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EGFR Inhibition by Novel Thiazole Derivatives: Insights from Docking Studies and Experimental Validation

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ABSTRACT: Molecular docking studies were conducted on promising compounds to elucidate their enzymatic activities based on binding interactions with the receptor. Among the compounds investigated, PVS 03 demonstrated the highest docking score of -7.811, indicating a strong affinity towards the receptor compared to others. Notably, it formed hydrophobic bonds with C10, C17, C18, and C14, which are crucial for anticancer activity. The compounds were synthesized via traditional methods, with reaction progress monitored using the TCL method. Percent yields revealed PVS 01 with the highest yield, whereas PVS 04 exhibited lower yield (Table 4). Additionally, % purity was assessed using the HPLC method, highlighting PVS 10's greater purity compared to PVS 04 in the series of novel thiazole derivatives. These derivatives were synthesized to evaluate their in vitro anticancer activity against Hep-G2 and MDAMB-231 cell lines. PVS 03 displayed superior anticancer activity compared to dasatinib. However, PVS 06 and 07 exhibited no inhibition against MDAMB-231 cells, and PVS 05 showed no inhibition against Hep-G2

cells. In an another series, novel 2,4-disubstituted thiazole derivatives were synthesized to screen their in vitro anticancer activity against MCF-7 (Breast Cancer) and A431 (Lung Cancer cell line) cells. PVS 2.7 demonstrated the most potent anticancer activity compared to dasatinib. Nonetheless, PVS 2.10 and PVS 2.4 did not inhibit A431 cells, while PVS 2.7 did not inhibit MCF-7 cells. These results collectively suggest that the novel thiazole derivatives hold promise as EGFR inhibitors with enhanced anticancer potential.

INTRODUCTION:

Cancer is a complicated illness resulting from aberrant cell growth and division. It is a huge public health issue globally and one of the main causes of mortality. According to the World Health Organization, cancer kills around 9.6 million people each year [1]. In recent years, cancer researchers have focused heavily on developing targeted medicines that selectively disrupt the signaling pathways involved in cancer growth and proliferation [2]. One strategy has been to target mutant or aberrantly produced oncogenic growth factor receptors and non-receptor tyrosine kinases, which play important roles in these signaling cascades. The EGFR (epidermal growth factor receptor) is a protein located on the surface of cells in the body. It regulates cell growth and division, and overexpression has been linked to the genesis and progression of numerous forms of cancer [3]. EGFR tyrosine kinase inhibitors (TKIs) are medications that target and suppress the EGFR protein's function. EGFR TKIs have been authorized to treat a wide range of cancers, including non-small cell lung cancer (NSCLC), pancreatic cancer, and head and neck cancer [4]. While they have shown encouraging outcomes, not all patients react to EGFR TKIs, and resistance might develop over time [5]. Ongoing research aims to develop novel therapeutic techniques to overcome resistance and enhance results for cancer patients.

Heterocyclic compounds are a varied family of chemicals found throughout nature that play important roles in a variety of biological activities [6]. Among heterocyclic compounds, those with the thiazole moiety exhibit a wide spectrum of biological activity [7]. The synthesis of the basic thiazole nucleus is well-established, and literature on the processes involved may help guide the development of derivatives [8]. Thiazoles and their derivatives are essential components of several metabolic processes and play a vital role in drug discovery [9]. Thiazoles are chemical compounds related to azoles that share the thiazole functional group [10]. Hantzsch and Waber initially described thiazole in 1887. Popp validated the structure in 1889 [11, 12]. Thiazole-containing compounds that include a thiazole amine-moiety demonstrate significant anticancer effects that vary depending on the substitution pattern at the thiazole ring [13]. Thiazole compounds have been intensively researched for their potential pharmacological uses, notably in the creation of anticancer medicines. Because of its potential to interact with biological targets, this one-of-a-kind scaffold is beneficial for a variety of natural, synthetic, and semi-synthetic medicines [14]. Tiazofurin, a thiazole-containing medication, has been found to be anticancer by blocking the enzyme inosine monophosphate dehydrogenase (IMPDH) [15]. Dasatinib, another thiazole-containing medication, has been licensed for the treatment of chronic myeloid leukemia (CML) and acute lymphoblastic leukemia (ALL) [16].

Dabrafenib, a thiazole-containing medication, is used to treat metastatic melanoma with a particular genetic mutation (BRAF V600E or V600K) [17]. Overall, thiazole compounds have significant potential for the development of anticancer medicines. Ongoing research in this field may lead to the development of even more effective therapies for different cancers.

Molecular docking is a computer approach that has gained popularity in recent years for drug discovery and design. To increase the effectiveness of virtual screening, successive filters may be used to reduce the number of compounds chosen for further biological investigation. These filters may include parameters such as drug similarity, pharmacokinetic characteristics, and projected toxicity [18]. Overall, molecular docking and virtual screening techniques are effective tools for accelerating drug development by discovering possible drug candidates with high binding affinity and selectivity for a target protein or enzyme. The virtual screening approach utilized in this work uses progressive filters to select a limited number of chemicals for biological examination. In this work, structure-based virtual screening techniques were applied [19]. In detail, (i) a library of EGFR tyrosine kinase was created based on the literature search. (ii) The binding mechanism of all recovered compounds was examined using molecular docking with the 3D structure of EGFR-TK (PDB ID: 1M17); (iii) The next filter was Lipinski's rule of five to evaluate drug-likeness, which has become an important tool for drug development. (iv) We next used SciFinder to determine the originality of compounds as Tyrosine Kinase Antagonists. (v) Finally, the virtually screened hits were synthesized and tested for inhibitory activity [20].

This research focuses on the design and synthesis of 2,4 disubstituted thiazole derivatives with possible anticancer characteristics. Building on past studies, our objective was to find physiologically active targets for cancer therapy. The synthesized prototypes were tested for anticancer activity against two cancer cell lines: HepG-2 and MCF-7. The most active compounds were then tested for inhibitory action against the EGFR kinase. Furthermore, molecular docking experiments were carried out to learn more about the binding mechanisms of the most effective drugs inside the EGFR kinase's active region.

Overall, this work examines the potential anticancer characteristics of thiazole derivatives and gives information on their mode of action using molecular docking experiments. The findings of this study may assist to guide the development of more effective cancer therapies.

MATERIALS AND METHODS:

Molecular docking study

The molecular docking Glide module (Schrodinger Inc., USA) was utilized to dock the drugs against the EGFR Tyrosine Kinase. The X-ray crystallographic structure of EGFR Tyrosine Kinase was obtained from the protein databank, accession ID 1M17. The protein structure was created using the "protein preparation wizard" panel. Prime was used at the pre-processing phases to assign bond ordering, add missing hydrogen, produce disulphide bonds, and modify missing side chains and loops. In the final refining step, the OPLS3 force field was employed to achieve full energy optimization, with heavy atoms' RMSD set to 0.3 Å. The LigPrep panel was used to create 3D structures for all of the produced compounds. The ionization state of each ligand structure was determined at a physiological pH of 7.2 ± 0.2 . The active site grid was allocated by centralizing the cognate ligand in the crystal structure and using the default box dimension. Finally, the molecular docking investigation was carried out utilizing Schrodinger's glide, which included loading the ready minimal energy 3D structure of the ligands and the receptor grid file into Maestro's work area and docking the ligands using extra precision (SP) docking methods.

Synthesis and characterization

Melting points were calculated using the open tube capillary technique and are uncorrected. The purity of the compounds was determined by elemental analysis, and the progress of the reactions was tracked using TLC plates (silica gel G) with mobile phases of chloroform: methanol (9:1) and acetone: n-hexane (8:2), with spots recognized by iodine vapours or ultraviolet light. The IR spectra were acquired using a Shimadzu 8201 PC FTIR spectrometer (KBr pellets). A Bruker AC 300 MHz spectrometer was used to record ^1H NMR spectra in DMSO d_6 , using TMS as an internal standard. Mass spectra were recorded on a Bruker Esquire LCMS with ESI, and elemental analyses were carried out on a Perkin-Elmer 2400 Elemental Analyzer.

Synthesis of thiazole derivatives Series 1

Synthesis of 2, 4 disubstituted thiazole derivatives:

Ammonium thiocyanate (2) (0.071 mol, 1 Eq.) was dissolved in acetone in a 250 mL round-bottom flask. The equivalent aroyl chloride (1) (0.071 mol, 1 Eq.) was added. The reaction mixture was then refluxed for five minutes. The synthesis of aroyl isothiocyanate (3) was detected by its yellow hue. The ammonium chloride precipitate was then filtered and washed with acetone to entirely eliminate the yellow liquid (aroyl isothiocyanate). A stirred solution of aroyl isothiocyanate (3) in acetone was cooled to 00 C before adding a secondary amine adduct (4) (0.071 mol, 1 Eq.) dropwise while keeping the temperature between 0 and 50 C. After the addition of secondary amine adducts (4), the reaction was maintained at 0-50°C until the product (5) precipitated out. Cold acetone was used to wash the product, which was then vacuum dried. Benzamidine derivatives (0.6288 moles, 2 eq.) were dissolved in acetonitrile in a 250 mL round-bottom flask. The equivalent triethyl amine was added, and the reaction was agitated for 10 to 15 minutes. The reaction mixture was then refluxed for 3-4 hours with 0.3144 moles of dichloro acetone (1eq.). The TLC detected the conclusion of the reaction. The reaction was completed when both reactants interacted with one another, as shown by TLC. After the reaction was completed, cold water was added to the reaction mixture, and the result precipitated out. After the product was sorted out. The chemical was purified using column chromatography.

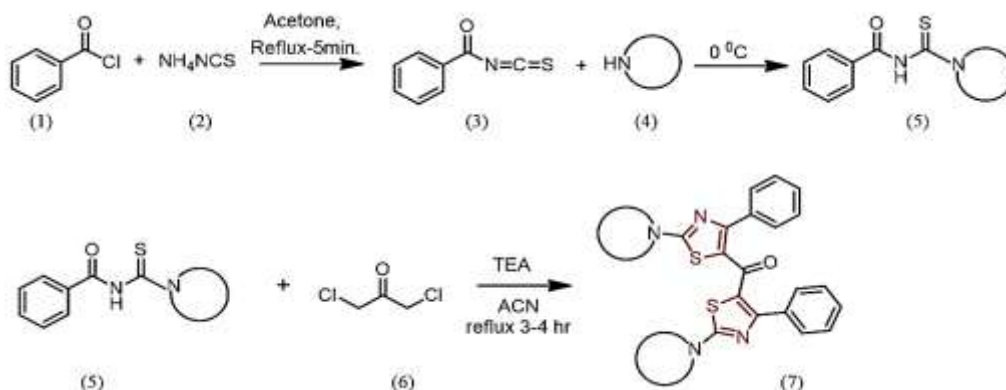
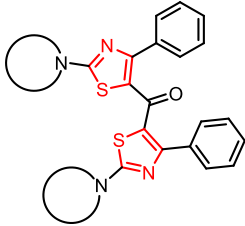


Figure 2: General method for the synthesis of thiazole derivatives Series 1

A total of 10 derivatives were synthesised which are summarized below in **table 1**.

Table 1: Novel Thiazole different derivatives Series 1

Compound Code	R Group	Core structure
PVS 1	N-methyl-1-phenylmethanamine	
PVS2	Dibutyl amine	
PVS3	2,2'-azanediyl diethanol	
PVS4	diisopropylamine	
PVS5	dimethylamine	
PVS6	diphenylamine	
PVS7	N-ethylpropan-2-amine	
PVS8	N-methylpropan-2-amine	
PVS9	N-ethylaniline	
PVS10	N-methylaniline	

SYNTHESIS OF THIAZOLE DERIVATIVES SERIES 2

Synthesis of ethyl 4-methyl-2-phenylthiazole-5-carboxylate.

A solution of benzo thioamide (40 mmol) and ethyl 2-chloro-3-oxo-butanoate (40 mmol) in ethanol (30 mL) was refluxed for three hours. The development of the reaction was tracked using TLC. Following the conclusion of the reaction, the solvent was distilled using a rotary evaporator, and the residue was dissolved in water. The reaction mixture was neutralized with sodium bicarbonate, extracted with ethyl acetate (3 x 50 mL), washed with brine, and distilled on a rotary evaporator, yielding crude product. The crude product was refined using column chromatography with hexane:ethylacetate (9:1) as eluent, yielding pure product.

Synthesis of 4-methyl-2-phenylthiazole-5-carboxylic acid The solution of ethyl 4-methyl-2-phenylthiazole-5-carboxylate and 10% aqueous NaOH was refluxed for two hours. Following completion of the reaction, the reaction mass was chilled in ice and acidified with concentrated HCl. The solid product produced was filtered and washed with water, yielding 4-methyl-2-phenylthiazole-5-carboxylic acid.

Synthesis of prop-2-yn-1-yl 4-methyl-2-phenylthiazole-5-carboxylate

DMAP (20 mmol) was added to an ice-cold solution of 4-methyl-2-phenylthiazole-5-carboxylic acid (10 mmol) in dichloromethane (30 mL) and agitated for 15 minutes, yielding a clear solution. EDC. HCl (15 mmol) was added to the reaction mixture and agitated for 15 minutes. At 0 °C, propargyl alcohol (15 mmol) was added and the mixture was stirred overnight. Following completion of the reaction, the reaction mixture was quenched with water and extracted in DCM. The organic layer was washed with brine, dried over sodium sulfate, and distilled using a rotary evaporator, yielding crude product. The crude product was refined using column chromatography with hexane: ethyl acetate (9:1) as eluent, yielding pure product.

Synthesis of (1-benzyl-1H-1,2,3-triazol-4-yl)methyl 4-methyl-2-phenylthiazole-5-carboxylate.

A solution of prop-2-yn-1-yl 4-methyl-2-phenylthiazole-5-carboxylate (5 mmol) with substituted benzyl azide (6 mmol), CuSO₄·5H₂O (1 mmol), and sodium ascorbate (1 mmol) in DMF:water (3:1) (4 mL) was agitated at room temperature for 10 hours. TLC monitors the course of the reaction. After the reaction was completed, the mixture was quenched with water and extracted with ethyl acetate. The organic layer was washed with brine, dried with anhydrous sodium sulphate, and distilled on a rotary evaporator, yielding crude product. The crude product was refined using column chromatography with hexane: ethyl acetate (8:2) as the eluent, resulting in pure product.

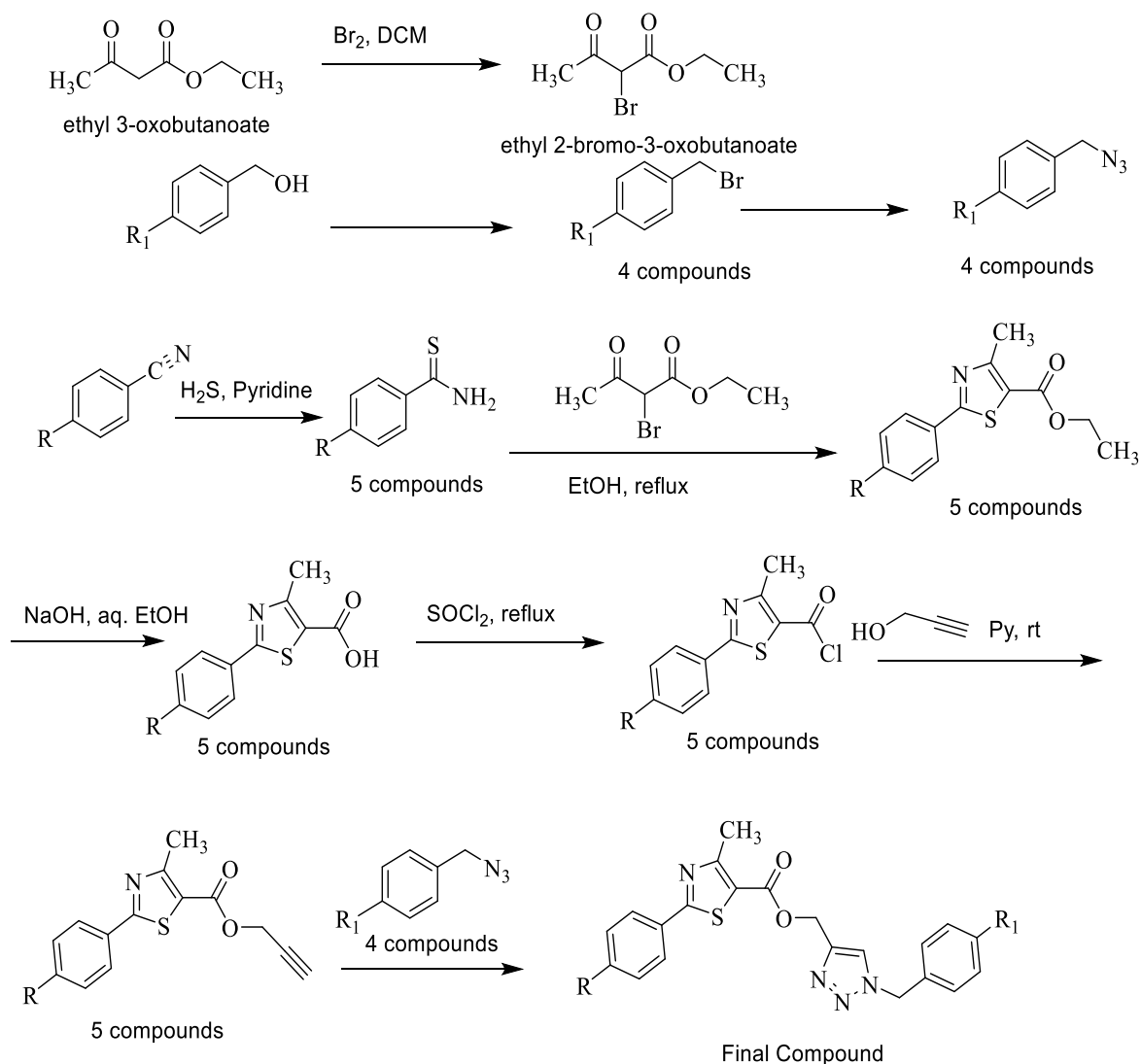
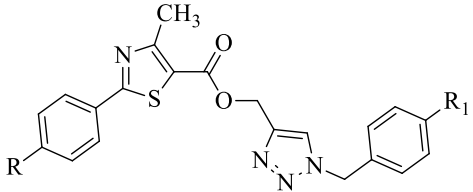


Figure 1: Method for the synthesis of thiazole derivatives Series 2

A total of 11 derivatives of Series 2 were synthesized which are summarized below in **table 1**.

Table 1: Novel Thiazole different derivatives Series 2

Compound Code	R Group	Core structure
PVS 2.4	4-chlorobenzyl	
PVS 2.5	4-chlorobenzyl, 4-bromophenyl	
PVS 2.6	4-chlorobenzyl, 4-chlorophenyl	
PVS 2.7	4-fluorobenzyl	
PVS 2.8	4-fluorobenzyl, 4-bromophenyl	
PVS 2.9	4-fluorobenzyl, 4-chlorophenyl	
PVS 2.10	4-methylbenzyl	
PVS 2.11	4-methylbenzyl, 4-bromophenyl	
PVS 2.12	4-methylbenzyl, 4-chlorophenyl	
PVS 2.14	4-fluorobenzyl, 4-fluorophenyl	
PVS 2.16	4-chlorobenzyl, 4-fluorophenyl	

MTT Assay

Cytotoxicity of the supplied samples on MDAMB-231, MCF-7 (human breast Cell), and HepG2 (Lungs) cell line was assessed by MTT Assay. The cells (10000 cells/well) were grown in 96-well plates for 24 hours in DMEM media with 10% FBS and 1% antibiotic solution at 37°C with 5% CO₂. The next day, cells were treated according to the client's instructions (varying concentrations were created in a full medium). After 24 hours of incubation, MTT (final concentration of 0.5 mg/ml) was added to the cell culture and incubated for an additional 2 hours. After the experiment, the culture supernatant was withdrawn, and the cell layer with matrix was dissolved in 100 µl DMSO (dimethyl sulfoxide) and read in an Elisa plate reader (iMARK, Biorad, USA) at 540 and 660 nm [23].

RESULTS AND DISCUSSIONS

Molecular docking study

Molecular docking is a computer approach that predicts the binding patterns and affinities of small compounds to their target macromolecules, making it useful for drug discovery and development. It may help guide the design and optimization of drug candidates, investigate the structure-activity connection of lead compounds, minimize the cost and time required for experimental procedures, and find novel therapeutic targets and drug leads [24]. In the research, molecular docking simulations were utilized to justify the reported biological effects of the new thiazole derivatives, which might help lead the design and development of more effective and selective anticancer medicines. To explain the observed biological effects, molecular docking simulations using PDB ID: 1M17 were used to discover the binding mechanism of the new thiazole derivatives. The compounds' H-bond acceptor (HBA) and hydrogen bond donor (HBD) groups were designed for optimal drug-receptor interaction. Dasatinib served as a benchmark for new derivatives. Among the compounds examined, PVS 03 (**Fig. 1** and **Table 2**) showed the highest docking score of -7.811 and a high affinity for the receptor compared to other compounds. It also generated hydrophobic bonds with C10, C17, C18, and C14, which are required for anticancer action. Among the compounds studied in series 2, PVS 2.7 exhibited the highest docking score of -7.724 and had a strong affinity towards the receptor compared to other compounds.

Table 2: Docking scores of docked molecules with standard Dasatinib

Compound Code	Docking Score, Receptor (1M17)
PVS3	-7.811
PVS5	-5.986
PVS2	-5.299
PVS4	-5.108
PVS9	-4.532
PVS10	-4.134
PVS1	-3.134
PVS5	-5.986
PVS6	-5.944
PVS7	-5.278
PVS8	-5.215
PVS 2.4	-6.146
PVS 2.5	-5.775
PVS 2.6	-6.243
PVS 2.7	-7.724
PVS 2.8	-6.326
PVS 2.9	-7.484
PVS 2.10	-6.056
PVS 2.11	-4.635
PVS 2.12	-5.23
PVS 2.14	-7.718
PVS 2.16	-7.406
DASATINIB	-6.617

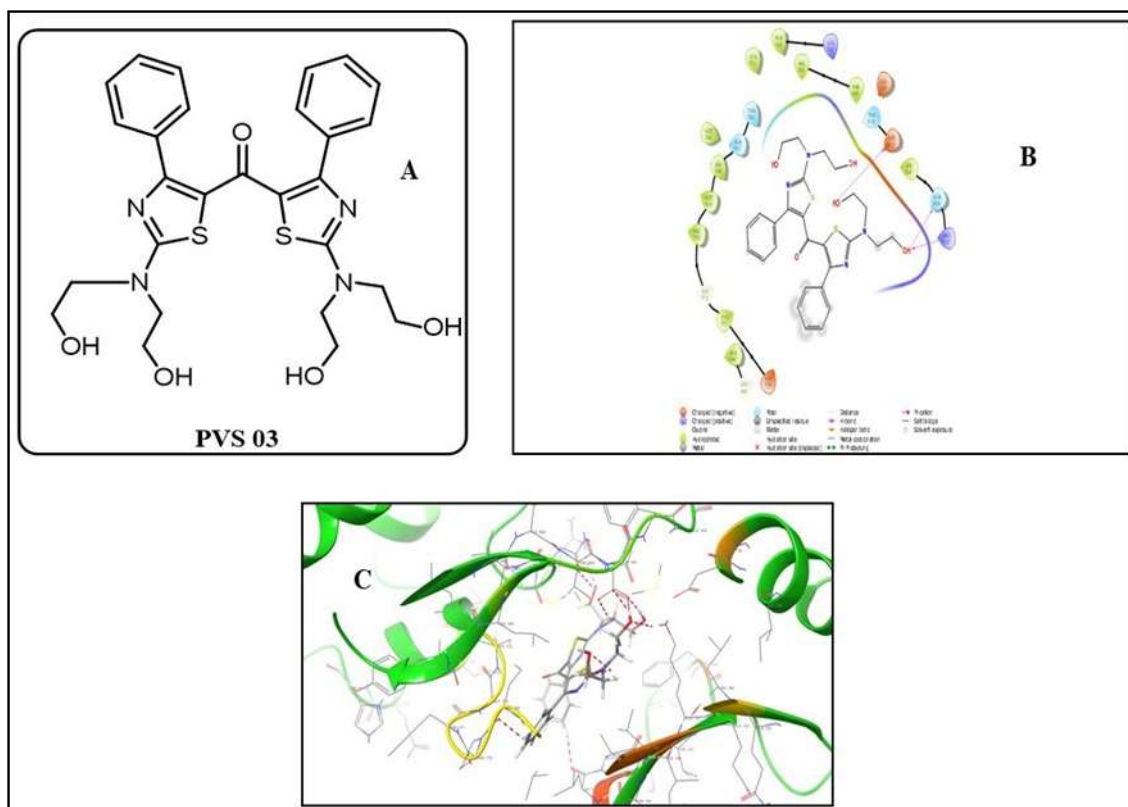


Figure 1: (A): Structure of PVS03 docked molecule; (B): 2D Structure of PVS 03 Docked Structure; (C): 3D or Ribbon Structure of PVS 03 Docked Structure

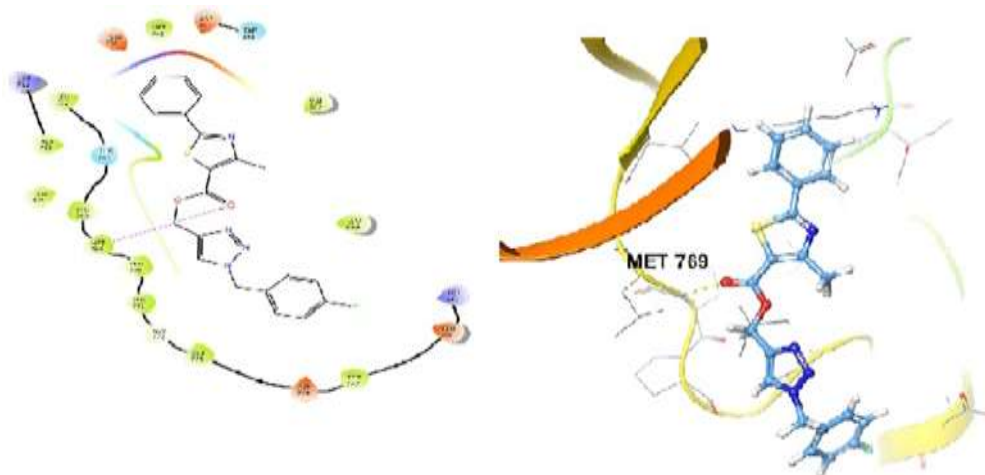


Figure 2: Structure of PVS 2.7 docked molecule; 2D Structure of PVS 2.7 Docked Structure; 3D or Ribbon Structure of PVS 2.7 Docked Structure

MTT Assay

The MTT assay is a standard method for determining cell viability and proliferation. In this investigation, the assay was carried out in RPMI medium supplemented with 10% FBS and 1% antibiotic solution at 37°C with 5% CO₂. The first tests were performed on two separate cell lines: MDAMB-231 human breast cells and HepG2 human lung cells. The cells were allowed to multiply for 24 hours before MTT was added at a final concentration of 0.5 mg/mL. The cultures were incubated for an additional 2 hours to enable MTT to convert to formazan. The impact of series 1 compounds PVS 03, 05, 08, 09, and 10 on

these cell lines' development was then investigated. The findings indicated that MDAMB-231 cells drained over 90% of the culture medium by 4 days after inoculation, but HepG2 cells used just 15% of the sugar. Figure 6 shows the action of PVS 03 at 250 mcg/mL.

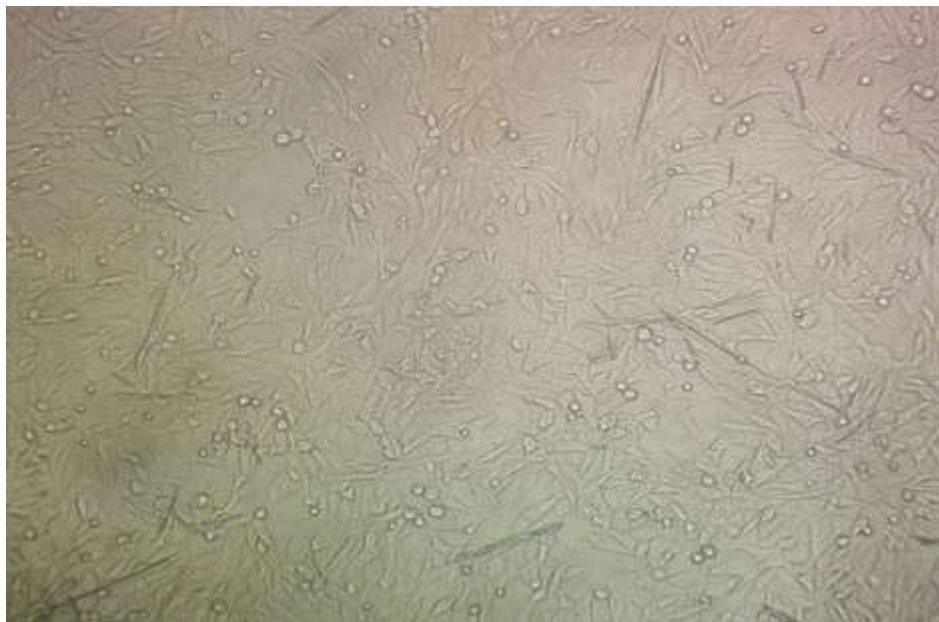


Figure 6: MTT assay observation at 250 mcg/ml concentration of PVS 03 molecule

This data suggested that MDAMB-231 cells multiply more quickly than HepG2 cells. Furthermore, the reduction in medium FBS content in MDAMB-231 cell cultures was associated with a significant drop in MTT-specific activity. In contrast, in the presence of compounds PVS 06, 07, and 02, the specific activity of MTT in both MDAMB-231 and HepG2 cells remained essentially constant across a 4-day growth period, suggesting no inhibition. These disparate findings motivated the researchers to perform more study utilizing a broader spectrum of tumor cell lines. To demonstrate broad-spectrum activity and therapeutic potential, substances must be tested on several cell lines. As a result, the researchers conducted identical studies with a variety of additional tumor cell lines. The findings of these studies would assist in determining the effectiveness of the chemicals against various kinds of malignancies and in the creation of new cancer medicines. In the second series, the impact of compounds PVS 2.7 and 2.9 on the growth of these cell lines was investigated. MCF-7 cells drained over 90% of the culture medium after 4 days of inoculation, but A431 cells used just 100% of the sugar within the same time period. Figure 6 shows the impact of PVS 2.7 at 100 mcg/mL.

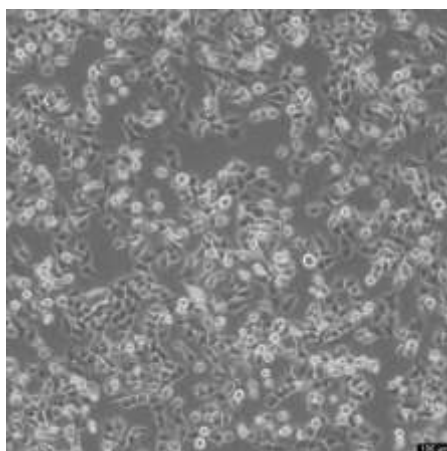


Figure 6: MTT assay observation at 100 mcg/ml concentration of PVS 2.7 molecule

In contrast, the presence of chemicals PVS 2.10, PVS 2.4, and PVS 2.6 results in a low percentage of inhibition and moderate anticancer efficacy against the A431 cell. While PVS 2.11, PVS 2.5, PVS 2.14, PVS 2.9, and PVS 2.8 exhibit higher inhibition and activity against the same cell line. Compounds PVS 2.7, PVS 2.9, PVS 2.11, and PVS 2.14 have increased activity against MCF-7 cells, whereas others exhibit moderate to low activity against the same cell line.

CONCLUSION:

In this work, we synthesized a new family of 2,4-disubstituted thiazole derivative chemicals intended to behave as EGFR inhibitors. These inhibitors were intended to create hydrogen bonds with the protein backbone, with peripheral groups orientated toward two hydrophobic pockets known as binding Regions I and II. The binding mechanism of dasatinib was compared to compound PVS 03, which had the highest activity in the substituted series. We found that substituting the thiazole nitrogen in dasatinib with a C-CN function might provide a new class of EGFR inhibitors that do not need water bridging, as dasatinib does. This was substantiated by PVS 03's cytotoxic impact on the tumor cell lines tested. The anticancer efficacy of the synthesized thiazole derivatives was tested against two tumor cell lines: Hep-G2 and MDAMB-231. PVS 03 had superior antitumor efficacy as compared to dasatinib. PVS 06 and 07 did not inhibit MDAMB-231 cells, but PVS 05 did not inhibit Hep-G2 cells. In another series, the anticancer efficacy of produced thiazole derivatives was tested against two tumor cell lines, MCF-7 and A431. PVS 2.7 had superior antitumor efficacy as compared to dasatinib. However, PVS 2.10, PVS 2.4, and PVS 2.6 did not suppress A431 cells. Overall, our results indicate that new thiazole compounds may be promising candidates for the development of EGFR inhibitors with better anticancer properties. The findings further emphasize the need of testing these drugs' anticancer characteristics on various cell lines to determine their broad-spectrum action.

REFERENCES:

- [1] Das R, Kumar H, Choithramani A, Bothra G, Shard A. Polymeric Nanoparticles to Entrap Natural Drugs for Cancer Therapy. Polymeric nanoparticles for the treatment of solid tumors. 2022 Nov 15:167-211.
- [2] Cheng F, Guo D. MET in glioma: signaling pathways and targeted therapies. Journal of Experimental & Clinical Cancer Research. 2019 Dec;38:1-3.
- [3] London M, Gallo E. Epidermal growth factor receptor (EGFR) involvement in epithelial-derived cancers and its current antibody-based immunotherapies. Cell biology international. 2020 Jun;44(6):1267-82.
- [4] Shah RR, Shah DR. Safety and tolerability of epidermal growth factor receptor (EGFR) tyrosine kinase inhibitors in oncology. Drug safety. 2019 Feb 8;42(2):181-98.
- [5] Rebuzzi SE, Alfieri R, La Monica S, Minari R, Petronini PG, Tiseo M. Combination of EGFR-TKIs and chemotherapy in advanced EGFR mutated NSCLC: Review of the literature and future perspectives. Critical Reviews in Oncology/Hematology. 2020 Feb 1;146:102820.
- [6] Drug evaluation: Deferritin GT-56-252; NaHBED for iron overload disorders I Drugs; 2007;104:270-281.
- [7] Graham R. Lawton, Haitao Ji, Pavel Martáse, Linda J. Roman, and Richard B. Silverman, Synthesis and enzymatic evaluation of 2- and 4-aminothiazole-based inhibitors of neuronal nitric oxide synthase, Beilstein Journal of Organic Chemistry, 2009, 5, 28
- [8] Bang-Chi Chen, Rulin Zhao, Bei Wang, Roberto Droghini, Jean Lajeunesse, Pierre Sirard, Masaki Endo, Balu Balasubramanian and Joel C. Barrisha, A new and efficient preparation of 2-aminothiazole-5-carbamides: applications to the synthesis of the anti-cancer drug dasatinib, ARKIVOC 2009 vi 32-38.
- [9] SR Pattan, Synthesis and Biological Evaluation of Some Substituted Amino Thiazole Derivatives, Asian J. Research Chem. 22; 2009; 196-201.
- [10] Korrapati. V. V. Prasada Rao, Synthesis of potential related compounds of Cefdinir, ARKIVOC 2006 xv 22-27.
- [11] Chang-Ling Liu, Zheng-Ming Li, Synthesis and biological activity of novel 2- methyl-4-trifluoromethyl-thiazole-5-carboxamide derivatives, Journal of Fluorine Chemistry 125;2004;1287-1290.
- [12] A.Th. Chaviara, Copper II Schiff base coordination compounds of dien with heterocyclic aldehydes and 2-amino-5-methyl-thiazole: synthesis, characterization, antiproliferative and antibacterial studies. Crystal structure of CudienOOC12, Journal of Inorganic Biochemistry 98; 2004;1271-1283.
- [13] Gülhan Turan-Zitouni, Synthesis of some 2-[benzazole-2-ylthioacetyl amino] thiazole derivatives and their antimicrobial activity and toxicity, European Journal of Medicinal Chemistry 39;2003;267-272.
- [14] Petrou A, Fesatidou M, Geronikaki A. Thiazole ring-A biologically active scaffold. Molecules. 2021 May 25;26(11):3166.
- [15] Kaur H, Goyal A. A review on thiazole as anticancer agents. Int J Pharm Drug Anal. 2018;6:509-22.

- [16] Niu ZX, Wang YT, Zhang SN, Li Y, Chen XB, Wang SQ, Liu HM. Application and synthesis of thiazole ring in clinically approved drugs. *European Journal of Medicinal Chemistry*. 2023 Feb 1;115172.
- [17] Sharma PC, Bansal KK, Sharma A, Sharma D, Deep A. Thiazole-containing compounds as therapeutic targets for cancer therapy. *European Journal of Medicinal Chemistry*. 2020 Feb 15;188:112016.
- [18] Kimber TB, Chen Y, Volkamer A. Deep learning in virtual screening: recent applications and developments. *International Journal of Molecular Sciences*. 2021 Apr 23;22(9):4435.
- [19] Zahid H. Chohan, Synthesis, Characterization And Biological Properties Of Tridentate Nno, Nns And Nnn Donor Thiazole-Derived Furanyl, Thiophenyl And Pyrrolyl Schiff Bases And Their CoLl, CuLl, NiLl And ZnLl Metal Chelates, Metal-Based Drugs, Vol. 7,1,2000.
- [20] Zahid H Chohan, Biologically Active Transition Metal Chelates Of NiLl, CuLl And ZnLl With 2-Aminothiazole-Derived Schiffbases: Their Synthesis, Characterization And The Role Of Anions No, So₄²⁻, Co⁴⁺-And Chco- On Their Antibacterial Properties, Metal-Based Drugs, 1999, 6, 3.
- [21] Robert G. Gentles, Initial SAR Studies on Apamin-Displacing 2-Aminothiazole
- [22] Blockers of Calcium-Activated Small Conductance Potassium Channels, 2000, BMCL.
- [23] A. Verma, Synthesis, characterization and biological evaluation of mutual prodrug of indomethacin and aminothiazole with reduced ulcerogenicity, AAPS, 2009;21-25.
- [24] Mosmann T. Rapid colorimetric assay for cellular growth and survival: application to proliferation and cytotoxicity assays. *J Immunol Methods*. 1983 Dec 16;65(1-2):55-63. doi: 10.1016/0022-1759(83)90303-4. PMID: 6606682.
- [25] Yuriev E, Holien J, Ramsland PA. Improvements, trends, and new ideas in molecular docking: 2012–2013 in review. *Journal of Molecular Recognition*. 2015 Oct;28(10):581-604.
- [26] Kar S, Leszczynski J. Open access in silico tools to predict the ADMET profiling of drug candidates. *Expert Opinion on Drug Discovery*. 2020 Dec 1;15(12):1473-87.
- [27] Chagas CM, Moss S, Alisaraie L. Drug metabolites and their effects on the development of adverse reactions: Revisiting Lipinski's Rule of Five. *International Journal of Pharmaceutics*. 2018 Oct 5;549(1-2):133-49.