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CHEMICAL DOCKING TESTS, SYNTHESIS, ANTIOXIDANT AND ANTIBACTERIAL QUALITIES OF 3-[4-(4-HYDROXY PHENYL)-1, 3- OXAZOLE -2-YL]-2-PHENYL-1, 3-THIAZOLIDIN-4-ONE

Chanda W. Awaghade[*1], Meghasham N. Narule[2], Niren Kathale[3]

[*1]Department of Chemistry, Sardar Patel Mahavidyalaya, Chandrapur.
[2]Department of Chemistry, Vidya Vikas Arts, Commerce & Science College, Samudrapur, Dist.-Wardha, 442305, India.
[3]Department of Chemistry, Sardar Patel Mahavidyalaya, Chandrapur.

***Corresponding Chanda W. Awaghade**

Department of Chemistry, Sardar Patel Mahavidyalaya, Chandrapur.

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ABSTRACT

In present study, creating a novel antibacterial agent and Chemical docking tests can be distinguished techniques are designed as an aid to the development of therapeutic agents of 3-[4-(4-hydroxy phenyl)-1, 3- Oxazole -2-yl]-2-phenyl-1, 3-thiazolidin-4-one **(3a-l)** was synthesis by cyclisation in presence of glacial acetic acid of 4-(2-schiffs base-1, 3-thiazol-4-yl) Phenol **(2a-l)**. 4-(2-amino-1, 3- Oxazole -4-yl) Phenol **(1a-l)** was prepared by stirred for 6 hours with different aldehydes to give 4-(2-schiffs base-1, 3-thiazol-4-yl) Phenol **(2a-l)**. Chemical docking tests study of the synthesized derivatives was conducted to evaluate their binding pattern with S. aureus gyrase and also show antibacterial and antifungal activities when compare with standard drugs Norfloxacine and Griseofulvin, these compounds exhibit antibacterial and antifungal properties against bacterial cultures, including *Escherichia coli*, *Pseudomonas aeruginosa*, *Staphylococcus aureus*, and *Proteus vulgaris*, as well as fungal cultures, including *Aspergillus niger* and *Candida albicans*. The compounds structure has been verified through elemental analysis, ^{1}HNMR, C^{13}NMR, and infrared spectroscopy. Therefore, in order to achieve a potential pharmacophores, these compounds will be further tested for antibacterial activity.

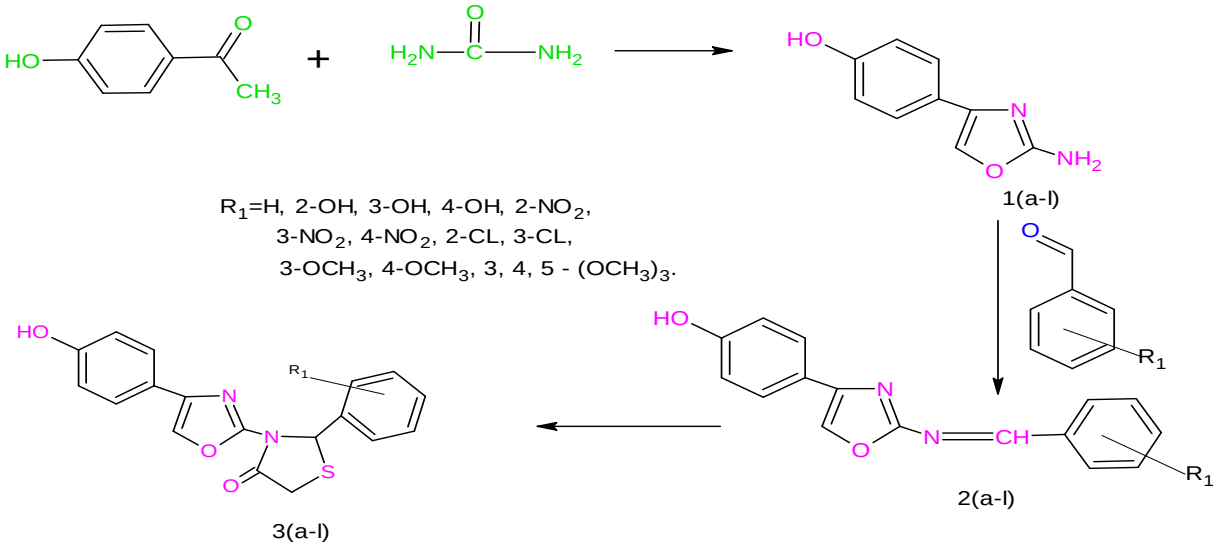
KEYWORDS: Chemical docking tests, Heterocyclic, Oxazole, Thaizolidine, Biological activities, etc.

1. INTRODUCTION

Heterocycles containing nitrogen and oxygen atoms involve a wide range of uses, including agrochemical, medicinal, veterinary, sanitizers, antioxidants, copolymers, corrosion inhibitors, dyestuff and in the production of a wide range of organic chemical substances such as alkaloids, morphine, vinblastine, reserpine, and a variety of antibiotics, such as cephalosporin, penicillin and include heterocyclic components.[1,18] Oxazole and its derivatives play a very essential role in the field of medicinal chemistry. Oxazole is a doubly unsaturated 5-membered ring having one oxygen atom at position 1 and a nitrogen at position 3 separated by a carbon in-between. It was first prepared in 1947, has a boiling point of 69 °C and is a stable liquid at room temperature. The structure of Oxazole derivatives exerts divergent weak interactions like hydrophobic effect, Vander Waals force, hydrogen bonds, coordination bonds, ion-dipole and pi-pi bond; hence the derivatives exhibit potential application in agricultural, biotechnology, medicinal, chemical and material sciences. Substitution pattern in Oxazole derivatives play a pivotal role in delineating the biological activities like antimicrobial, anticancer, antitubercular anti-inflammatory, antidiabetic, antiobesity and antioxidant.[19,21] etc. Schiff bases derived from an amino and carbonyl compound are an important class of ligands that coordinate to metal ions via azomethine nitrogen and have been studied extensively.[22] Chemical docking tests has proved to be an important tool to help understanding how chemical compounds interact with their molecular targets, and for

drug discovery and development. As a matter of fact, the number of studies is reporting- the use of Chemical docking tests to identify structural determinants necessary for efficient ligand-receptor binding, and the development of more accurate docking methods, have heavily increased since its first appearance.[23,26]

The reaction sequence leading to the formation of desire heterocyclic compounds are outline in scheme 1. Thiourea and 4-hydroxyacetophenone in ethanol to form starting material 4-(2-amino-1, 3- oxazole -4-yl) Phenol (1a-l) was prepared by stirred for 6 hours with different aldehydes to give 4-(2-schiffs base-1, 3-thiazol-4-yl) Phenol (2a-l) was then undergo cyclisation in presence of glacial acetic acid gives 3-[4-(4-hydroxy phenyl)-1, 3-oxazole -2-yl]-2-phenyl-1, 3-thiazolidin-4-one (3a-l)



Scheme 1-Reaction scheme1.

2. Experimental

2.1 MATERIALS AND METHODS

The melting points were determined with the use of an open capillary tube, and the outcomes were unaltered. Infrared spectra of KBr pellets were recorded using a Perkin-Elmer spectrophotometer model 157. TMS was employed as the internal standard in the Bruker-300 Varian MHz FT NMR spectrometer to record 1H NMR spectra in either CDCl3 or DMSO. The spots were located using iodine vapors, and the purity of the compounds was assessed using thin-layer chromatography (TLC) on silica gel G plates. Tables 3 and 4 include details on the characterization of the compounds.

2.2 Synthesis starting material

2.2.1 4-(2-amino-1, 3- oxazole-4-yl) Phenol

In order to create compound (1), a cold solution of 4-hydroxyacetophenone (0.01 mol) was added drop-by-drop to a urea solution (0.01mol) in ethanol while the mixture was continually agitated (0.01mol). Four more hours were spent stirring the reaction mixtures. The solvent was removed using distillation and the leftover material was cleaned with petroleum ether, dried and crystalized from ethanol. Yield 70%:M.P.213^{0}C: IR (KBr):3249 (OH), 3153(NH_2), 1595(ArH), (C-S-C), (N=C): 1NMR (300 MHz DMSO) d 8.7-8.9(4H, s, ArH), (1H, s, ArH).

2.2.2 Synthesis of 4-(2-schiffs base-1, 3-thiazol-4-yl) Phenol

4-(2-amino-1, 3- oxazole -4-yl) Phenol **(**1) (0.01mole) and different aldehydes (0.01mole) in methanol were stirred for 6 hours, reaction liquid was poured over crushed ice after being agitated for 6-7 hours, and the solid that obtained was cleaned with ether, dried and crystalized from ethanol. Yield 70%:M.P.213^{0}C: IR (KBr):3249 (OH), 3153(NH_2), 1595(ArH), (C-S-C), (N=C): 1NMR (300 MHz DMSO) d 8.7-8.9(4H, s, ArH), (1H, s, ArH).

2.2.3. 3a: Synthesis of 3-[4-(4-hydroxy phenyl)-1, 3-oxazole -2-yl]-2-phenyl-1, 3-thiazolidin-4-one

Compound 3 (0.01 Mole) undergo cyclisation in 100% ethanol, and the experiment also included a handful drops of glacial acetic acid. The reaction liquid was poured over crushed ice after being agitated for 6-7 hours, and the solid that obtained was cleaned with ether, dried and crystalized from ethanol. Yield 71%:M.P.128^{0}C.

Table 1: IR, H^1NMR, C^{13}NMR & FSB Mass data of compounds 3(a-l).

Compounds	IR(KBr)	H^1NMR (300MHz DMSO)	C^{13}NMR (300MHz, DMSO-d6) & FSB Mass
3a	3477.0 (OH), 3348(N=C), 2980.4(C-O-C), 2362.4 (C-S-C), 1804.9(C-C), 1622.8 (C=O), 1507.6 (ArH), 707.4(C-N-C),	10.67(1H, s, OH), 7.88(4H, s, ArH), 6.35(5H, s, ArH).	150.09, 149.06, 146.33. 145.85, 144.60, 143.20, 119.38, 116.26, 112.56, 112.14, 78.96, 78.54, 78.10, 40.05.
3b	3477.22 (OH), 3348.2(N=C), 2980.0(C-O-C), 2362.1 (C-S-C), 1804.2(C-C), 1622.5 (C=O), 1507.1 (ArH), 707.2(C-N-C).	10.9(1H, s, OH), 7.8 (4H, s, ArH), 6.2(5H, s, ArH).	150, 149.02, 146.1. 145.35, 144.50, 143.3, 119.1, 116.27, 112.36, 112.44, 78.56, 78. 78.10, 40.05.
3c	3477.3 (OH), 3348.3(N=C), 2980.5(C-O-C), 2362.4 (C-S-C), 1804.9(C-C), 1622.8 (C=O), 1507.6 (ArH), 707.4(C-N-C).	10.62(1H, s, OH), 7.88(4H, s, ArH), 6.35(5H, s, ArH).	150.07, 149.06, 146.33. 145.85, 144.60, 143.20, 119.48, 116.26, 112.56, 112.14, 78.96, 78.54, 78.10, 40.05.
3d	3477.5 (OH), 3348.5(N=C), 2980.2(C-O-C), 2362.4 (C-S-C), 1804.9(C-C), 1622.8 (C=O), 1507.6 (ArH), 707.4(C-N-C).	10.67(1H, s, OH), 7.88(4H, s, ArH), 6.35(5H, s, ArH).	150.5, 149.05, 146.33. 145.55, 144.50, 143.20, 119.38, 116.26, 112.56, 112.14, 78.96, 78.55, 78.10, 40.5.
3e	3477.6 (OH), 3348.6(N=C), 2980.4(C-O-C), 2362.4 (C-S-C), 1804.9(C-C), 1622.8 (C=O), 1507.6 (ArH), 707.4(C-N-C).	10.62(1H, s, OH), 7.82(4H, s, ArH), 6.32(5H, s, ArH).	150.6, 149.06, 146.3, 145.3, 144.4, 143.1, 119.38, 116.26, 112.56, 112.14, 78.96, 78.54, 78.10, 40.1.
3f	3477.3 (OH), 3348(N=C), 2980.4(C-O-C), 2362.4 (C-S-C), 1804.9(C-C), 1622.8 (C=O), 1507.6 (ArH), 707.4(C-N-C).	10.63(1H, s, OH), 7.88(4H, s, ArH), 6.35(5H, s, ArH).	150.09, 149.06, 146.33. 145.85, 144.60, 143.20, 119.38, 116.26, 112.56, 112.14, 78.96, 78.54, 78.10, 40.05.
3g	3477.4 (OH), 3348(N=C), 2980.4(C-O-C), 2362.4 (C-S-C), 1804.9(C-C), 1622.8 (C=O), 1507.6 (ArH), 707.4(C-N-C).	10.64(1H, s, OH), 7.88(4H, s, ArH), 6.35(5H, s, ArH).	150.09, 149.06, 146.33. 145.85, 144.60, 143.20, 119.38, 116.26, 112.56, 112.14, 78.96, 78.54, 78.10, 40.05.
3h	3477.4 (OH), 3348(N=C), 2980.4(C-O-C), 2362.4 (C-S-C), 1804.9(C-C), 1622.8 (C=O), 1507.6 (ArH), 707.4(C-N-C).	10.67(1H, s, OH), 7.88(4H, s, ArH), 6.35(5H, s, ArH).	150.09, 149.06, 146.33. 145.85, 144.60, 143.20, 119.38, 116.26, 112.56, 112.14, 78.96, 78.54, 78.10, 40.05.
3i	3477.2 (OH), 3348(N=C), 2980.4(C-O-C), 2362.4 (C-S-C), 1804.9(C-C), 1622.8 (C=O), 1507.6 (ArH), 707.4(C-N-C).	10.67(1H, s, OH), 7.88(4H, s, ArH), 6.35(5H, s, ArH).	150.09, 149.06, 146.33. 145.85, 144.60, 143.20, 119.38, 116.26, 112.56, 112.14, 78.96, 78.54, 78.10, 40.05.
3j	3477.1 (OH), 3348(N=C), 2980.2(C-O-C), 2362.4 (C-S-C), 1804.9(C-C), 1622.8 (C=O), 1507.6 (ArH), 707.4(C-N-C).	10.67(1H, s, OH), 7.88(4H, s, ArH), 6.35(5H, s, ArH).	150.09, 149.06, 146.33. 145.85, 144.60, 143.20, 119.38, 116.26, 112.56, 112.14, 78.96, 78.54, 78.10, 40.05.
3k	3477.7 (OH), 3348(N=C), 2980.4(C-O-C), 2362.4 (C-S-C), 1804.9(C-C), 1622.8 (C=O), 1507.6 (ArH), 707.4(C-N-C).	10.67(1H, s, OH), 7.88(4H, s, ArH), 6.35(5H, s, ArH).	150.09, 149.06, 146.33. 145.85, 144.60, 143.20, 119.38, 116.26, 112.56, 112.14, 78.96, 78.54, 78.10, 40.05.
3l	3477.5 (OH), 3347(N=C), 2980.2(C-O-C), 2362.1 (C-S-C), 1804.3(C-C), 1622.3 (C=O), 1507.4 (ArH), 707.1(C-N-C).	10.7(1H, s, OH), 7.9(4H, s, ArH), 6.25(5H, s, ArH).	150.1, 149.2, 146.2, 145.7, 144.63, 143.21, 119.28, 116.16, 112.36, 112.24, 78.16, 78.34, 78.8, 40.0.

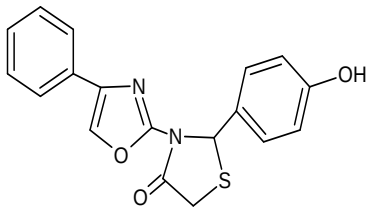
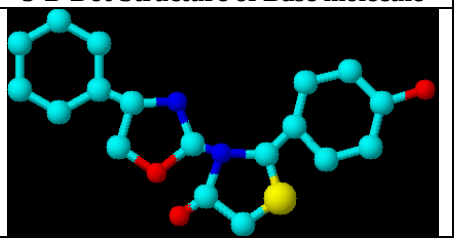
Table 2-Characterization data of compounds 3(a-l).

Comp	R*	Mol Formula	RF Value Eluent[a]	M. P. (°C)	Yield (%)	Analysis fond (calcd)% (obs)			
						C	H	N	S
3a	-H	$C_{18}H_{14}O_3N_2S$	0.81	148	82	63.9 (63.7)	4.1 (4.2)	8.28 (8.1)	9.4 (9.5)
3b	2-OH	$C_{18}H_{14}O_4N_2S$	0.91	156	66	60.3 (60.1)	3.9 (3.7)	7.8 (7.4)	8.9 (8.5)
3c	3-OH	$C_{18}H_{14}O_4N_2S$	0.87	168	72	60.3 (60.1)	3.9 (3.7)	7.8 (7.4)	8.9 (8.5)

3d	4-OH	$C_{18}H_{14}O_4N_2S$	0.65	177	74	60.3 (60.1)	3.9 (3.7)	7.8 (7.4)	8.9 (8.5)
3e	2-NO_2	$C_{18}H_{14}O_5N_3S$	0.41	173	67	56.2 (56.1)	3.6 (3.4)	10.9 (10.8)	8.3 (8.2)
3f	3-NO_2	$C_{18}H_{14}O_5N_3S$	0.57	172	66	56.2 (56.1)	3.6 (3.4)	10.9 (10.8)	8.3 (8.2)
3g	4-NO_2	$C_{18}H_{14}O_5N_3S$	0.74	179	89	56.2 (56.1)	3.6 (3.4)	10.9 (10.8)	8.3 (8.2)
3h	2-Cl	$C_{18}H_{13}O_3N_2SCl$	0.52	188	62	58.0 (58.0)	3.4 (3.3)	7.5 (7.4)	8.6 (8.5)
3i	4-Cl	$C_{18}H_{13}O_3N_2SCl$	0.65	185	72	58.0 (58.0)	3.4 (3.3)	7.5 (7.4)	8.6 (8.5)
3j	2-OCH3	$C_{19}H_{15}O_4N_2S$	0.93	180	68	62.1 (62.2)	4.1 (4.2)	7.6 (7.5)	8.7 (8.5)
3k	4-OCH3	$C_{19}H_{15}O_4N_2S$	0.80	192	74	62.1 (62.2)	4.1 (4.2)	7.6 (7.5)	8.7 (8.5)
3l	3, 4, 5 $(OCH_3)_3$	$C_{21}H_{20}O_6N_2S$	0.45	183	79	58.8 (58.6)	4.6 (4.3)	6.5 (6.4)	7.4 (7.3)

*Solvent for crystallization: aq. Ethanol for 3a-i; methanol for 3j-l. a Eluents for TLC: ethyl acetate-acetone (6:4) for 3a, 3b, 3c, 3d, 3f ethyl acetate-acetone (7:3) for 3e, 3g, 3h, 3j, 3k, 3l.

Table 3: Base molecule 3-[4-(4-hydroxyphenyl)-1, 3-thiazol-2-yl]-2-phenyl-1, 3-thiazolidin-4-one.

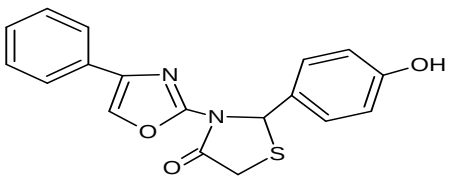
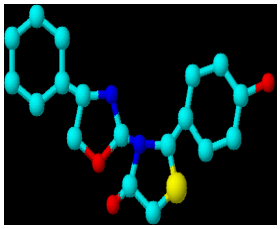
2-D Structure of Base molecule	3-D Dot Structure of Base molecule
	

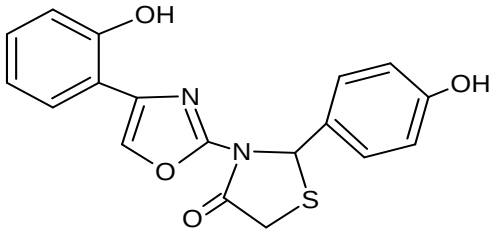
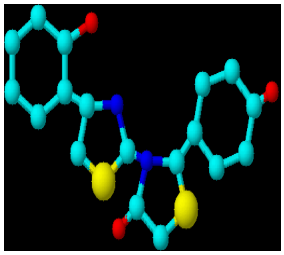
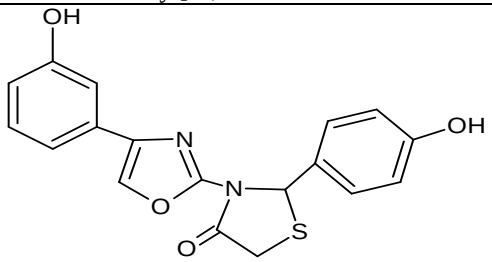
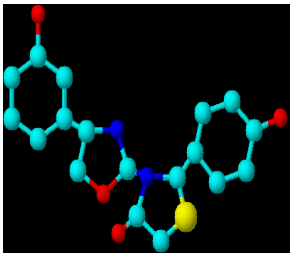
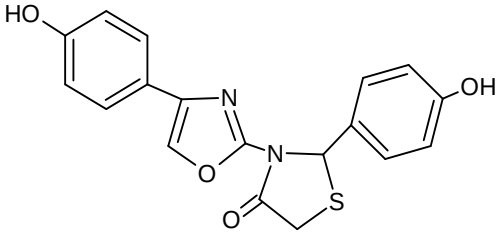
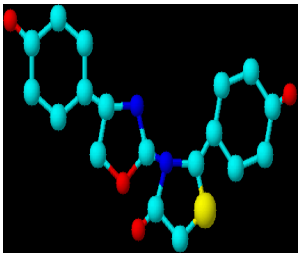
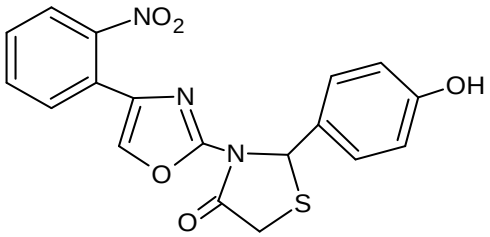
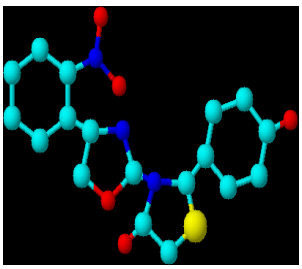
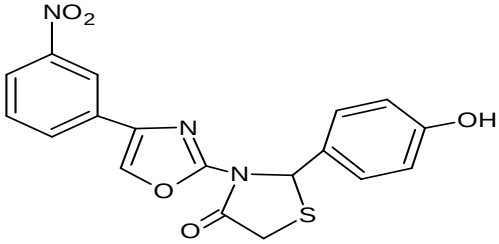
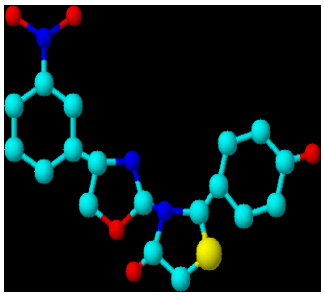
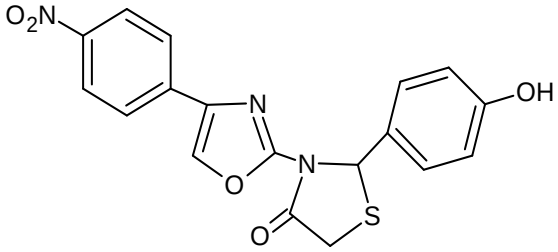
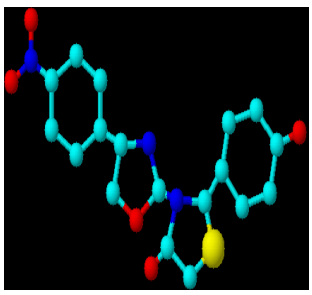
3. Function of CDK Activities

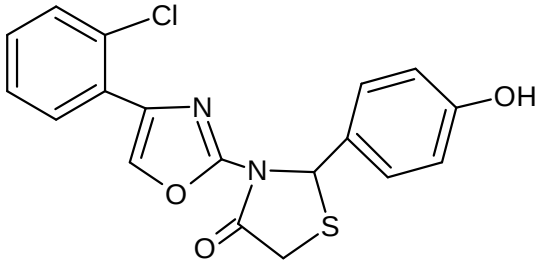
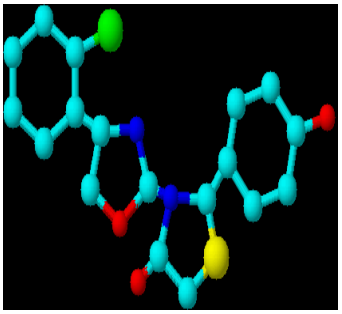
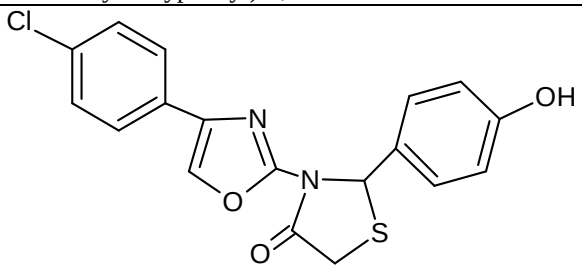
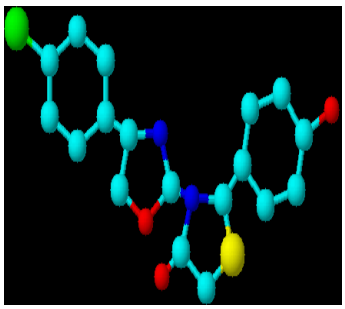
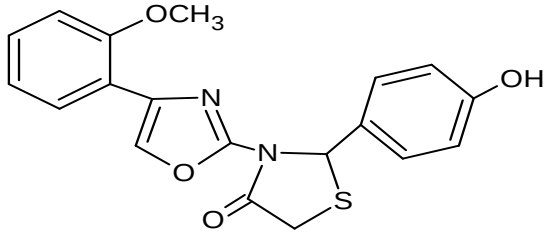
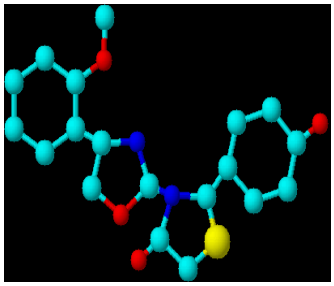
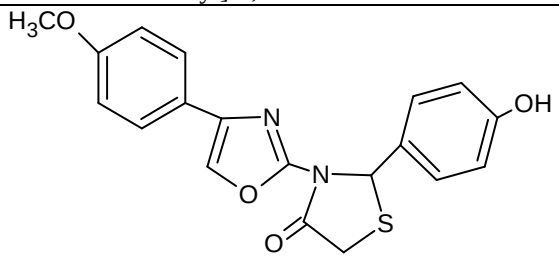
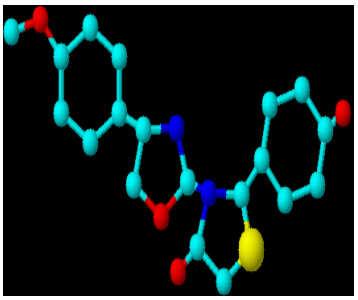
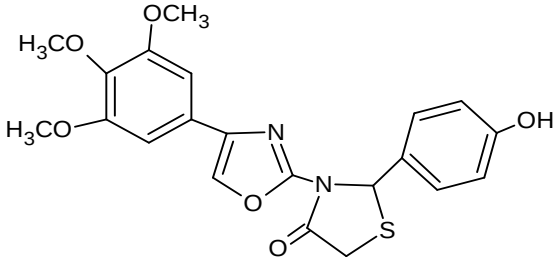
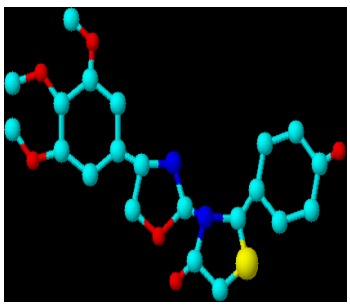
In the protein databank, there exist many CDK2 electronic structures. The choice of 3EZR was made because of a natural inhibitor that is present in one of the key active sties. Additionally, this structure is flawless and entire.

To selectively induce apoptotic cell death via the E2F pathway in tumor cells, cycling A and cycling E-associated cycling dependent kinase-2 (CDK2) activity must be inhibited. The natural CDK-inhibitory (CDKI) tumor suppressor protein p27 KIP1's cycling groove recognition motif (CRM) served as the inspiration for the design and synthesis of a series of cyclic peptides, whose biological activity and structural characterization by NMR and X-ray crystallography are reported[30]. Cdk7 and Cdk9, which regulate transcription, are reportedly inhibited by cycling-dependent kinase inhibitors in chronic lymphocytic leukemia cells. Here, we examined the new cycling-dependent kinase inhibitor SNS-032, which inhibits Cdk2, Cdk7, and Cdk9 with strong and specificity Cyclooxygenase-2 (COX-2) over expression has been linked to a number of human malignancies, including head and neck, lung, and colon. Additionally, deregulation of cell cycle events and concurrently enhanced cycling-dependent kinase activity are linked to cancer (CDK). In this study, CDK2 is a crucial cell cycle regulatory protein that regulates how cells move from the G1 to the S phase. By inhibiting CDK2 activity, we provide many lines of evidence that demonstrate the CDK2's functional role in interleukin-1 (IL-1)-induced COX-2 production in the H358 human non-small cell lung cancer cell line.

Table 4- Substituted 3-[4-(4-phenyl)-1, 3-thiazol-2-yl]-2-phenyl-1, 3-thiazolidin-4-one.

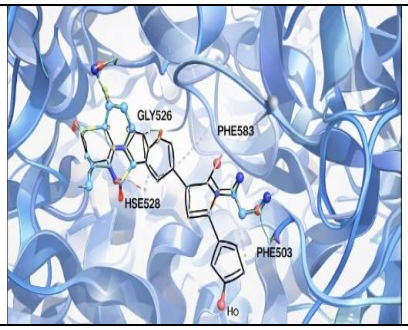
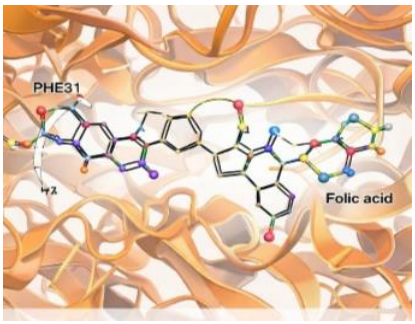
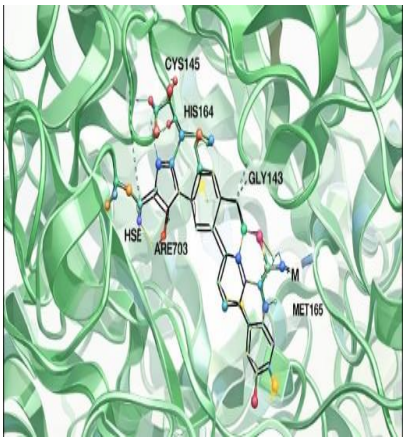
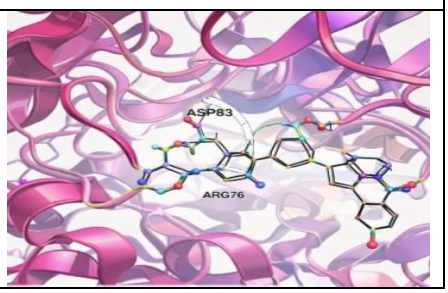
Compounds	2D Structure name	R2	3D Structure
1	 2-(4-hydroxyphenyl)-3-(4-phenyl-1,3-oxazol-2-yl)-1,3-thiazolidin-4-one	-H	

2	 2-(4-hydroxyphenyl)-3-[4-(2-hydroxyphenyl)-1,3-oxazol-2-yl]-1,3-thiazolidin-4-one	2-OH	
3	 2-(4-hydroxyphenyl)-3-[4-(3-hydroxyphenyl)-1,3-oxazol-2-yl]-1,3-thiazolidin-4-one	3-OH	
4	 2-(4-hydroxyphenyl)-3-[4-(4-hydroxyphenyl)-1,3-oxazol-2-yl]-1,3-thiazolidin-4-one	4-OH	
5	 2-(4-hydroxyphenyl)-3-[4-(2-nitrophenyl)-1,3-oxazol-2-yl]-1,3-thiazolidin-4-one	2-NO_2	
6.	 2-(4-hydroxyphenyl)-3-[4-(3-nitrophenyl)-1,3-oxazol-2-yl]-1,3-thiazolidin-4-one	3-NO2	
7	 2-(4-hydroxyphenyl)-3-[4-(4-nitrophenyl)-1,3-oxazol-2-yl]-1,3-thiazolidin-4-one	4-NO_2	

8	 3-[4-(2-chlorophenyl)-1,3-oxazol-2-yl]-2-(4-hydroxyphenyl)-1,3-thiazolidin-4-one	2-Cl	
9	 3-[4-(4-chlorophenyl)-1,3-oxazol-2-yl]-2-(4-hydroxyphenyl)-1,3-thiazolidin-4-one	4-Cl	
10	 2-(4-hydroxyphenyl)-3-[4-(2-methoxyphenyl)-1,3-oxazol-2-yl]-1,3-thiazolidin-4-one	2-OCH_3	
11	 2-(4-hydroxyphenyl)-3-[4-(4-methoxyphenyl)-1,3-oxazol-2-yl]-1,3-thiazolidin-4-one	4-OCH_3	
12	 2-(4-hydroxyphenyl)-3-[4-(3,4,5-trimethoxyphenyl)-1,3-oxazol-2-yl]-1,3-thiazolidin-4-one	3, 4, 5 $(OCH_3)_3$	

Five-diphenyl-4-phenyl-[2, 3'] bithiazolyl-4'-one is created in fifteen molecules of 2-Cyclohexa-1 and examined for its ability to inhibit the CDK2 (PDB ID 3EZR) enzyme using molecular docking methods. Investigating potential binding energies, different interaction poses, and potential hydrogen bonding will help us better understand how efficient these compounds are in inhibiting CDKs, especially CDK2.

Table 5-Information about the protein structures shown in docking diagram.

Sr. No.	Protein	Enzyme	Structur
1.	Cyclooxygenase-2 (COX-2) PDB ID: 5IKR,	Type: Oxidoreductase enzyme Biological Role: Converts arachidonic acid into prostaglandins, which cause inflammation and pain. Medical Importance: Target of anti-inflammatory drugs (like celecoxib). Selective COX-2 inhibition reduces pain with fewer stomach side effects. Docking Insight:Aromatic compounds interact through hydrophobic interactions and hydrogen bonding in the active channel.	
2.	Epidermal Growth Factor Receptor (EGFR)	PDB ID: 1M17, Type: Receptor Tyrosine Kinase Biological Role: EGFR controls cell growth, survival, and division. It is located on the surface of cells. Medical Importance: Overexpressed in many cancers (lung, breast, colon). Target of anticancer drugs like gefitinib and erlotinib. Docking Insight: Ligands bind in the ATP-binding pocket of the kinase domain. Hydrogen bonding with residues like MET793 is important for strong inhibition.	
3.	Main Protease (Mpro) PDB ID: 6LU7	Type: Viral protease Biological Role: Cleaves viral polyproteins during replication of SARS-CoV-2.Medical Importance: Important antiviral drug target (COVID-19 research). Inhibition blocks viral replication. Docking Insight: Key catalytic residues: CYS145 and HIS41. Strong hydrogen bonding here indicates good antiviral potential. Protein Function Disease Target Application EGFR Cell growth signaling Cancer Anticancer drugs COX-2 Inflammation mediator Pain/Arthritis Anti-inflammatory DNA Gyrase DNA replication Bacterial infection Antibiotics Mpro Viral protein processing COVID-19 Antiviral drugs	
4.	DNA Gyrase PDB ID: 1KZN,	Type: Bacterial enzyme Biological Role: Introduces negative supercoils into DNA during replication. Medical Importance: Target of antibiotics like ciprofloxacin. Present in bacteria, not humans → good antibacterial target. Docking Insight: Ligands bind near the DNA cleavage site, interacting with ARG and ASP residues.	

3.1. Synthesized molecules (Ligand)

To study inhibition of enzyme with synthesized molecules (called as Ligand), fifteen molecules are selected as listed in Table 5.

3.2. Receptor enzyme

Target protein CDK2 is chosen because of its electronic structure, which has the PDB reference ID 3EZR. The protein file was obtained from an internet database and contains a natural inhibitor called 3-methoxy-4-[4-(4-methylpiperazin-1-yl)-1H-benzimidazol-2-yl]-1H-indazol-6-yl aniline.[17] There is no possibility for misunderstanding owing to atoms or amino acids lacking from the specified enzyme structure. Kollmann charges were used after all heteroatom's (i.e., non-receptor atoms like water, ions, etc.) were removed. Using Auto Dock 19's Add sol function, the Salvation parameters were added to the final macromolecule structure. The location of the natural inhibitor in the enzyme is employed as the active site of the chosen enzyme and is utilized unaltered.

Table 6- Surface Dot 3-D structure of new moieties.

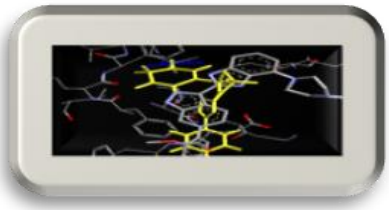
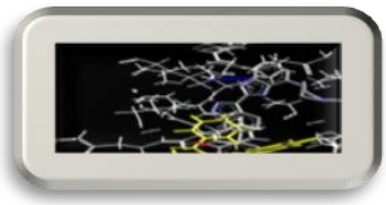
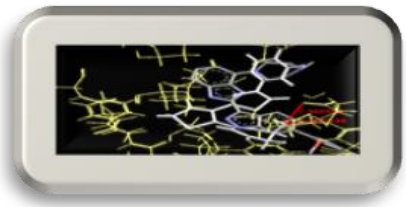
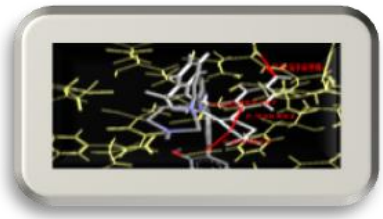
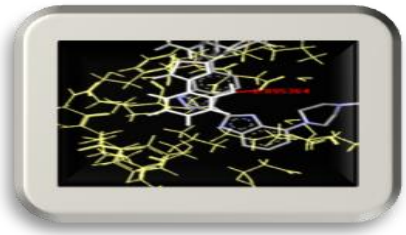
Sr. No	Surface Dot 3-D structure	Binding Energy In Kcal/mole	H-bond distance	Amino acids
1		**-11.6863**	2.744652	955-DEF
2		**-10.7636**		958- DEF
3		**-10.0056**	2.452949	145 –ASP
4		**-10.0197**	2.633822	83-LEU
5		**-10.0197**	2.895364	145- ASP

Table 5 displays each docked molecule's obtained binding energies. The range of noted docking energies, -9.68543 to -11.0 653 kcal.mol.1, is greater than what can be achieved when employing natural inhibitors. There are certain compounds whose binding energy is hidden. Since the binding energies of all components are negative, stable complex formation is conceivable. Hydrogen bond (HB) formation is increasing the stability of certain molecules.

3. Biological activities

Comparative study of 4-(2-amino-1, 3- oxazole -4-yl) Phenol (1) and compounds 3-[4-(4-hydroxy phenyl)-1, 3-oxazole -2-yl]-2-phenyl-1, 3-thiazolidin-4-one **3(a-l)** have been observed by using Norfloxacine and Griseofulvin as standards. The enhancement in biological activity of compound **(1)** as compared with the newly synthesized **3(a-i)** has been observed. The synthesized compounds were tested at 100 ug/ml concentrations against *Escherichia coli*, Pseudomonas *aeruginosa*, *Staphylococcus aureus*, *Proteus vulgaris* and fungal cultures such as *Aspergillus niger* and *Candida albicans* for its antibacterial and antifungal screening as shown in Tables **7**.

Table 7- Data for in vitro antibacterial and anti-fungal activities (in mm).

Comp.	Minimum inhibitory concentration's g/ml					
	E. *Coli*	S. *aurous*	Ps. *aeruginosa*	P. *Vulgaris*	A. *niger*	C. *albicans*
3a	17	17	19	16	17	20
3b	16	10	12	13	24	18
3c	18	12	14	16	15	15
3d	14	10	13	17	16	20
3e	12	14	15	21	18	21
3f	14	16	16	10	17	19
3g	11	13	15	17	17	23
3h	15	17	17	18	14	21
3i	12	10	13	NA	18	12
3j	17	18	12	14	12	17
3k	14	10	12	11	16	14
3l	12	13	12	10	18	16

NA: not active; -: no inhibition of growth.

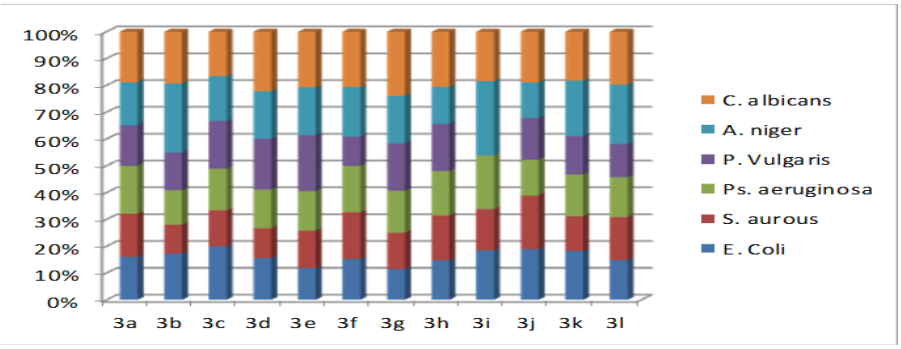


Fig 1- Biological activity of the compounds 3(a-l).

4. Antioxidant activity

The proportion of free radical scavenging activity revealed by the test compounds 3a-l was quantified using the 1, 1-diphenyl picryl hydrazyl (DPPH) assay technique. Drug stock solutions with concentrations of 1 mg mL-1 in methanol were diluted to produce final concentrations of 2, 4, 6, 8, and 10 mg mL-1. The findings were read after adding a DPPH methanol solution (1 mL, 0.3 M mol) to 2.5 mL of drug solutions with different concentrations and letting the mixture react at room temperature. The proportion of antioxidant activity was determined from the observations made after 30 minutes of observation by measuring the absorbance values at 518 nm. Methanol was applied as the solvent, while ascorbic acid was used as the reference. The estimated percentage of inhibition based on concentration is shown in Figure **2**. The outcomes are shown in Table **8**. Ascorbic acid was the usual medication.

Table 8- Antioxidant activity of new compounds 3(a-l).

Compounds	%Inhibition 20ug	%Inhibition 40ug	%Inhibition 60ug	%Inhibition 80ug	%Inhibition 100ug/ml
3a	22	33	41	52	58
3b	24	35	41	53	59
3c	25	34	42	51	55
3d	22	33	44	54	58
3e	26	31	44	57	59
3f	26	24	22	55	35
3g	23	24	26	53	56
3h	21	23	26	46	51
3i	22	25	28	41	47
3j	23	26	31	38	45
3k	20	26	31	39	44
3l	21	26	33	39	43
	2ug/ml	**4ug/ml**	**6ug/ml**	**8ug/ml**	**10ug/ml**
Ascorbic acid	**10**	**15**	**20**	**33**	**56**

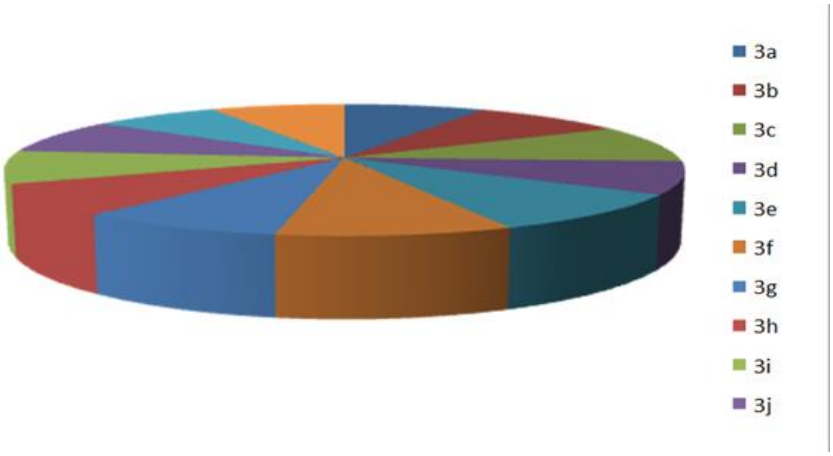


Fig 2- Antioxidant activity of compounds 3(a-l).

5. RESULT AND DISCURSION

The most popular method Chemical docking tests use is in structure-based virtual screening to find novel active chemicals that target a specific protein, it has yielded some success stories in this regard. In view of the above mentioned pharmacological activities of Thaizolidine, Thiourea and 4-hydroxyacetophenone in ethanol to form starting material 4-(2-amino-1, 3- oxazole -4-yl) Phenol **(1)** was prepared by stirred for 6 hours with different aldehydes to give 4-(2-schiffs base-1, 3- oxazole -4-yl) Phenol **(2)** was then undergo cyclisation in presence of glacial acetic acid gives 3-[4-(4-hydroxy phenyl)-1, 3-oxazole -2-yl]-2-phenyl-1, 3-thiazolidin-4-one **3 (a-l)**. The compounds **3(a-l)** possessing (hydroxyl phenyl, nitro phenyl, chlorophenyl, methoxyphenyl, N (di-methylphenyl) have shown good antioxidant activity within the series of compounds synthesized. Hence these compounds shall be exploited further for antibacterial activities to attain a potential pharmacophores.

6. CONCLUSION

The result of this study indicate that the present synthetic method is a simple efficient, inexpensive and easy synthesis of biologically active compounds 3-[4-(4-hydroxy phenyl)-1, 3- oxazole -2-yl]-2-phenyl-1, 3-thiazolidin-4-one **3(a-l).** These compounds showing good result tested at 100ug/ml concentration against *Escherichia coli*, Pseudomonas *aeruginosa*, *Staphylococcus aureus*, *Proteus vulgaris* and fungal cultures such as *Aspergillus niger* and *Candida albicans as compare to simple Thaizolidine*. The compounds 3-[4-(4-hydroxy phenyl)-1, 3- Oxazole -2-yl]-2-phenyl-1, 3-thiazolidin-4-one **3(a-l)** have shown good antioxidant activity. One essential element of Chemical docking tests that merits additional development is the scoring function. Examples of successful applications demonstrate the ability of computational methods to filter hits from a large database and create new tiny molecules. However, experimental technique is still needed to achieve realistic interactions between tiny compounds and receptors. Scoring functions that are both accurate and computationally inexpensive could advance Chemical docking tests applications.

Declaration of competing interest

The authors affirm that they have no financial stake in the outcome of the work described in the publication.

Data availability

Data will be made available on request.

Supplementary data

Supplementary data to this manuscript can be found online.

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