,4-oxadiazole-linked bis-indole derivatives **[Scheme-6]** were evaluated the anticancer activity against selected human cancer cell lines, that is breast (MCF-7), oral (KB), colon (Colo-205), and lung(A-549) origin by employing the sulforhodamine B (SRB) assay method.



[Scheme-6]

Qi DQ, etal, (2015) were designed and synthesized a series of pyrazole-based 1,3,4-oxadiazole derivatives **[Scheme-7]**. The fluorescence properties of all the compound were analyzed in dimethyl sulfoxide media and were evaluated for their n vitro inhibitory activity against commercial enzyme xanthine oxidase (OX) by measuring the formation of uric acid from xanthine.

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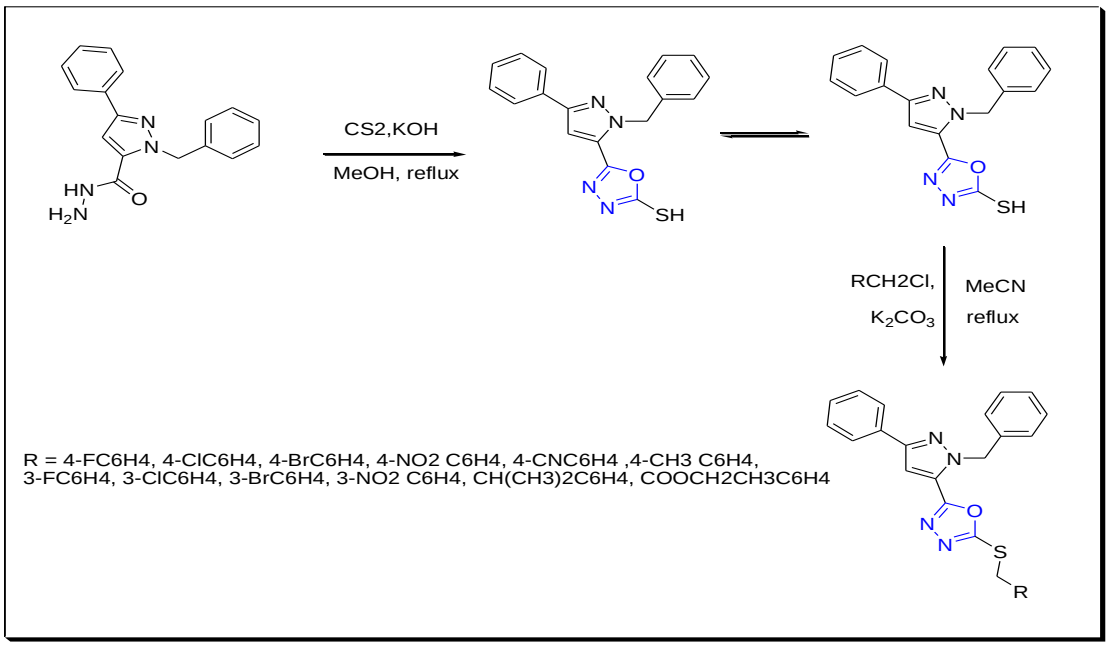
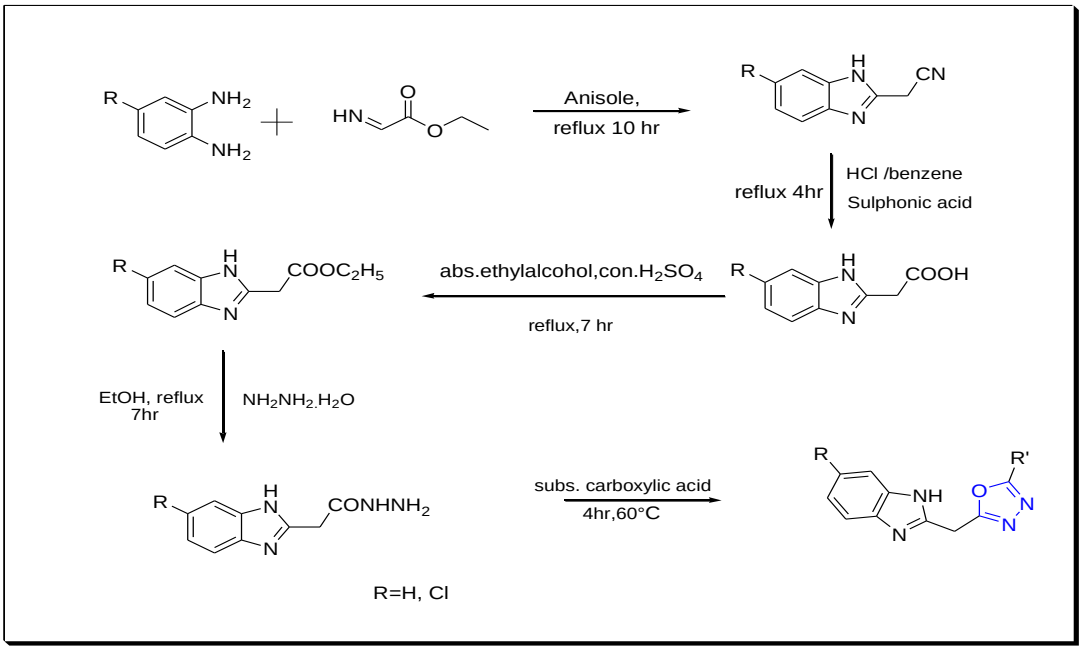


[Scheme-7]

Akhtar M.d. et. al. (2016), synthesized a newer novel series of benzimidazole linked oxadiazole derivatives **[Scheme-8]** designed as potential EGFR and erbB2 receptor inhibitors with anticancer and apoptotic activity.



[Scheme-8]

Nisha M. Jagtap,et al. (2016), were synthesized a newer novel series of N-substituted-2-thione-1,3,4-oxadiazole-3(2H)-yl derivatives **[Scheme-9]** by microwave method and having in vitro anticancer activity against MCF-7 cell lines.

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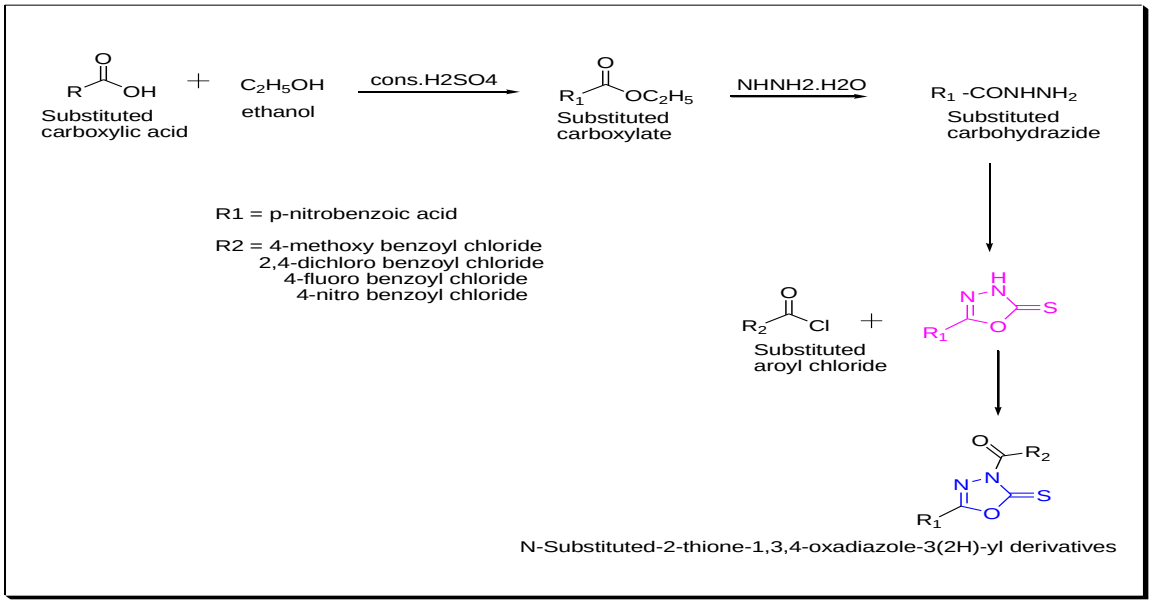
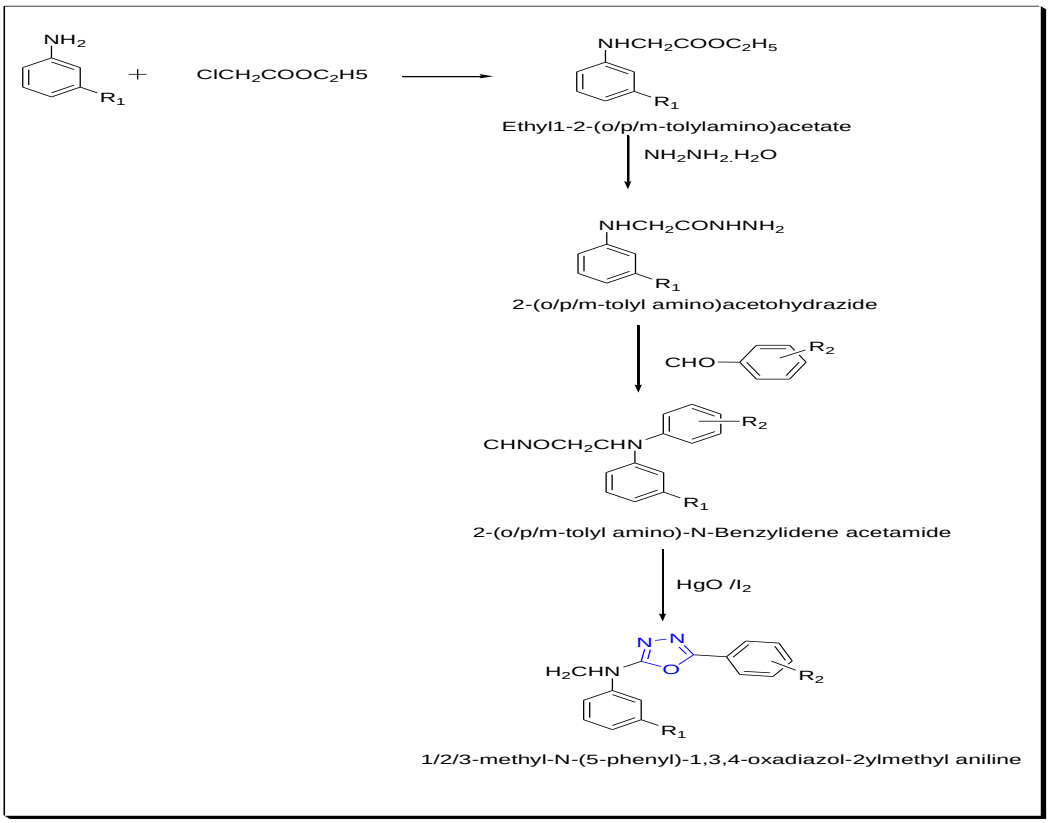


[Scheme-9]

Rawat B.S. et al, (2017) synthesized and Characterization of Substituted Aniline Oxadiazole Derivatives **[Scheme-10]**. Isomeric forms of ortho/meta/ p-toluidine, is converted to 3- methyl-N-(5- substituted phenyl)-1, 3, 4 oxadiazol-2yl-methyl aniline and evaluated for anti-inflammatory activity.



[Scheme-10]

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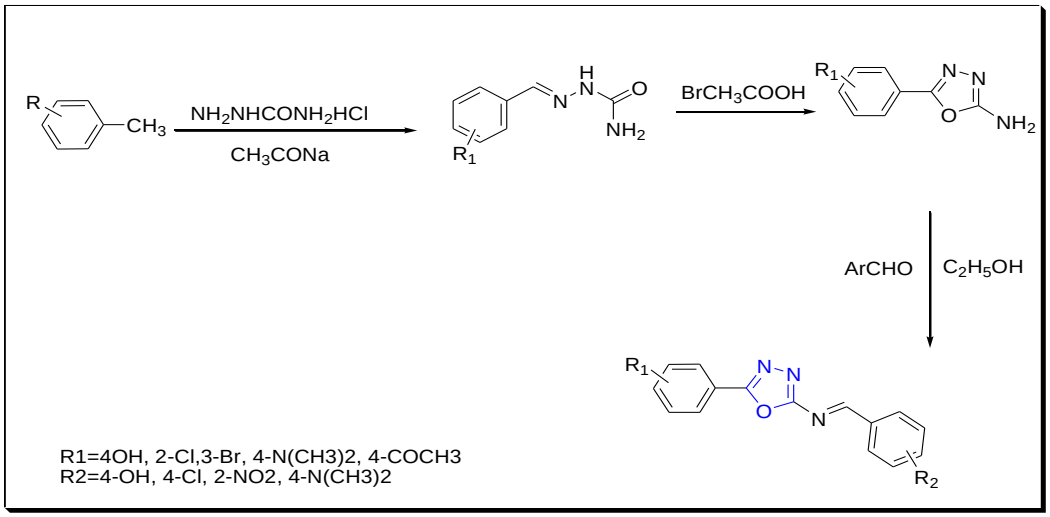
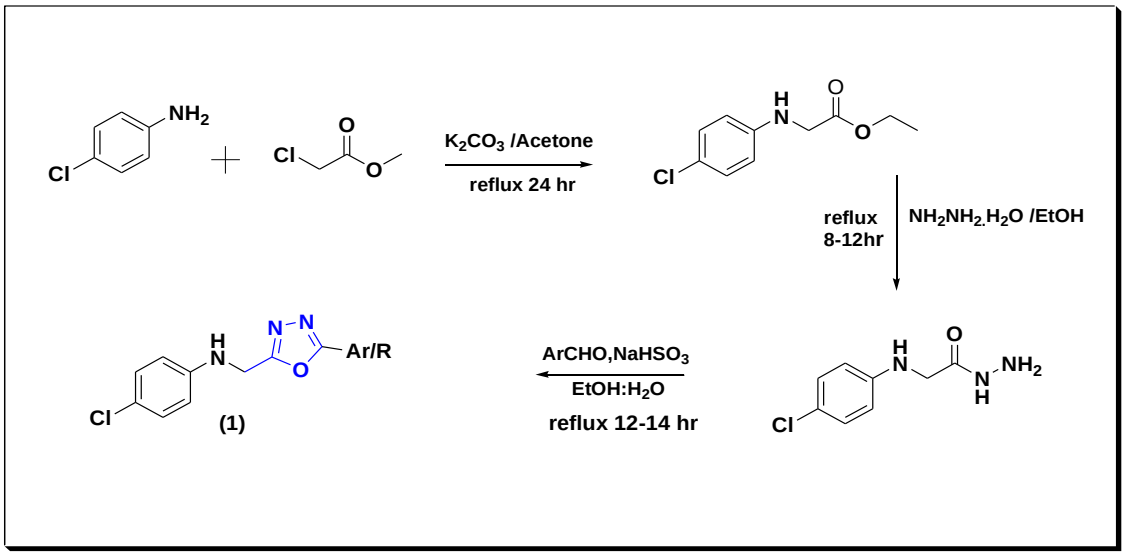
Roy PP, et al., (2017) were synthesized a novel series of 2, 5-disubstituted 1, 3, 4-Oxadiazole derivatives **[Scheme-11]** using different aromatic benzaldehyde and. the evaluated for their anticancer activity against Ehrlich Ascites Carcinoma (EAC) bearing albino mice**.**



[Scheme-11]

Ahsan M.J.et al.(2017), synthesized two novel series 2-(5-{[(4-Chlorophenyl) amino] methyl}-1,3,4-oxadiazol-2-yl) phenol and 2-[(2,4-dichlorophenoxy) methyl]-5-(3,4-dimethoxyphenyl)-1,3,4-oxadiazole. Compound showed maximum cytotoxicity with the mean (GIs) of 71.56 and 72.68 respectively **(1)** and **(2)** also inhibited the polymerization of tubulin with, an IC50 of 2.8 and 2.2 µM, respectively **[Scheme-12].**



[Scheme-12 (1)].

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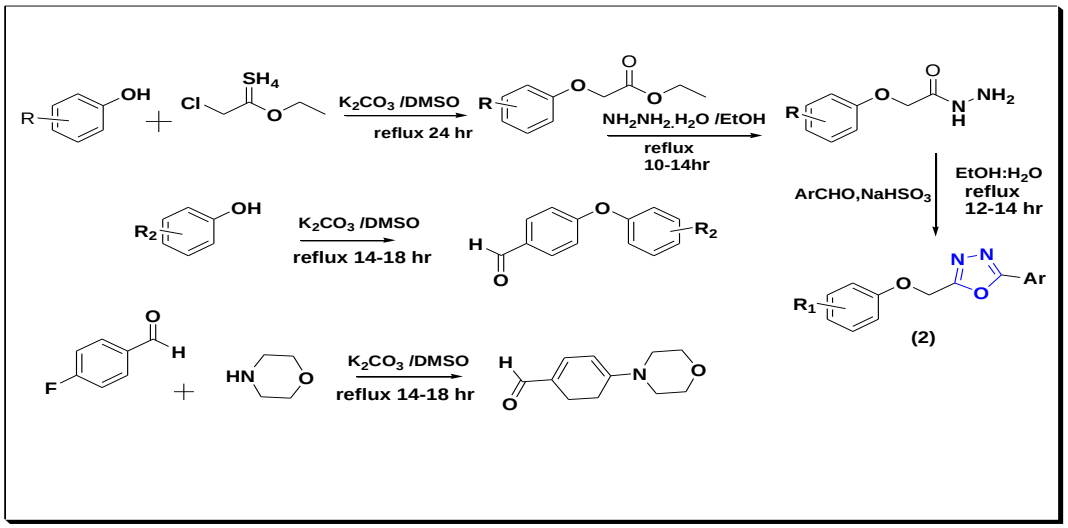
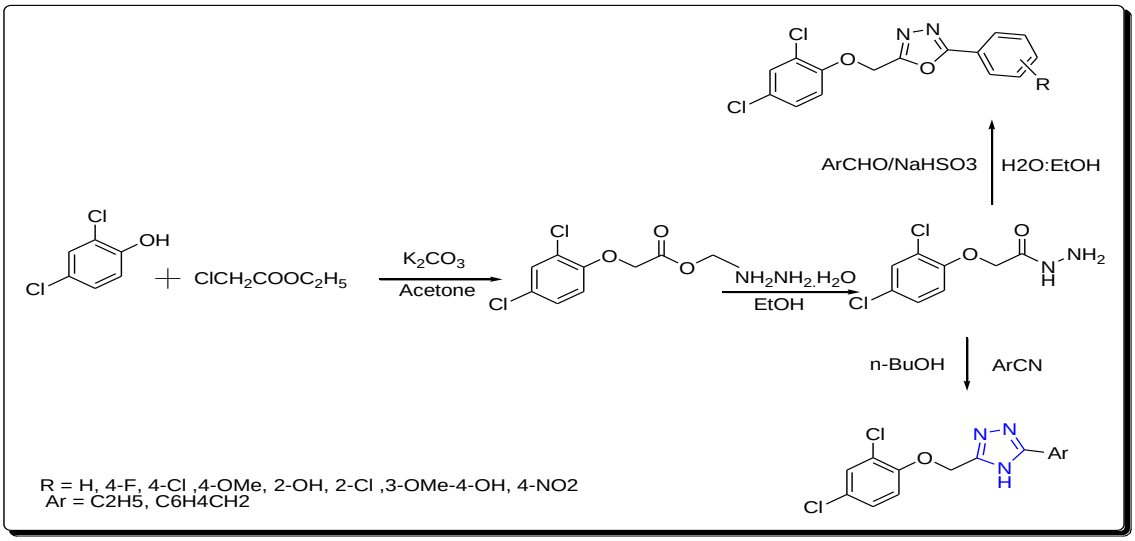


[Scheme-12 (2)].

Ahsan M.J. (2018), were synthesized, characterizes of a newer novel series of oxadiazole and triazole derivatives **[Scheme-13].**evaluated for anticancer activity and comparable to that of the standard anticancer drug, 5-fluorouracil, and better than that of Imatinib.



[Scheme-13].

Fathi, et al. (2018) were synthesized & designed A new series of 1,3,4-oxadiazole/chalcone hybrids **[Scheme-14]**were having anti-tumor activity & evaluated as inhibitors of EGFR, Src, and IL-6.

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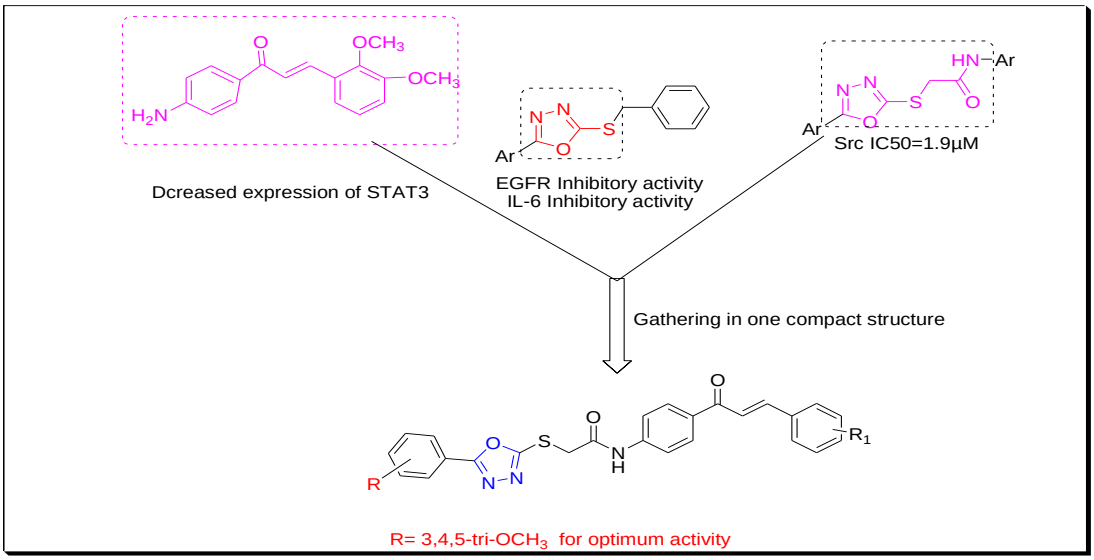
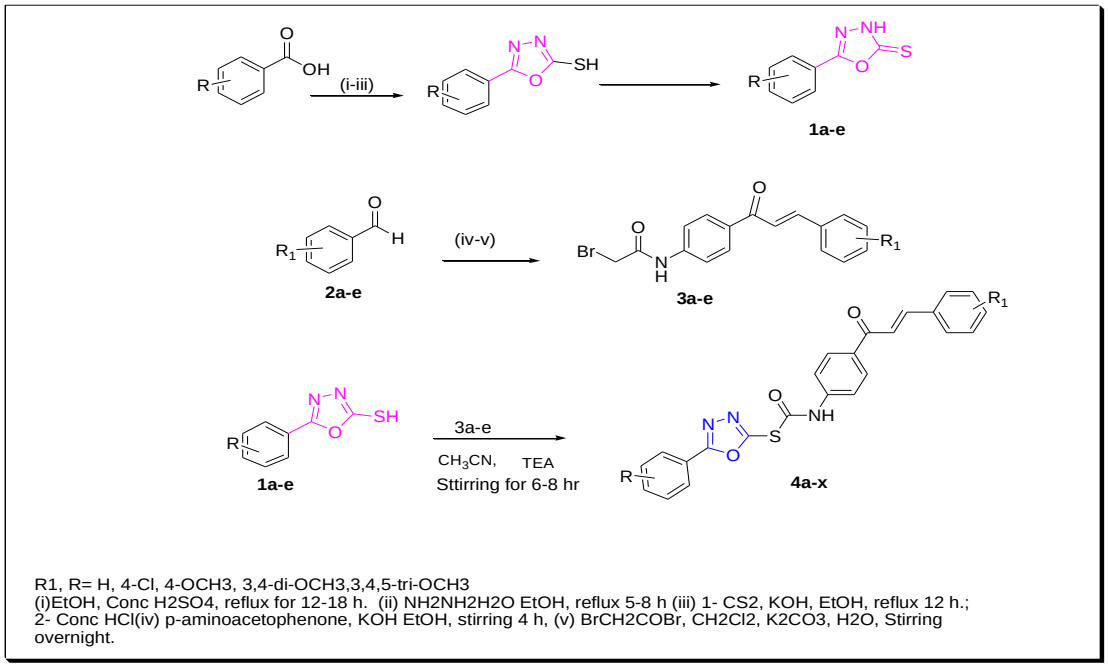


[Scheme-14]



[Scheme-14]

Polothi R.et al., (2019) Synthesis a series of novel analogs of 1,3,4-oxadiazole embedded with 1,2,4-oxadiazole derivatives **[Scheme-15]** as tubulin binding agents and evaluated for their in vitro anticancer activity against three human cancer cell lines (MCF-7, A459 and MDA MB 231).

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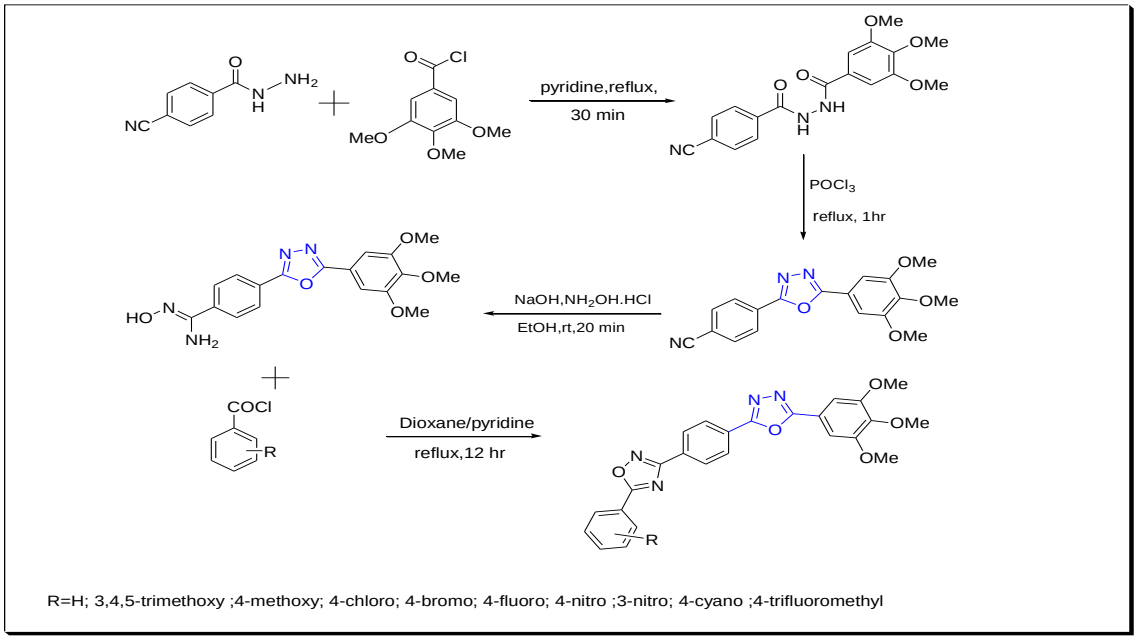
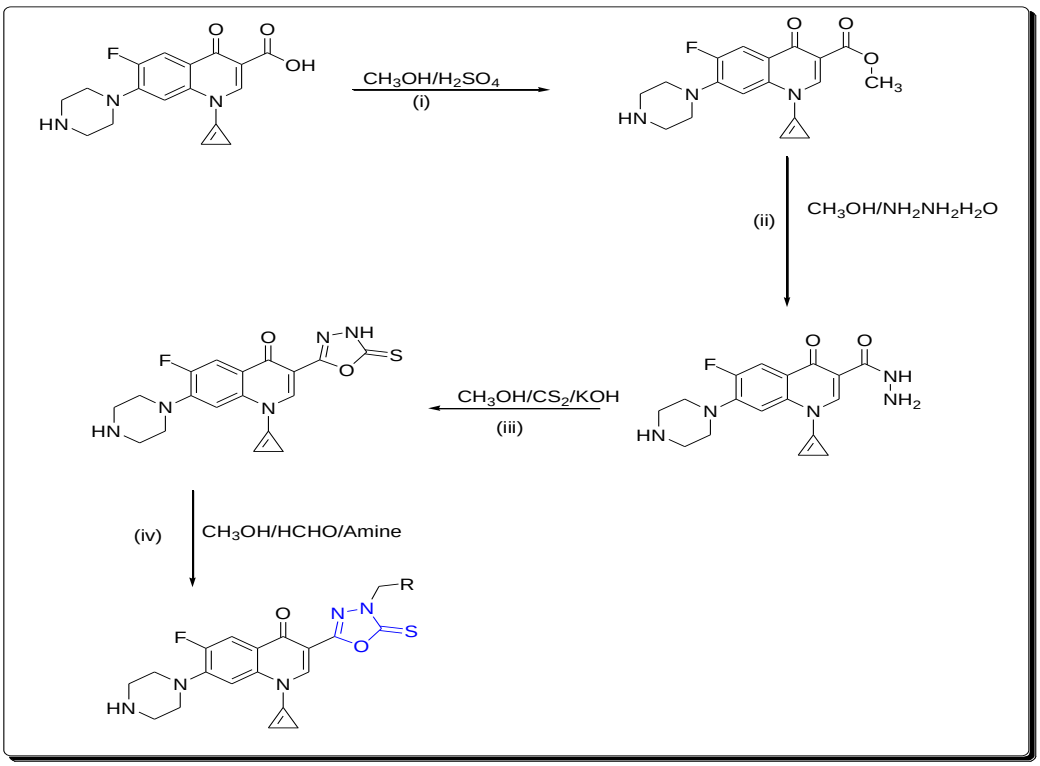


[Scheme-15]

Singhai et al. (2019), Synthesized a newer novel series of substituted 1,3,4-oxadiazole derivative **[Scheme-16]** starting from amine with 1-cyclopropyl-6-fluoro-7(piperazin-1-yl)-3-(5-thioxo-4,5-dihydro-1,3,4-oxadiazol-2-yl) quinolin-4(1H)-one (III)and evaluated for anti-bacterial activity against all Gram-positive and Gram-negative organisms.



[Scheme-16]

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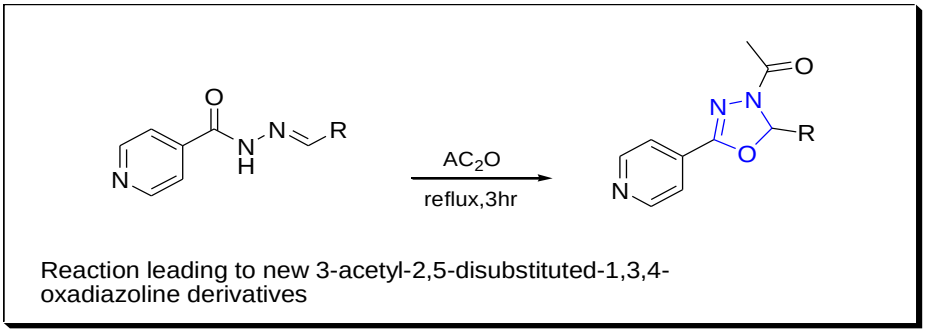
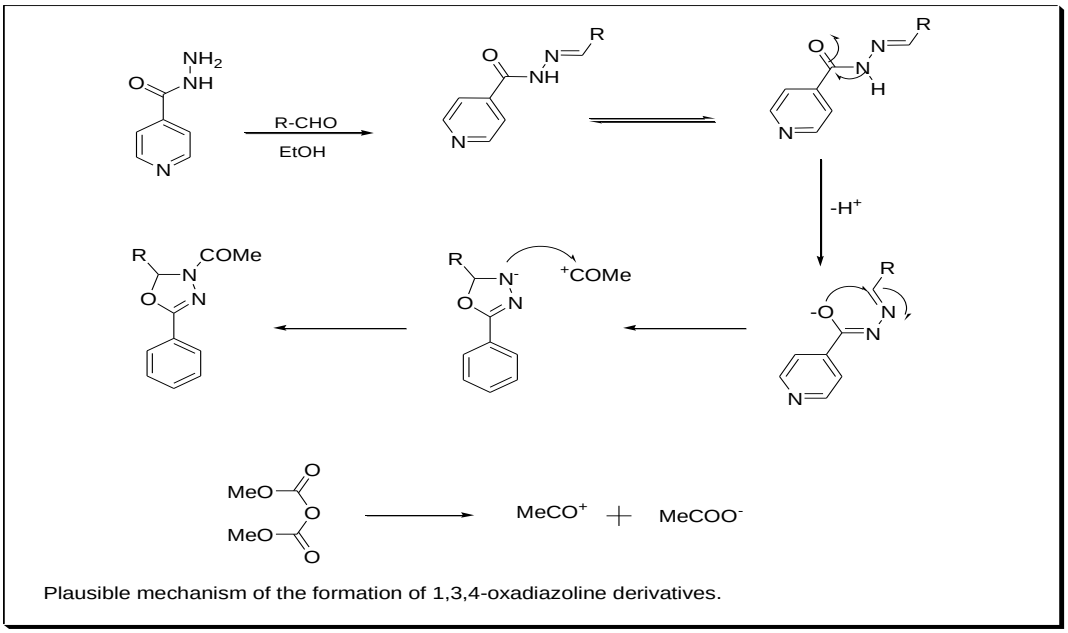
Lukasz Popiołek et.al. (2019) Synthesized of New 3-Acetyl-2,5-disubstituted-1,3,4-oxadiazoline Derivatives **[Scheme-17]** and evaluated them for their in vitro antimicrobial activity.



Reaction leading to new 3-acetyl-2,5-disubstituted-1,3,4-oxadiazoline derivatives



Plausible mechanism of the formation of 1,3,4-oxadiazoline derivatives.

[Scheme-17]

Çevik et al. (2019), were synthesized a novel series 2-[(5-(4-(5(6)-substituted-1H-benzimidazol-2-yl) phenyl)-1,3,4-oxadiazol-2-yl) thio]-1-(4-substitutedphenyl) ethan-1-ones derivatives **[Scheme-18]** have evaluated for DNA Topo inhibition and cytotoxicity. Anticancer activity of these compounds was assessed against two different human cancer cell lines A549 (human lung adenocarcinoma) and HepG2 (human liver cancer cell line), as well as normal mouse embryonic fibroblast cells (NIH3T3).

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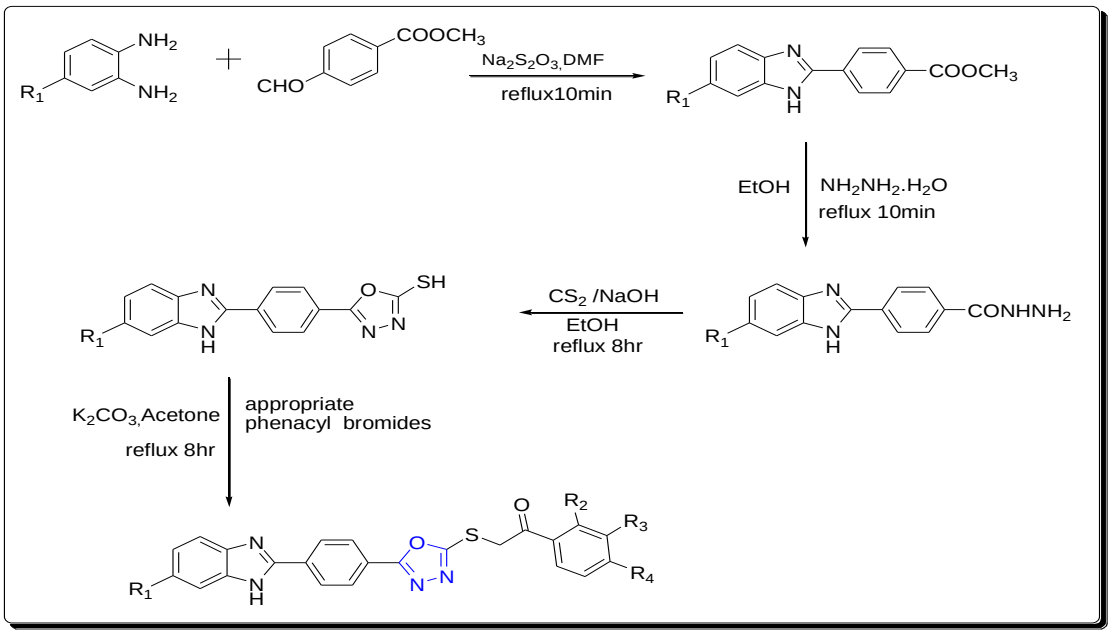
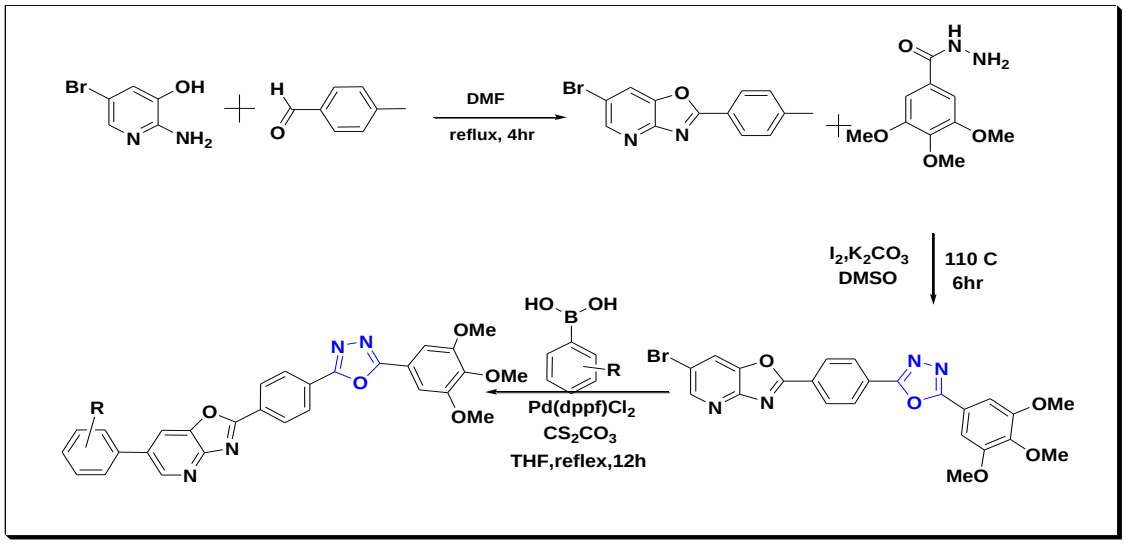


[Scheme-18]

Kokkiligadda, et al., (2020) were Synthesized of 1,3,4-oxadiazole incorporated oxazole [4,5-b] pyridine derivatives **[Scheme-19]** and evaluated for in vitro cytotoxicity. Anti-cancer activity against four different human cancer cell lines including (MCF-7), (A549), (Colo-205), (A2780) by the MTT method using etoposide as the standard drug.



[Scheme-19]

Vema et al. (2020), synthesized a newer novel series of 1,3,4-Oxadiazole linked Resveratrol derivatives **[Scheme-20]**. the compounds were evaluated against four different human cancer cells including **MCF-7,(IC 50 = 1.56, 0.45 µM**, respectively) **MDA MB-231** (Breast)**(IC 50 = 1.22, 1.98 µM**, respectively). and **A549** (Lung) cell lines **(IC 50 = 0.11, 1.11 µM**, respectively.

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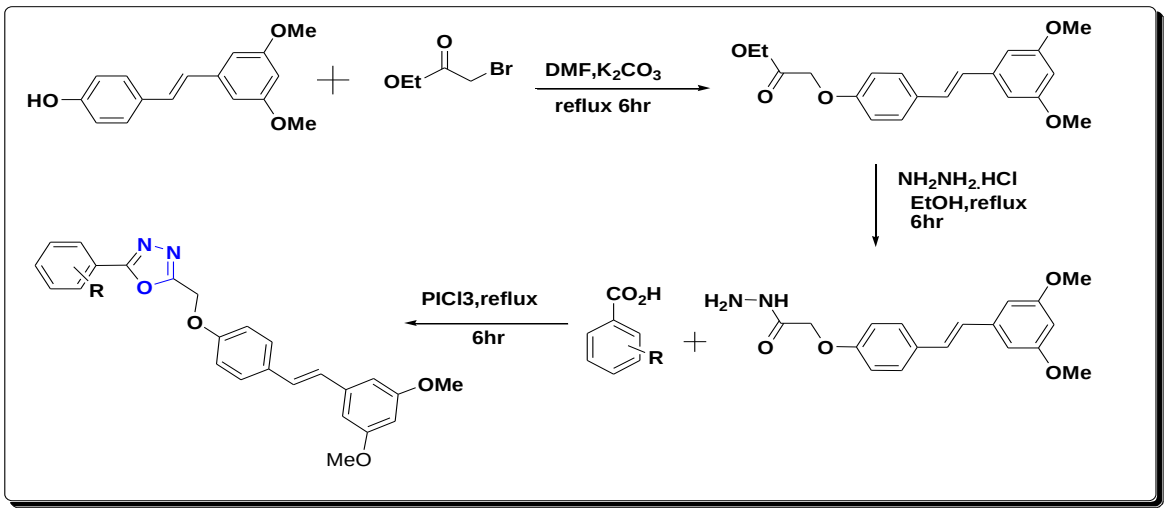
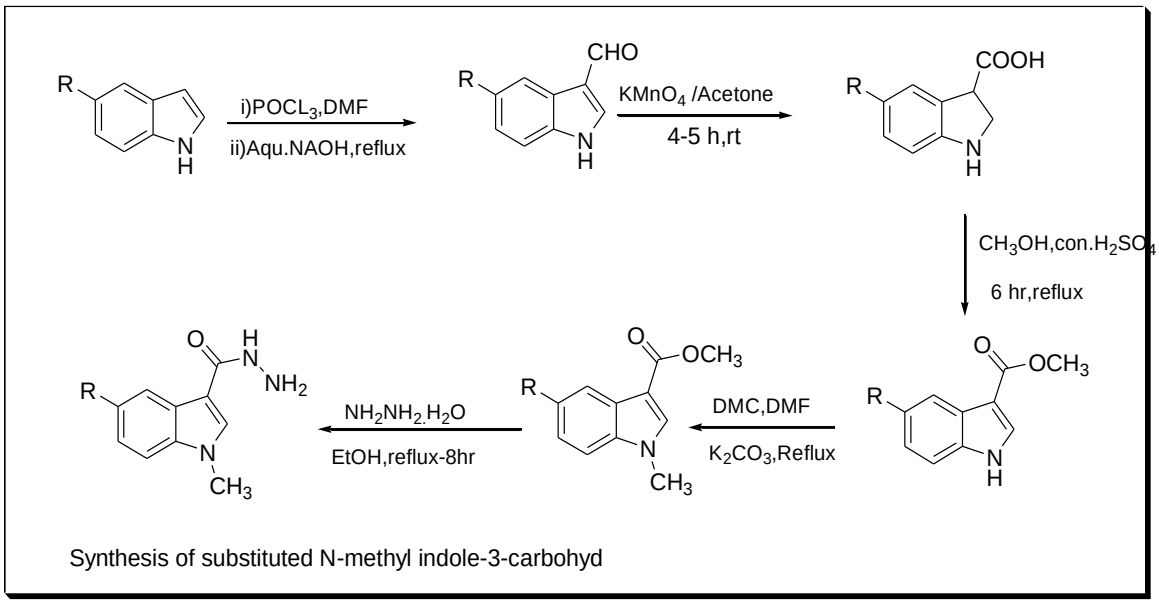


[Scheme-20].

Sreenivasulu et al. (2020) synthesized and designed a newer series of ten novel 2,5-bis(indolyl)-1,3,4-oxadiazoles derivatives **[Scheme-21].** The in vitro cytotoxicity effects of synthesized compounds were evaluated against four different human cancer cells including A549, MDA-MB-231, MCF-7 and HeLa IC50 value of 3.3 µM, 2.6 µM, a1.8 µM and 6.34 µM respectively.



[Scheme-21].

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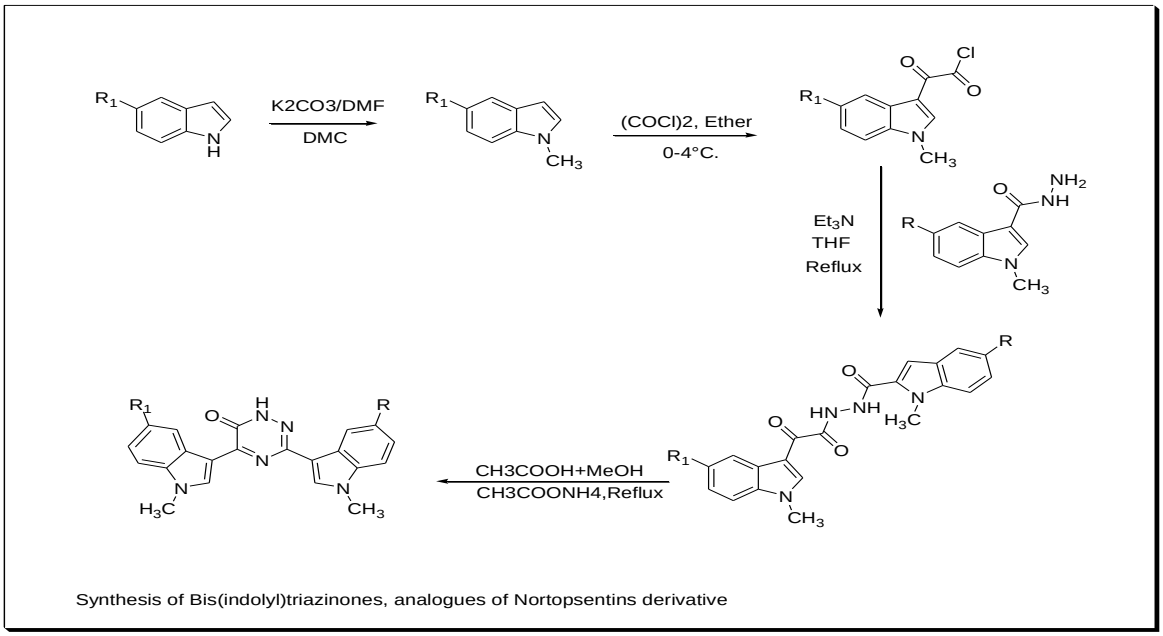
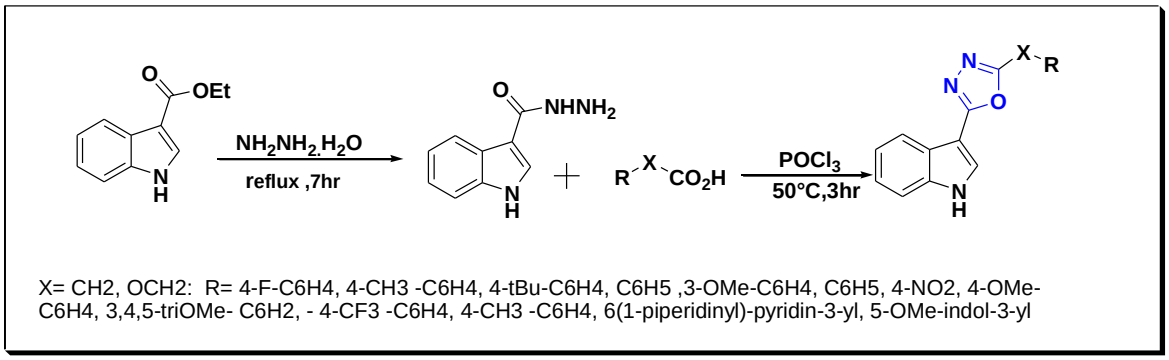


[Scheme-21].

R. Hamdy (2020) were synthesized A novel series of 2-(1H-indol-3-yl)-5-substituted-1,3,4-oxadiazoles derivatives **[Scheme-22]** were designed, evaluated having anti-proliferative activity against human cancer cell lines MDA-MB-231, HeLa, KG1a; sub-micromolar IC50 values of 0.52–0.88 µM respectively.



[Scheme-22]

Eid E. Salama et.al. (2020) were synthesized and characterized of new 2-amino-1,3,4-oxadiazole derivatives **[Scheme-23]** and evaluated for their anti-bacterial activity against gram-negative bacteria Salmonella typhi.

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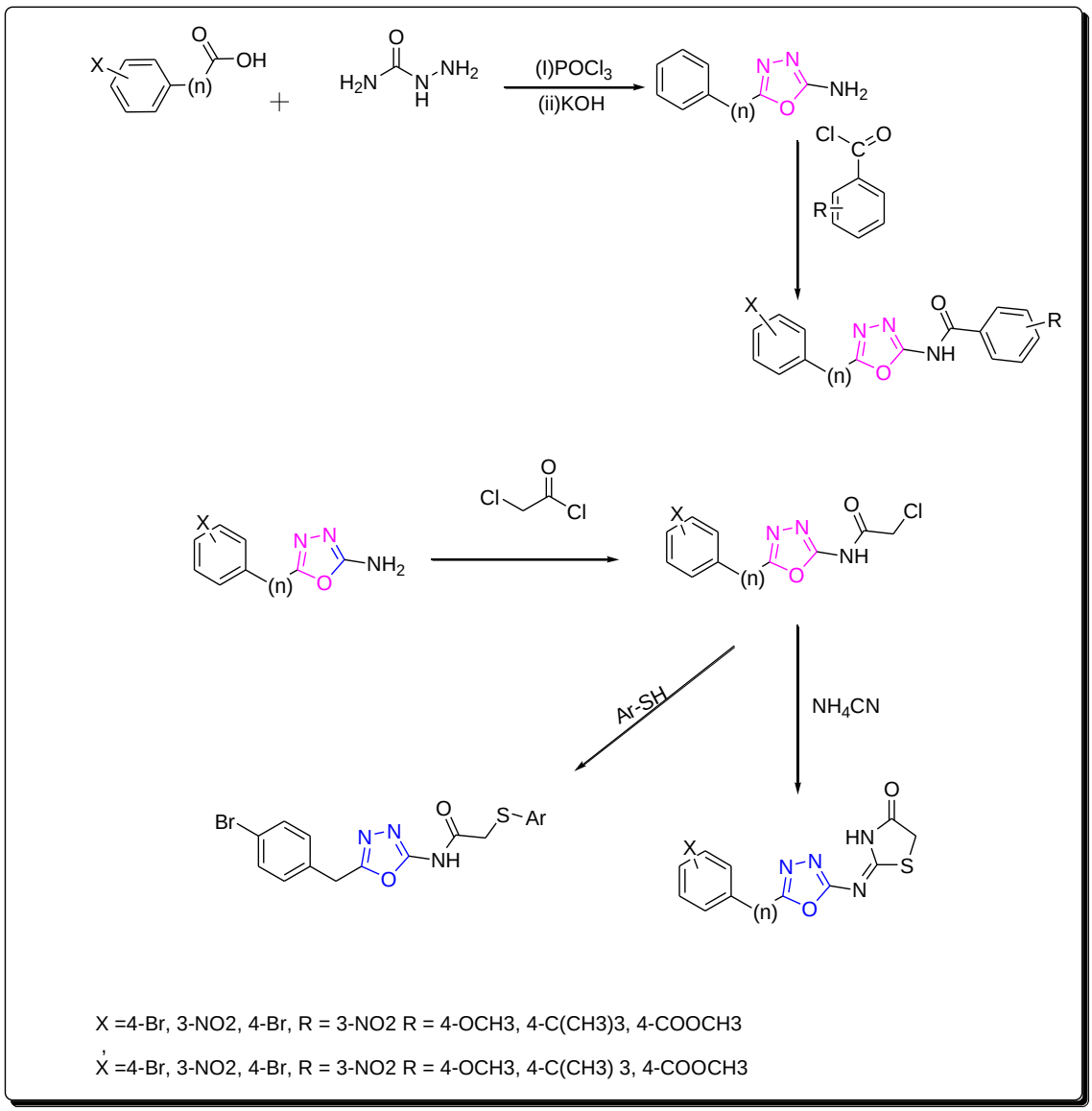

[Scheme-23]

Kadambar A.K., et.al (2020) were synthesized of one-pot three-component azide-alkyne cycloaddition of 5-chloro-1- phenyl-pyrazole-4-carbaldehyde with 2-(prop-2-yn-1-ylthio)-5-((substituted phenoxy) methyl1,3,4-oxadiazole and sodium azide **[Scheme-24]** having in vitro anti-inflammatory activity being comparable with that of the standard drug diclofenac sodium.

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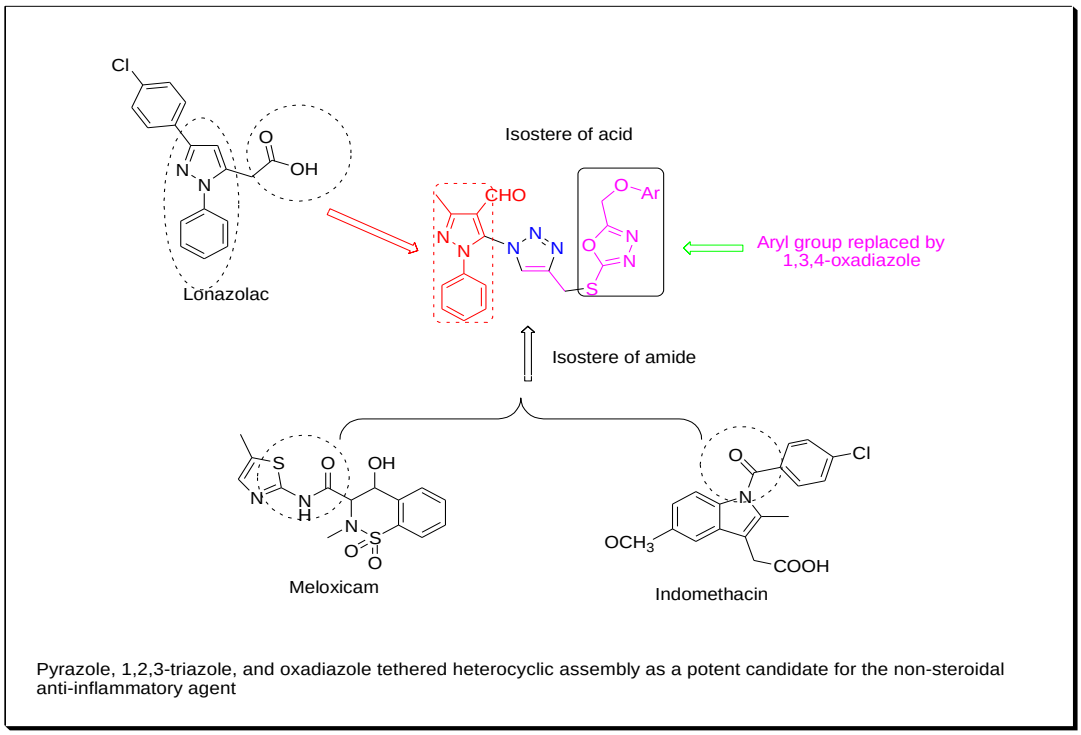
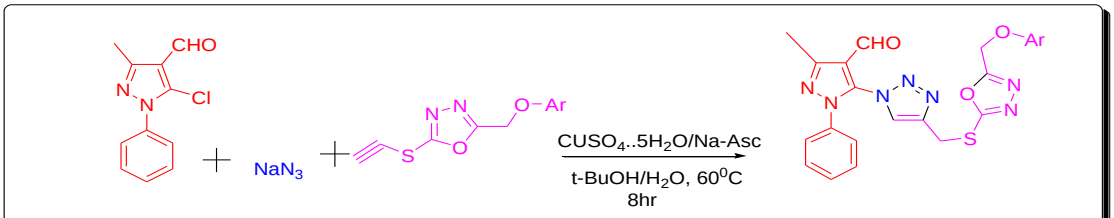


Pyrazole, 1,2,3-triazole, and oxadiazole tethered heterocyclic assembly as a potent candidate for the non-steroidal anti-inflammatory agent



The substrate scope of one-pot three-component azide-alkyne cycloaddition reaction

Ar= 4-Methylphenyl; 2,3,5-Trimethylphenyl; 2-Chlorophenyl; 4-Chlorophenyl; 4-Chloro-3-methylphenyl; 2,4-Dimethylphenyl; 4-Nitrophenyl; 2,4-dichlorophenyl; 3-Chlorophenyl; 2-Naphthyl Phenyl; 2-methylphenyl

[Scheme-24]

Naclerio G.A., et. Al. (2021) were synthesized newer N-(1,3,4-oxadiazol-2-yl) benzamides derivatives **[Scheme-25]** antibacterial activity against Gonorrhea& other Gram-positive and Gram-negative pathogens.

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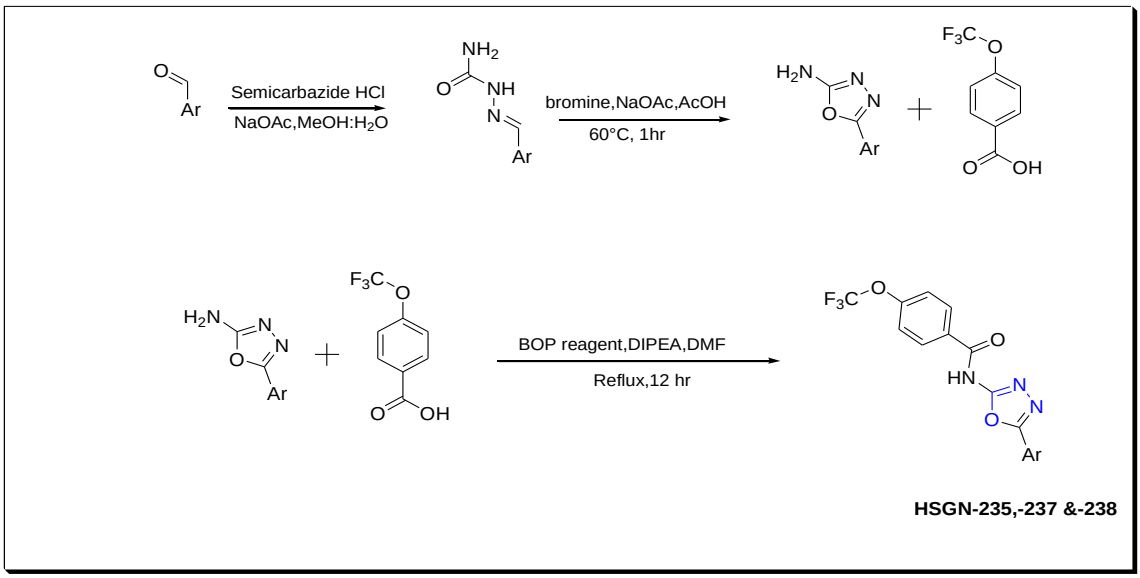

[Scheme-25]

II. CONCLUSION:

The pharmacological potential of 1,3,4-oxadiazole nucleus is cleared from the literature and clinically used drugs. The literature revealed that 1,3,4-oxadiazole possess diverse biological potential, easy synthetic routes for the synthesis and taken the attention of researchers. Though it can be concluded that antimicrobial, antifungal, anti-inflammatory and anti-cancer are the four major areas of clinical use in which much efforts has been done, some other potential targets also showed good results such as enzyme inhibitors and antiviral but these are still to be explored. From these observations important of the nucleus is highlighted.

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