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A Review: 1,2,4-oxadiazole as Potential Anticancer Scaffold 2020-2024.

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ABSTRACT

Cancer is one of the common dangerous diseases caused by uncontrolled cell growth leading to tumour formation. Compounds containing hetero atom in cyclic ring are playing a vital role for the development of potent anticancer agents. Numerous anti-cancer agents are available in market which contain hetero atom in cyclic ring. Among the heterocyclic ring oxadiazole is of great interest in the recent era due to their potential anti-cancer activity. 1,2,4-oxadiazole is a five-member ring containing heterocyclic compound which contain two nitrogens at 2nd and 4th position and one oxygen at 1st position. The 1,2,4-oxadiazole formed hydrogen bond with biomacromolecule and showed various pharmacological activity. Literature survey revealed that 1,2,4-oxadiazole showed potent antibacterial, anti-inflammatory, anti-tuberculous, anti-fungal, anti-diabetic and anticancer activities activity. In this review work, we discuss 1,2,4-oxadiazole derivatives as anticancer agents that have been reported in the last five years only (2020–2024) as there was no report or their activities described in any article in 2019. This work summarized chemical structure of oxadiazole derivatives, anticancer activity of 1,2,4-oxadiaozole derivatives. Overall, this review underscores the pivotal role of 1,2,4-oxadiaozole advancing our understanding of anticancer activity and guiding to researcher to develop better anticancer agents in field of medicinal chemistry.

Keywords: Anti-cancer, Oxadiazole, Structure activity relationships, Breast cancer, Colon cancer.

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INTRODUCTION

Now a day's cancer is a life-threatening disease impacting human health. Medicinal researchers have discovered several chemotherapeutic agents but several of them showed drug resistance and have several side effects. Oxadiazole is a crucial pharmacophores that are responsible for binding to the active site residues of receptor that are responsible for cancer [1]. Oxadiazole is a heterocyclic aromatic scaffold that is capable of connecting with a variety of substituent's and exhibits anti-cancer activity by targeting various enzymes or signalling pathways [2].

Oxadiazole have four different isomer among them 1,2,4-oxadiazole is an important pharmacophore reported with significant biological activity. Due to metabolic profile and hydrogen binding ability of 1,2,4-oxadiazole it act as anti-bacterial, anti-inflammatory, anti-tubercular, anti-HIV, anti-fungal, anti-diabetic, anti-oxidant, anti-cancer and cathepsin K (Cat K), monoamine oxidase and tyrosinase inhibitory activity [3-5]. In this review article we mainly focused on anticancer activity of 1,2,4-oxadiazole derivatives against various cancer cell lines. This article aims to describe the chemistry of 1,2,4-oxadiazole, marketed medicine of 1,2,4-oxadiazole, recent different derivatives of 1,2,4-oxadiazole reported as anticancer agents from 2020 to 2024.

Chemistry of oxadiazole

Oxadiazole is an azole category five membered heterocyclic ring which is contains one oxygen and two nitrogen atom. Oxadiazole are great bio-isosteres of amides and esters and follow huckle rule. The (-N=C-O-) azole group of oxadiazole is responsible for its lipophillic nature that influence the ability of oxadiazole derivatives to reach the targeted receptor by transmembrane diffusion [6].

Based on the position of oxygen and nitrogen atom in oxadiazole ring, four constitutional isomers of oxadiazole are formed. All isomers 1,3,4-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole and 1,2,3-oxadiazole are shown in **Figure 1**.

Figure 1: Chemical structure of four different isomer of oxadiazole

Marketed analog of 1,2,4-oxadiazole

The 1,2,4-oxadiazole scaffold have vital pharmacological activity. Some of the marketed products that contain 1,2,4-oxadiazole scaffold are listed below in **Table 1**. The 1,2,4-oxadiazole scaffold also present in natural products Phidianidine A, Phidianidine B and Quisqualic (**Figure 2**). Phidianidine A and Phidianidine B are indole alkaloids isolated from sea slug Opisthobranch Phidiana militaris [7]. Phidianidines are reported *in vitro* cytotoxicity against human cervical (HeLa) and colon adenocarcinoma (CaCo-2) [8, 9]. Quisqualic acid is an alanine derivative and obtained from seeds of Quisqualis indica. It showed affinity to metabotropic glutamate receptor and use in neurodegenerative disorders, epilepsy, and stroke [10, 11].

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Table 1: Marketed analog containing 1,2,4-oxdiazole scaffold [12-14].

S. No.	Drug Name	Pharmacological Application
1.	**Oxolamine**	Cough suppressant
2.	**Prenoxdiazine**	Cough suppressant
3.	**Butalamine**	Vasodilator
4.	**Fasiplon**	Anxiolytic drug
5.	**Pleconaril**	Antiviral drug
6.	**Ataluren**	Duchenne muscular dystrophy treatment
7.	**Proxazole**	Gastrointestinal disorders
8.	**Opicapone**	Parkinson's disease
9.	**Azilsartan medoxomil**	Hypertension
10.	**Ozanimod**	Immunosuppressants
11.	**Amenamevir**	Antiviral to treat herpes infections
12.	**Naldemedine**	Constipation treatment

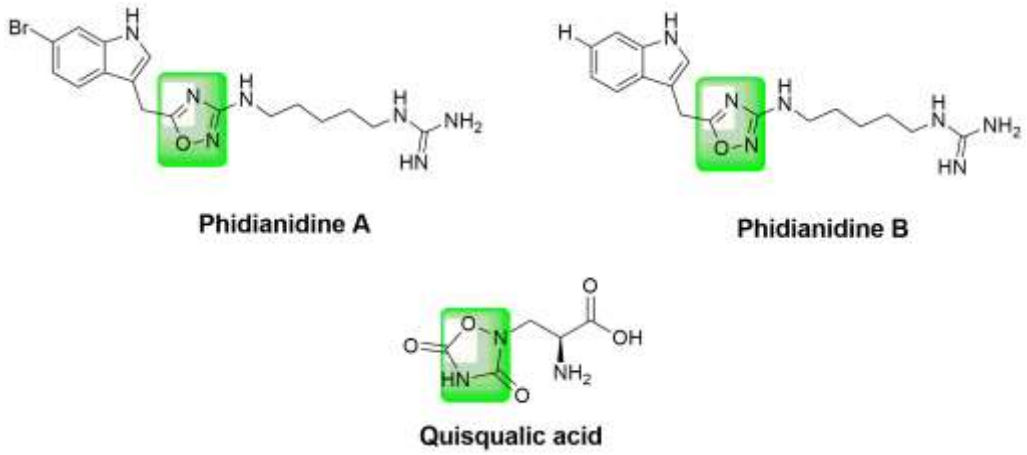

Figure 2: Naturally occurring derivatives containing 1,2,4-oxadiazole scaffold

Different types of cancer and their receptor

Anticancer activity of 1,2,4-oxadiaozle derivatives

Mohamed A.M.et al., 2024, have reported a series of quinazoline-4-one linked 1,2,4-oxadiazole derivatives as anti-proliferative agent. The chemical structure of all synthesized derivatives was confirmed by IR, NMR, MASS, and elemental techniques. All the synthesized derivatives are follows Lipinski rule of five. Compound 1, 2 and 3 showed higher anti-proliferative activity compared to standard drug Erlotinib (**Table 2**). Compound 1, 2 and 3 also reported potent activity against epidermal growth factor receptor (EGFR) and BRAFV600E gene. Compound 1 arrest cell cycle at the G2/M transition phase [15].

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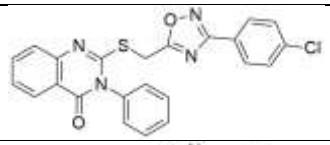
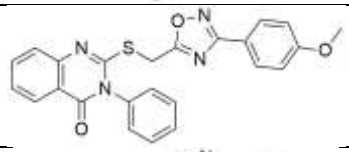
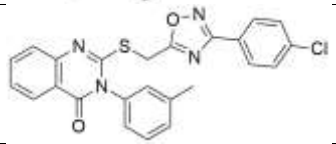
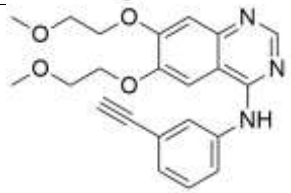
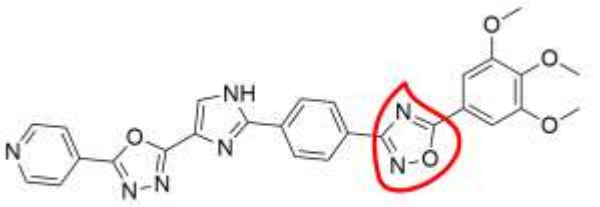
Table 2: Chemical structure of quinazoline-4-one linked 1,2,4-oxadiazole derivatives along with anti-proliferative activity

Compound No.	Compound chemical structure	A-549 IC_{50} nM	MCF-7 IC_{50} nM	Panc-1 IC_{50} nM	HT-29 IC_{50} nM	EGFR inhibition IC_{50} nM	BRAFV inhibition IC_{50} nM
Comp. 1		22 ± 2	26 ± 2	24 ± 2	24 ± 2	57 ± 4	48 ± 4
Comp. 2		24 ± 2	28 ± 3	26 ± 2	25 ± 2	64 ± 5,	51 ± 5
Comp. 3		28 ± 2	31 ± 3	29 ± 2	30 ± 3	72 ± 5	57 ± 5
Standard		30 ± 3	40 ± 3	30 ± 3	30 ± 3	80 ± 5	60 ± 5

Khedkar NR et al., 2024, have designed a series of novel 1,2,4-oxadiazole derivatives by fragment based drug discovery (FBDD) approach. All the designed derivatives was synthesized and evaluated for anti-cancer activity by MTT assay against prostate cancer (PC3 & DU-145), lung cancer (A549), and liver cancer (HEPG2) cell lines. Target specific activity of all synthesized derivatives also against endothelial growth factor receptor (EGFR) also evaluated. MTT assay study result revealed that derivatives **4, 5 and 6** are more potent anti-cancer agents compared to standard drug etoposide. All the derivatives also screened against normal Vero cell line and study result revealed that no compound showed any effect on normal cell lines. **Compound 4** was reported as a highly potent derivative and showed higher cytotoxicity against different cancer cell line reported in **Table 3.** No derivatives reported potent EGFR inhibitory activity compared to standard drug [16].



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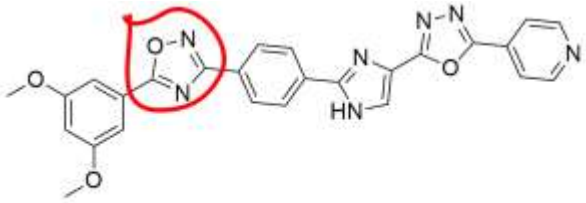

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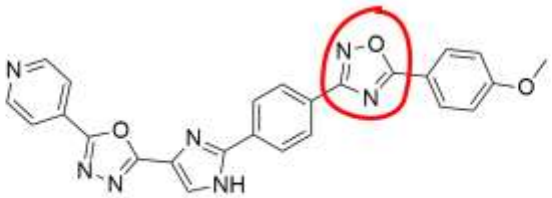

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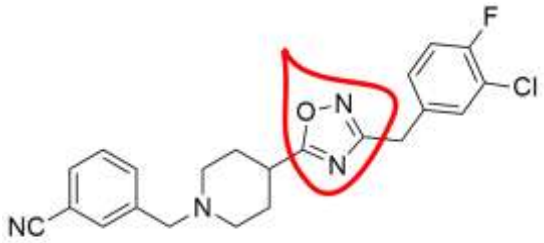
Table 3: Inhibitory activity of oxadiazole derivatives against different cancer cell line

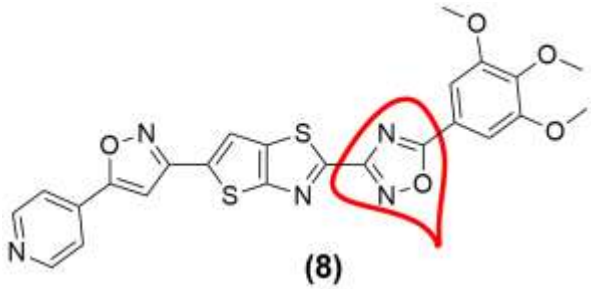
Name	VERO (IC_{50} µm)	PC3 (IC_{50} µm)	DU-145 (IC_{50} µm)	A549 (IC_{50} µm)	HEPG2 (IC_{50} µm)
Comp. 4	14.96± 6.98	0.12± 0.095	0.43 ± 0.075	0.13 ± 0.06	0.11 ± 0.039
Comp. 5	15.09±4.33	0.98±0.043	0.88±0.067	0.86±0.059	0.273±0.052
Comp. 6	16.66±6.12	1.29±0.97	1.74±0.85	1.10±0.88	1.243±0.91

Song Liu et al., 2024 have synthesized a series of 5-(piperidin-4-yl)-1,2,4-oxadiazole derivatives as anticancer agents by targeting human caseinolytic protease P (HsClpP). **Compound 7** reported as highly potent HsClpP agonistic activity in the α-casein hydrolysis assay with EC_{50} = 1.30 µM and inhibited the proliferation of HCCLM3 (Cellosaurus cell line) cells with IC_{50} = 3.1 µM. The **compound 7** reported potent tumor growth inhibitory activity and compared to the kinase inhibitor sorafenib [17].



(7)

Rambabu Vasamsetti and its coworker (2024) have reported a 1,2,4-oxazole derivatives linked with isothieno[2,3-*d*]thiazole-isoxazole-pyridine. Anticancer activity of all the synthesized derivatives ware reported against four different cancer cell lines such as MCF-7 (breast cancer), A549 (lung cancer), Colo-205 (colon cancer) and A2780 (ovarian cancer). Etoposide was taken as positive control to compared anti-cancer activity by using of MTT assay. Etoposide showed IC_{50} values against MCF-7, A549, Colo-205 and A2780 cancer cell lines 2.19 ± 1.87, 3.34 ± 0.152, 0.17 ± 0.034 µM 1.38 ± 0.56 µM respectively. **Compound 8** reported as highly potent derivatives compared to standard [18].



(8)

MCF-7 IC_{50} = 0.02 ± 0.007 µM

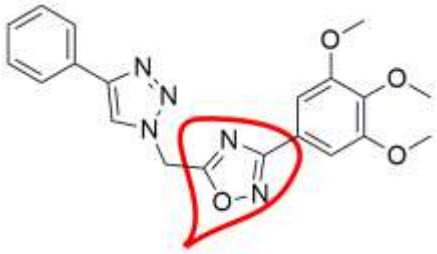
A549 IC_{50} = 0.01 ± 0.009 µM

Colo-205 IC_{50} = 0.13 ± 0.052 µM

A2780 IC_{50} = 0.11 ± 0.083 µM

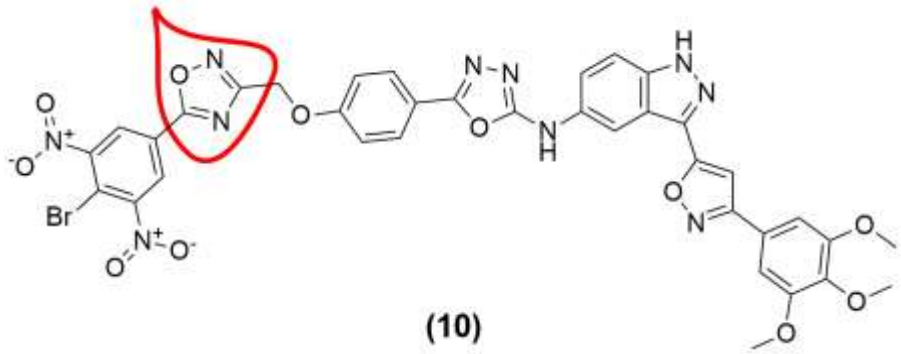
Mahmoud, M. A., *et al.,*2024, have designed and synthesized a novel series of 1,2,4-oxadiazole derivatives as dual inhibitors of endothelial growth factor receptor (EGFR) and veso endothelial growth factor receptor (VEGFR-2). Anti-proliferative activity of all synthesized 1,2,4-oxadiazole derivatives was reported against A549, MCF-7, Panc-1 and HT-29 cancer cell lines with erlotinib as the reference drug. **Compound 9** was

reported as highly significant anti-proliferative derivative against A549, MCF-7, Panc-1 and HT-29 cancer cell line with IC_{50} value 26± 2, 30± 3, 28± 2 and 28± 2 nM respectively. **Compound 9** also reported as potent dual inhibitor against EGFR and VEGFR-2 with IC_{50}= 76±06 and 2.40±0.02 respectively. Erlotinib and sorafenib was used as a positive control for EGFR and VEGFR inhibitory activity with IC_{50}= 80±05 and 0.17±0.01 nM respectively [19].



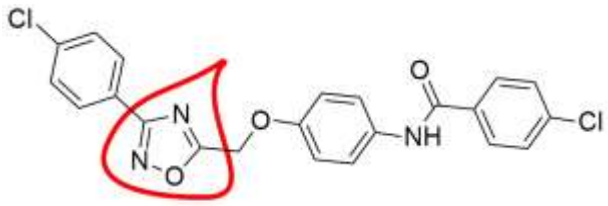
(9)

Lingam, J *et al.,*2023, have synthesized ten derivatives of 1,2,4-oxadiazole linked with 1,3,4-oxadiazole, indazole and isoxazole ring and evaluated their anti-cancer activity against breast cancer (MCF-7, MDA MB-231), lung cancer (A549), and prostate cancer (DU-145) cell lines by MTT assay using etoposide as a standard drug. **Compound 10** showed potent anti-cancer activity in reference to standard drug. **Compound 9** also showed binding with active site amino acid residues of the tubulin protein [20]



(10)

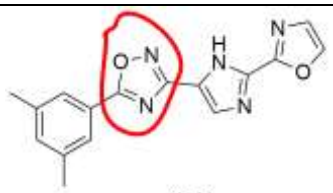
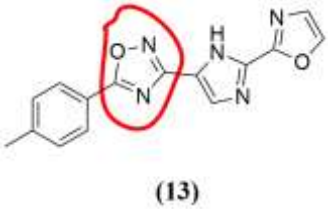
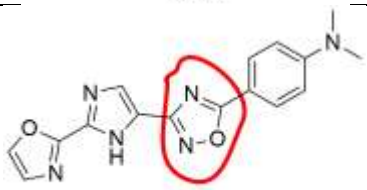
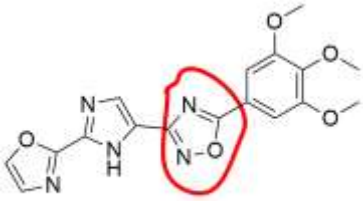
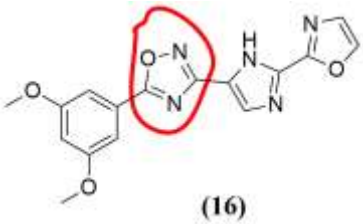
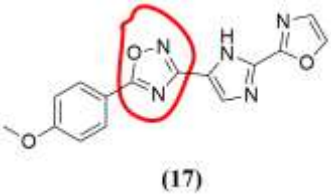
Dhanalakshmi, B *et al.,* 2023, reported designing, synthesis and anti-proliferative activity of 4-aminophenol benzamide analogues of 1,2,4-oxadiazole. Chemical structure of all synthesized derivatives was confirmed by ^{1}HNMR, ^{13}CNMR, IR and LC-MS spectroscopic techniques. The *in-vitro* anti-proliferative activity of all synthesized derivatives was reported against MDA-MB-468 and MDA-MB-231 cancer cell lines. The study results revealed that **compound 11** significantly promoted apoptosis against both MDA-MB-468 and MDA-MB-231 cancer cells with IC_{50} values of 22.31 µM and 26.27 µM, respectively. **Compound 11** also reported binding interaction with active sites amino acid residues of MAPK and exhibited the highest docking score of −7.06 kcal/mol [21].



(11)

Suresh Bairi *et al.,* 2022, have design and synthesized a novel series of 1,2,4-oxadiazole incorporated (2-(oxazol)-1H-imidazole derivatives. All the synthesized derivatives were evaluated for anti-cancer activity against PC3, U-145, A549 and MCF-7 cancer cell lines by MTT assay. Total six derivatives **12, 13, 14, 15, 16** and **17** were showed more potent activity compared to etoposide reference drug reported in **Table 4** [22].

Table 4: Anti-cancer activity of 1,2,4-oxadiazole incorporated (2-(oxazol)-1H-imidazole derivatives

Name	PC3 (IC_{50} µm)	A549 (IC_{50} µm)	MCF-7 (IC_{50} µm)	DU-145, (IC_{50} µm)
 (12)	1.91±0.96	2.05±1.84	2.11±1.88	2.56±1.45
 (13)	2.77±1.55	2.30±1.65	2.66±1.73	2.80±1.83
 (14)	2.41±1.80	2.58±1.58	3.42±2.11	2.18±1.68
 (15)	0.23±0.056	0.06±0.0087	0.01±0.0065	0.19±0.054
 (16)	0.97±0.085	0.22±0.074	0.09±0.0092	0.76±0.051
 (17)	1.64±0.72	1.84±0.81	1.44±0.67	1.80±0.55
Etoposide	2.39±1.56	3.08±0.135	2.11±0.024	1.97±0.45

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Ravi Kumar Bommera *et al.,* 2021, have reported synthesis of 5-fuoruracil linked 1,2,4-oxadiazole derivatives. All the synthesized derivatives were investigated for their anti-cancer activity against four human cancer cell lines such as breast cancer (MCF-7, MDA MB-231), lung cancer (A549) and prostate cancer (DU-145) by using MTT method. Among them, compounds **18, 19, 20, 21** and **22** demonstrated more promising anticancer activity than standard **(Table 5) [**23].

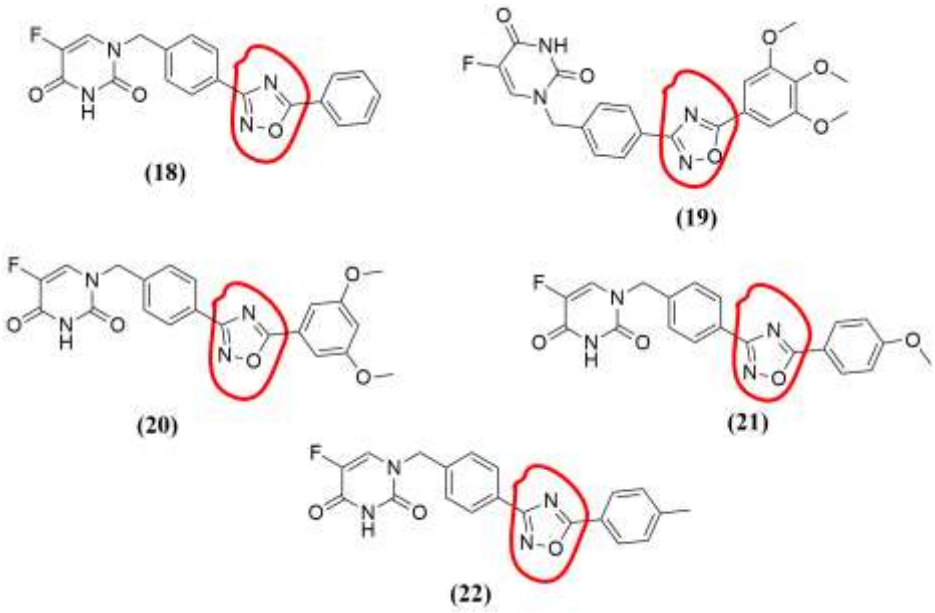

Table 5: Anti-cancer activity of 5-fuoruracil linked 1,2,4-oxadiazole derivatives

No.	MCF-7 IC_{50} (nM)	A-549 IC_{50} (nM)	DU-145 IC_{50} (nM)	MDAMB-231 IC_{50} (nM)
Compound 18	0.76 ± 0.044	0.18 ± 0.019	1.13 ± 0.55	0.93 ± 0.013
Compound 19	0.011 ± 0.009	0.053 ± 0.0071	0.017 ± 0.0062	0.021 ± 0.0028
Compound 20	0.88 ± 0.073	1.44 ± 0.32	1.28 ± 0.27	1.95 ± 0.19
Compound 21	1.78 ± 0.22	1.67 ± 0.49	2.10 ± 1.09	2.34 ± 1.10
Compound 22	2.17 ± 1.66	1.88 ± 0.25	2.65 ± 1.26	2.14 ± 0.94
Standard	2.11 ± 0.024	3.08 ± 0.135	1.97 ± 0.45	1.91 ± 0.84

Shamsi, F *et al.,* 2020 have reported a series of 1,2,4-oxadiazoles derivatives as anti-cancer agents by targeting carbonic anhydrase IX (CAIX) enzyme. Study result revealed that the thiazole/thiophene-sulfonamide conjugates of 1,2,4-oxadiazoles showed anti-cancer activities with low potencies compared to standard drug. **Compound 23** reported anti-proliferative activity with IC_{50} = 11.1 µM and CAIX inhibitory activity with IC_{50} = 4.23 µM. Based on structure activity of **compound 23** a newer series of eleven derivatives was designed, synthesized and evaluated for anti-proliferative and CAIX inhibitory activity. Among them compound enhanced the anti-proliferative activity against colorectal cancer cell line (HCT-116) which is just double compared to **compound 23** (IC_{50} = 6.0 ± 3 µM). **Compound 24** also showed more CAIX inhibitory activity comparison to compound **23** with IC_{50} = 0.74 ± 0.11 µM. **Compound 24** also decreases the expression of CAIX, induces apoptosis and ROS production [24].

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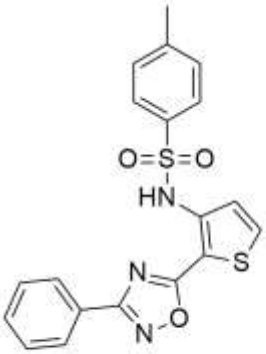

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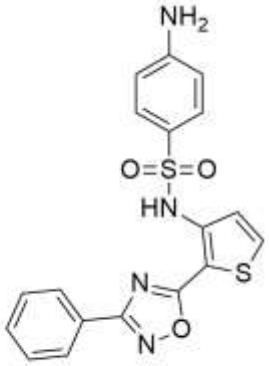
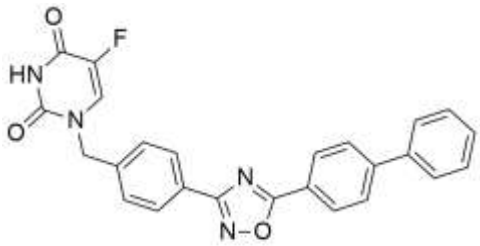


(24)

El Mansouri *et al.,* 2020, have designed and synthesized a newer series of uracil analogues-1,2,4-oxadiazole hybrid derivatives. Structure characterization of all the synthesized derivatives was done by different spectroscopic methods such as HRMS, FT-IR, ^{1}HNMR, and ^{13}C NMR. The cytotoxicity of all the derivatives was reported against melanoma (A-375), fibrosarcoma (HT-1080), breast (MCF-7 and MDA-MB-231), and lung (A-549) cancer cell lines. The derivative **25** showed highly potent cytotoxicity against HT-1080 and MFC-7 cancer cell lines compared to standard drug doxorubicin. The **compound 25** induced apoptosis through caspase-3/7 activation and S-phase arrest in HT-1080 and A549 cells [25].



(25)

CONCLUSION

Cancer is a life threatening disease which is responsible for higher numbers of death in world wide. Therefore, there is need to develop therapeutic agents which treat cancer more effectively without harming healthy cells [26-28].

1,2,4-Oxadiazole scaffold containing derivatives has been reported as potent bioactive agent and exhibiting various pharmacological activities. Literature survey revealed that various substituted 1,2,4-oxadiazole compounds have significantly useful in the treatment of cancer. 1,2,4-oxadiazole derivatives reported from 2020-2024 are described in this article. Marketed drug containing 1,2,4-oxadiazole ring along with their pharmacological uses also reported in this present article. Based on the studies we conclude that further designing and synthesis of 1,2,4-Oxadiazole derivatives will enhance therapeutic activity and efficacy against cancer.

AUTHOR CONTRIBUTIONS

Conceptualization, R.K.C.; validation, H.P.; formal analysis, H.P.; investigation, H.P.; resources, R.K.C.; data curation, H.P.; writing—original draft preparation, H.P.; writing—review and editing, R.K.C.; visualization, H.P.; supervision, R.K.C.; funding acquisition, R.K.C. All authors have read and agreed to the published version of the manuscript.

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