WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
SJIF Impact Factor 8.453
Volume 14, Issue 5, 746-759. Research Article ISSN 2277–7105

IN-SILICO MOLECULAR DOCKING AND ITS ANTIULCER ACTIVITY OF ARALKYLBENZAZOLES

A. Sarala*, S. K. Senthil Kumar, A. Aakash[1], R. Hariramsun[2], E. Sathiya[3], J. Shinee Princiya[4] and S. Jayakumar[5]

*Associate Professor, Department of Pharmaceutical Chemistry, Arunai College of Pharmacy, Tiruvannamalai, Tamilnadu, India.

Principal Cum Professor, Department of Pharmaceutics, Arunai College of Pharmacy, Tiruvannamalai, Tamilnadu, India.

[1,2,3,4,5]B. Pharmacy Final Year Students, Arunai College of Pharmacy, Tiruvannamalai, Tamilnadu, India.

Article Received on
07 January 2025,

Revised on 27 Jan. 2025,
Accepted on 17 Feb. 2025

DOI: 10.20959/wjpr20255-35689

***Corresponding Author**
A. Sarala
Associate Professor, Department of Pharmaceutical Chemistry, Arunai College of Pharmacy, Tiruvannamalai, Tamilnadu, India.

ABSTRACT

This study explores the in-silico molecular docking analysis of Aralkylbenzazoles to evaluate their antiulcer activity. Ulcers, primarily caused by Helicobacter pylori infection and prolonged use of nonsteroidal anti-inflammatory drugs (NSAIDs), remain a global health concern. Conventional treatments often exhibit adverse effects, necessitating the search for alternative therapeutics. In this research, a set of Aralkylbenzazoles was selected, and their molecular interactions with the target protein, VEGFR2 (PDB ID: 3VHE), were analyzed using computational docking methods. SwissDock was utilized for virtual screening and docking, while ADME profiling was conducted via SWISSADME to assess the drug-likeness properties of the compounds. The docking results revealed that Compound 12 exhibited the highest binding affinity (-9.173 kcal/mol) compared to the standard drug Rebamipide (-6.727 kcal/mol), suggesting its potential as a promising antiulcer candidate. Additionally, ADME analysis confirmed favorable pharmacokinetic properties, ensuring effective absorption and minimal side effects. This study underscores the significance of computational drug discovery in identifying novel antiulcer agents with enhanced efficacy and safety profiles.

KEYWORDS: Molecular docking, Aralkylbenzazoles, Antiulcer activity, Helicobacter pylori, SwissDock, VEGFR2, Computational drug discovery, ADME analysis, Drug-likeness, In-silico analysis, Lipinski's Rule, Pharmacokinetics, Binding affinity, Lead optimization, Structure-based drug design.

INTRODUCTION

Ulcer

An Ulcer can be referred to a surface/region in the digestive system where the tissue has been ruined or damaged by the gastric juice or other digestive enzymes that are produced my stomach. An ulcer is a discontinuity or break in a bodily membrane that impedes the organ, of which that membrane is a part of, from continuing its normal functions. As many as 70-90% of such ulcers are associated with Helicobacter pylori, a spiral-shaped bacterium that lives in the acidic environment of the stomach. The common major type of ulcer that mostly affects the global population is the peptic ulcer diseases, which occurs in the stomach or small intestine, the secreted gastric acid by the stomach compartment destroys the protective cover of the small intestine or the stomach (Duodenum) giving rise to acid-related disorders.

Antiulcer activity

Anti-ulcer medications, also known as gastroprotective agents or anti-ulcerants, are drugs designed to prevent or treat ulcer in the gastrointestinal (GI) tract. Ulcers are open sores that develop in the lining of the stomach, duodenum (first part of the small intestine), or esophagus. Anti-ulcer exerts their action by blocking the H+/K+-ATPase enzyme, which is the final step of gastric acid secretion in the stomach. H. pylori secrete CagA, (Cytoxin-associated gene A), which is a poisonous substance produced by the bacterium after translocation into host cell, it alters cell shape, increase cell motility, redirect cell junction activity and thus responsible for gastric carcinomas and gastric ulcer.

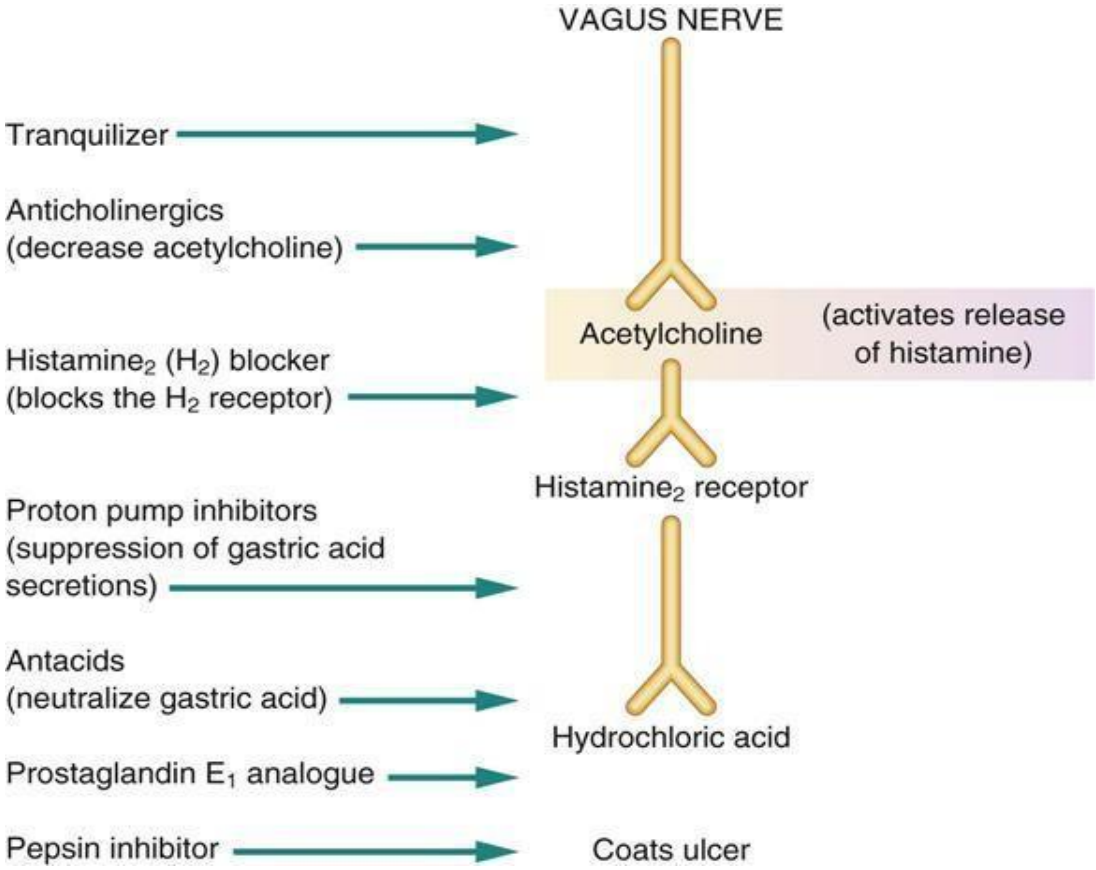


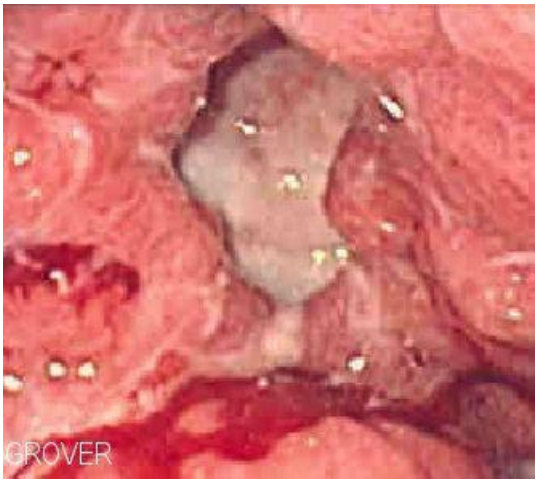
Fig. Actions of the Antiulcer drug groups.

Mechanisms of action

Mucosal protection: Protecting the gastrointestinal mucosa from damage and promoting healing.

Anti-inflammatory effects: Reducing inflammation and inhibiting pro-inflammatory cytokines.

Antioxidant activity: Neutralizing free radicals and reducing oxidative stress.



Endoscopic image of gastric ulcer

Aralkylbenzazoles

Aralkylbenzazoles are a class of heterocyclic compounds that have gained significant attention in the field of medicinal chemistry due to their diverse biological activities.

Definition

Aralkylbenzazoles are a fusion of aryl and alkyl groups attached to a benzazole ring system. The general structure consists of:

An aryl group (e.g., phenyl)

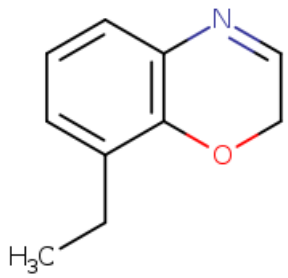
An alkyl group (e.g., methyl, ethyl)

A benzazole ring (e.g., benzimidazole, benzoxazole)

Classification

Aralkylbenzazoles can be classified based on the type of benzazole ring and the substitution pattern:

- Benzimidazoles
- Benzoxazoles
- Benzothiazoles



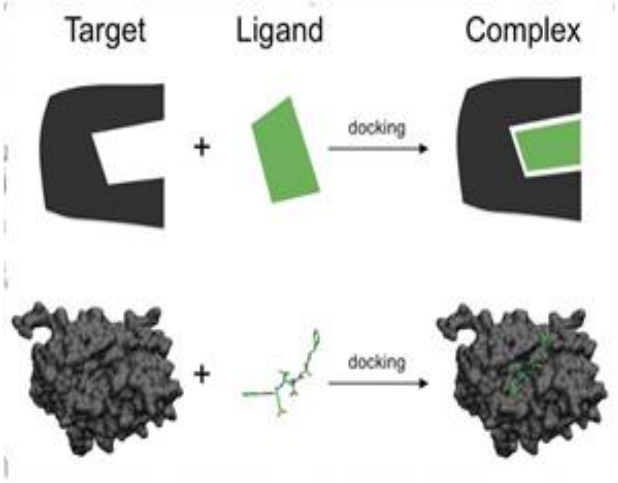
Structure of aralkylbenzazoles

Molecular docking

Molecular docking is a computational technique used to predict the preferred orientation of one molecule (Typically a small ligand) when bound to a target macromolecule (Usually a protein). This approach plays a pivotal role in drug discovery and design by helping researchers understand how potential drug candidates interact with biological targets at the molecular level. The primary goal of molecular docking is to model the interaction between the ligand and the target protein, providing insights into binding affinities and the structural features that influence these interactions. By simulating these docking scenarios, scientists can identify promising compounds, optimize lead candidates, and streamline the drug

development process. Molecular docking relies on various algorithms and scoring functions to evaluate the binding modes and affinities, making it an essential tool in pharmacology, biochemistry, and structural biology.

For example, protein-ligand docking. More recently, docking is also applied to predict the binding mode between two macromolecules, for instance protein-protein docking.



Major steps involved in mechanics of molecular docking

Molecular Docking is the process in which the intermolecular interaction between 2 molecules was studied in In-silico. In this process, the Macromolecule is the protein receptor. The micro molecule is the Ligand molecule which can be acted as an inhibitor.

The Docking process involves the following steps

Step I – Preparation of protein: Three dimensional structure of the Protein should be retrieved from Protein data bank (PDB); afterward the retrieved structure should be pre-processed. This should admit removal of the water molecules from the cavity, stabilizing the charges, filling the missing residues, generation the side chains etc. according to the parameters available.

Step II – Active site prediction: After the preparation of protein, the active site of protein should be predicted. The receptor might possess lots of active sites merely the one of the concern should be picked out. Mostly the water molecules and hetero atoms are removed if present.[14-15]

Step III – Preparation of ligand: Ligands can be retrieved from several databases such as ZINC, Pub Chem or can be sketched applying Chem sketch tool. While picking out the ligand, the LIPINSKY'S RULE OF 5 should be utilized. Lipinski rule of 5 assists in discerning amongst non-drug like and drug like candidates. It promises high chance of success or failure due to drug likeness for molecules abiding by with 2 or more than of the complying rules.

For choice of a ligand allowing to the LIPINSKI'S

Less than five hydrogen bond donors

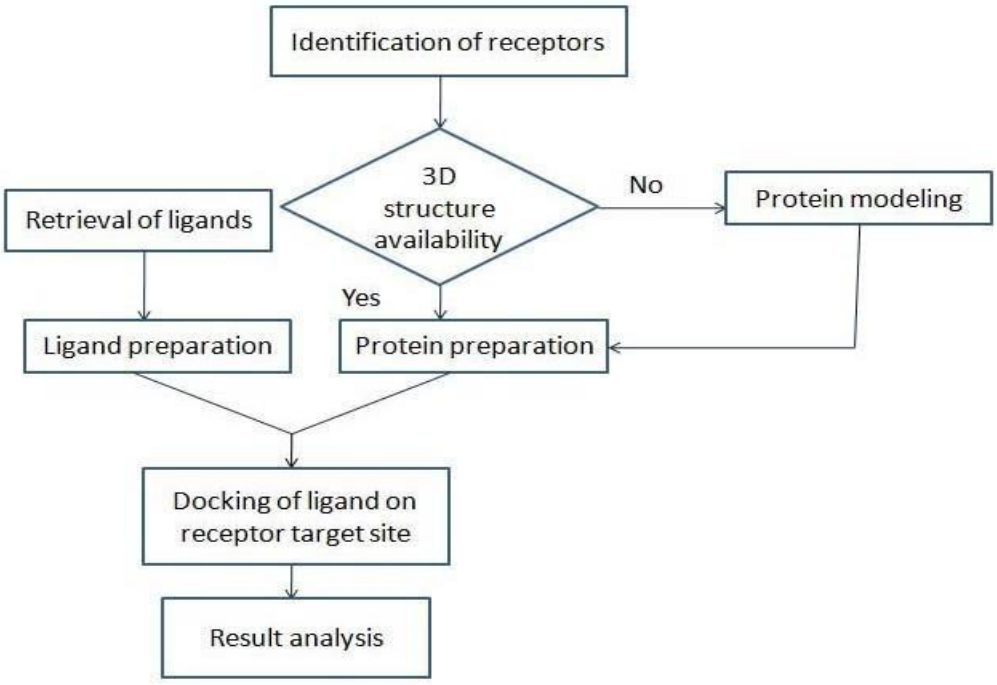
Less than ten hydrogen bond acceptors

Molecular mass less than 500 Da

High lipophilicity (Expressed as LogP not over 5)

Molar refractivity should be between 40-130

Step IV- docking: Ligand is docked against the protein and the interactions are analyzed. The scoring function gives score on the basis of best docked ligand complex is picked out.



Basic steps of molecular docking

MATERIALS AND METHODS

In this study, we use the new SwissDock, based on the Attracting cavities and Autodock Vina docking engines old version.

1. Protein preparation

Crystal structure of human VEGFR2 kinase domain with a novel pyrrolopyrimidine inhibitor, PDB ID 3VHE, resolution 1.55Å was retrieved from the protein data bank and entered into the SWISSADME as a result of this study. The Crystal structure of human VEGFR2 Kinase domain with a novel pyrrolopyrimidine underwent protein preparation before docking began. They used the protein preparation SWISSADME.

The next step in the preprocessing includes deleting water molecules farther than 5' from heteroatom states, H-bond acceptor, H-bond donar, solubility, GI absorption, BBB permeant, pain. Still being done are preprocessing minimization and optimization. Finally, the workspace's centroid was used to build the grid. All ligand can be docked using this protein.

2. Ligand preparation

The 2D structure (SDF) of various compound was selected from the antiulcer activity. The molinspiration tools were created to construct high-quality ligand preparation, and all the ligand's two-dimensional (2D) or three-dimensional (3D) SDF (structures Data Flies) structure were obtained at the workspace. The ligand preparation steps involved sketching individual designs in molinspiration structure the copy the smiles proceed to SWISSDOCK, and saving the final energy- minimized structure in SDF format for protein-ligand docking. The ligand was arranged in the proper bond orders by using tools.

3. Docking analysis

A molecular docking study of the selection of various compound of antiulcer activity for high though the put virtual screening was performed against the ulcer VEGFR2 (PDB ID: 3VHE). With flexible docking on SWISS DOCK between ligands and the target protein active site, a molecular docking investigation of the various compounds was conducted against the tumour. For docking, an additional accuracy mode is provided. While ligands were flexible, the protein was fixed during molecular docking. Among ligands, the best configuration with the highest docking score of virtual screening was scored by extra precision flexible docking.[15]

4. ADME Analysis

The ADME properties of selected lead molecules were calculated using the ADME and molecular properties module of the SWISSADME. The molinspiration tool in the SWISSADME is used to predict the "drug-likeness" features of various compounds from antiulcer activity.[16]

The physicochemical properties include formula, molecular weight, No. heavy atoms, No. aromatic heavy atoms, fraction Csp3, No. rotatable bonds. No. H-bond acceptors, No. H-bond donors, molar refractivity, TPSA [topological polar surface area]. The lipophilicity includes iLOGP, XLOGP3, WLOGP, MLOGP, Silicos-IT Log P, consensus LogP. The predicted water solubility compounds includes ESOL log S, ESOL solubility [mg/ml], ESOL solubility[mol/l], ESOL class, Ali log S,Ali solubility[mg/ml],Ali solubility[mol/l], Ali class, Silicos-IT log S, Silicos-IT solubility[mg/ml], Silicos- IT solubility [mol/l], Silicos-IT class.

The pharmacokinetics compounds include GI absorption, BBB permeant, Pgp substrate, CYP1A2 inhibitor, CYP2C19 inhibitor, CYP2C9 inhibitor, CYP2D6 inhibitor, CYP3A4 inhibitor, Log Kp (skin permeation). The predicted drug-likeness compounds include Lipinski, Ghose, Veber, Egan, Muegge, bioavailability, PAINS, Brenk, Lead-likeness, Synthetic accessibility.

RESULTS AND DISCUSSIONS

Ulcers can be effectively treated. Symptoms can vary greatly or affect everyone. Because, the symptoms of these ulcer behave like burning pain in the abdominal often at night, nausea and vomiting, bloating and discomfort, loss of appetite, heart burn, blood in stool, etc., There is a specific treatment available in the world. So, we realize the vigorous condition of these disease. By concern of these disease, we try to promote drug likeness property to act against ulcer disease with help of Anti-ulcer activity of various Aralkylbenzazoles compounds.

Table: List of aralkylbenzazoles compounds.

Compound no	Iupac name	Molecular formula
1	6-(pyridin-2-ylmethyl)-1,3- benzothiazol-2-amine	C13H11N3S
2	N-methyl-6-(pyridin-2-ylmethyl)-1,3- benzothiazol-2-amine	C14H13N3S
3	(2-amino-1,3-benzothiazol-6-yl)- pyridin-2-ylmethanol	C13H11N3OS
4	N-ethyl-5-(2-pyridin-2-ylethyl)-1,3- benzothiazol-2-amine	C17H19N3S
5	5-(2-pyridin-2-ylethyl)-1,3-benzothiazol- 2-amine	C15H15N3S
6	5-[2-(4-methylpyridin-2-yl)ethyl]-1,3- benzothiazol-2-amine	C16H17N3S
7	5-[2-(3-methylpyridin-2-yl)ethyl]-1,3- benzothiazol-2-amine	C16H17N3S
8	5-[2-(5-methylpyridin-2-yl)ethyl]-1,3- benzothiazol-2-amine	C16H17N3S
9	4-methoxy-5-(2-pyridin-2-ylethyl)-1,3- benzothiazol-2-amine	C16H17N3OS
10	4-bromo-5-(2-pyridin-2-ylethyl)-1,3- benzothiazol-2-amine	C15H14BrN3S
11	4-bromo-5-[2-(3-methylpyridin-2- yl)ethyl]-1,3-benzothiazol-2-amine	C16H16BrN3S
12	4-bromo-5-[2-(5-methylpyridin-2- yl)ethyl]-1,3-benzothiazol-2-amine	C16H16BrN3S
13	4-bromo-N-methyl-5-(2-pyridin-2- ylethyl)-1,3-benzothiazol-	C16H17N3S

	2-amine	
14	4-bromo-N-ethyl-5-[2-(3-methylpyridin- 2-yl)ethyl]-1,3-benzothiazol-2-amine	C18H21N3S
15	5-(pyridin-2-ylmethoxy)-1,3- benzothiazol-2-amine	C13H11N3OS
16	5-(pyridin-2-ylmethylsulfanyl)-1,3- benzothiazol-2-amine	C13H11N3S2
17	5-(2-pyridin-2-ylethyl)-1,3-benzoxazol-2- amine	C15H15N3O
18	5-[2-(5-methylpyridin-2-yl)ethyl]-1,3- benzoxazol-2-amine	C16H17N3O
19	N-ethyl-5-(2-pyridin-2-ylethyl)-1,3- benzoxazol-2-amine	C17H19N3O
20	5-(2-pyridin-2-ylethyl)-1H-benzimidazol- 2-amine	C15H16N4
21	5-[2-(5-methylpyridin-2-yl)ethyl]-1H- benzimidazol-2-amine	C16H18N4
22	4-[2-(5-methyl-1H-imidazol-4-yl)ethyl]- 1,3-benzothiazol-2-amine	C13H14N4S
23	4-[2-(5-methyl-1H-imidazol-4-yl)ethyl]- 1H-benzimidazol-2-amine	C13H15N5
24	5-(2-pyridin-2-ylethyl)-1H-benzimidazol- 2-amine	C15H18N4O
25	5-[2-(5-methylpyridin-2-yl)ethyl]-1H- benzimidazol-2-amine	C16H19NOS
26	4-[2-(5-methyl-1H-imidazol-4-yl)ethyl]- 1,3-benzothiazol-2-amine	C18H22N4O3
27	4-[2-(5-methyl-1H-imidazol-4-yl)ethyl]- 1H-benzimidazol-2-amine	C20H28N4O
28	N-ethyl-4-[2-[5-(piperidin-1- ylmethyl)furan-2-yl]ethyl]-1,3-benzoxazol-2-amine	C21H27N3O2
29	5-[[5-[(dimethylamino)methyl]furan-2- yl] methylsulfanylmethyl]-N-ethyl-1,3- benzoxazol-2-amine	C18H23N3O2S
30	5-[[5-[(dimethylamino)methyl]furan-2- yl] methylsulfanylmethyl]-N-ethyl-1,3- benzoxazol-2-amine	C18H23N3O2S
31	2-[4-[[2-(ethylamino)-1,3-benzoxazol-5-yl]methylsulfanylmethyl]-1,3-thiazol-2- yl]guanidine	C15H18N6OS2
32	2-[4-[[2-(ethylamino)-1,3-benzoxazol-6-yl]methylsulfanylmethyl]-1,3-thiazol-2- yl]guanidine	C15H18N6OS2
33	N-ethyl-5-[[3-(piperidin-1- ylmethyl)phenoxy]methyl]-1,3-benzoxazol-2-amine	C22H27N3O2
34	N-ethyl-6-[[3-(piperidin-1- ylmethyl)phenoxy]methyl]-1,3-benzoxazol-2-amine	C22H27N3O2
35	5-[2-(4-methyl-3-trityl-2,4- dihydroimidazol-5-yl)ethyl]-1,3-benzothiazol-2-amine	C32H28N4S
36	N-ethyl-6-[2-(4-methyl-3-trityl-2,4- dihydroimidazol-5-yl)ethyl]-1H- benzimidazol-2-amine	C34H33N5
37	N-ethyl-6-[2-(4-methyl-3-trityl-2,4- dihydroimidazol-5-yl)ethenyl]-1,3- benzoxazol-2-amine	C34H30N4O
38	N-ethyl-5-[2-(4-methyl-1H-imidazol-5- yl)ethenyl]-1,3-benzoxazol-2-amine	C15H16N4O
39	N-(methoxymethyl)-6-[3-(oxolan-2- yl)propyl]-1,3-benzoxazol-2-amine	C15H15N3O3
40	N-ethyl-6-[2-(furan-3-yl)ethenyl]-1,3- benzoxazol-2-amine	C15H14N2O2
41	N-ethyl-6-[2-(furan-2-yl)ethyl]-1,3- benzoxazol-2-amine	C15H16N2O2
42	N-ethyl-N-[6-[2-(furan-2-yl)ethyl]-1,3- benzoxazol-2-yl]formamide	C15H16N2O2
43	N-ethyl-N-[5-[2-(3-formylphenyl)ethyl]- 1,3-benzoxazol-2-	C18H16N2O4

	yl]formamide	
44	N-ethyl-N-[6-[2-(3-formylphenyl)ethyl]- 1,3-benzoxazol-2-yl]formamide	C18H16N2O2
45	4-(2-pyridin-2-ylethyl)aniline	C13H14N2
46	2-(2-pyridin-2-ylethyl)aniline	C13H14N2
47	4-[2-(3-methylpyridin-2-yl)ethyl]aniline	C14H16N2
48	4-[2-(4-methylpyridin-2-yl)ethyl]aniline	C14H16N2
49	4-[2-(5-methylpyridin-2-yl)ethyl]aniline	C14H16N2
50	2-methoxy-4-(2-pyridin-2-ylethyl)aniline	C14H16N2O

The ADME Study Report of the compounds of aralkylbenzazoles

The captured various compounds were then subjected to ADME testing using SWISSADME software. The forecasted ADME property of various compound based on their structure, functional groups and molecular properties such as Mol/M.W (Molecular weight), BBB permeant (Blood-Brain Barrier parameter of compounds), GI (Gastrointestinal absorption), H-bond acceptors, H-bond donors, Violation and MLogP (Moriguchi octanol-water partition coefficient). Few compounds transgressed drug-likeness tests were removed as those compounds have poor ability to cross the biological membrane. The ADME report are mentioned under the following table.

Compound No.	M.W g/mol	BBB	GI Absorption	H-bond acceptors	H-bond donors	Violation	mLogP
1	241.31	No	High	2	1	0	1.93
3	257.31	No	High	3	2	0	1.08
5	269.36	No	High	2	1	0	2.45
6	283.39	No	High	2	1	0	2.70
7	283.39	No	High	2	1	0	2.70
8	283.39	No	High	2	1	0	2.70
9	299.3	No	High	3	1	0	2.12
10	348.26	No	High	2	1	0	3.09
11	362.29	No	High	2	1	0	3.33
12	362.29	No	High	2	1	0	3.33
15	257.31	No	High	3	1	0	1.35
16	273.38	No	High	3	1	0	2.20
22	258.34	No	High	2	2	0	1.52
23	241.29	No	High	2	3	0	1.10
25	301.41	No	High	3	1	0	1.47
29	345.46	No	High	4	1	0	1.94
31	285.30	No	High	4	2	0	1.54
Limit	≤500	No	High	≤ 10	≤ 5	0	≤ 4.15

The molecular docking score of aralkylbenzazoles

The docking studies of the ligands to protein active sites were done by the modern molecular docking programmed SWISSDOCK old version to determine compounds binding affinity. In

silico approach between selected ligands and Protein Data Bank ID: 3VHE of the Ulcer disease. The good drug-likeness properties containing the ligands's docking score, yield [%].

Compounds No.	Docking score [Kcal/mol]
12	-9.173
25	-8.806
8	-8.801
7	-8.609
11	-8.581
10	-8.524
6	-8.334
9	-8.330
3	-8.292
1	-8.176
5	-8.104
23	-7.782
31	-7.777
22	-7.655
29	-7.477
15	-7.375
16	-7.143
REBAMIPIDE	-6.727

From the docking results, docked ligand Compound 12 has a low crucial binding energy with VEGFR2 protein target (Ulcer). The docking score is **-9.173** [kcal/mol] shown here.

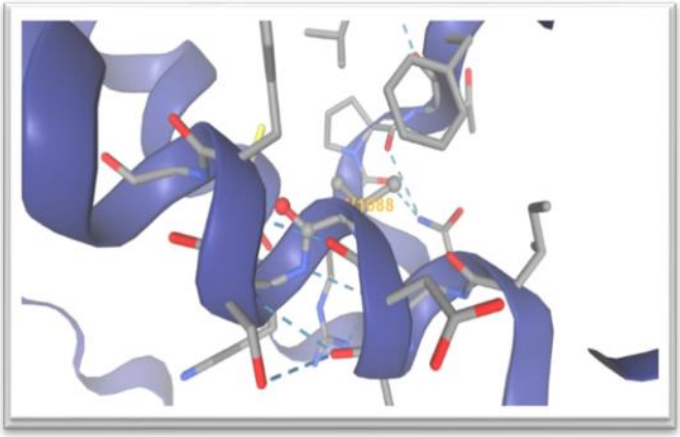


Fig: 3D Structure of docking interaction of compound 12 with VEGFR2.

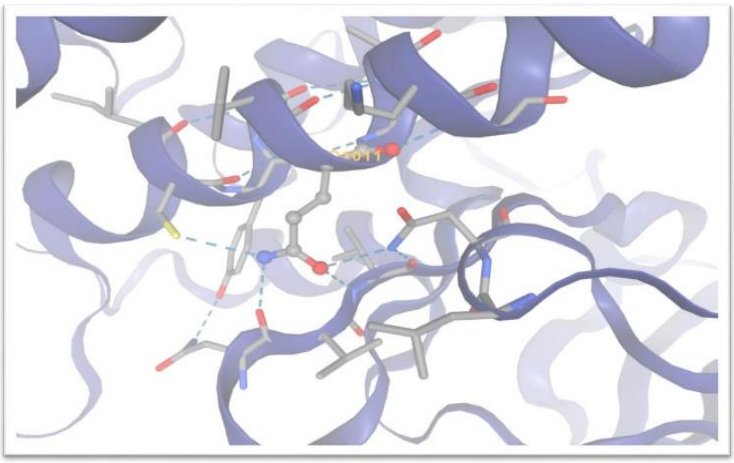


Fig: 3D Structure of docking interaction of Rebamipide with VEGFR2.

Compared to other selected compounds, Compound 12 had low binding energy. This top hit selected compound was compared with the standard drug Rebamipide, docking score is -6.727kcal/mol. The docking score of Compound 12 contains low binding energy of -9.173 kcal/mol. Moreover, C12 includes a molecular weight of 362.29g/mol. So, it can easily be transported when compared to other heavy molecular weight molecules. The BBB activity is inactive (NO). so, it does not cause any side effects in CNS. The MLogP of C12 (3.33) is less than 4.15, So it easily crosses the cell membranes. From the above discussion, we suggested Compound 12 had more effectiveness against the Ulcer.

CONCLUSION

This study successfully explored the in-silico molecular docking of Aralkylbenzazoles for their potential antiulcer activity. Using computational tools, we analyzed the binding interactions between various Aralkylbenzazoles and the VEGFR2 protein (PDB ID: 3VHE), a key target in ulcer treatment. The docking results revealed that Compound 12 exhibited the most promising binding affinity, with a docking score of -9.173 kcal/mol, outperforming the standard drug Rebamipide (-6.727 kcal/mol).

Further ADME analysis confirmed that Compound 12 has favourable pharmacokinetic properties, including high gastrointestinal absorption and compliance with Lipinski's Rule of Five, making it a strong candidate for further in-vitro and in-vivo studies. The findings indicate that Aralkylbenzazoles hold significant potential as antiulcer agents and warrant further experimental validation to establish their therapeutic efficacy.

Overall, this research highlights the effectiveness of molecular docking in drug discovery and provides a foundation for the development of novel antiulcer treatments based on Aralkylbenzazoles.

REFERENCE

1. Muhammad baba Muh'd.; Molecular docking and quantitative structure-activity relationship study of anti-ulcer activity of quinazolinone derivatives. Ahmadu Bello University, 2018.
2. Djahanguiri B. The production of acute gastric ulceration by indomethacin in the rat. Scand J Gastroenterol, 1968; 4: 265-267.
3. Ezealisiji KM, ljeomah SC, Agbo MO Anti-ulcer activity of African walnut Tetracarpidium conophorum nuts against gastric ulcers in rats Asian Pac J Trop Dis, 2014; 4: 998- 1001.
4. Chaudhary, S., Kapila, A., Sharma, R.B., Vashist, H., A review on peptic ulcer. Int. J. Recent Adv, Sci, Technol, 2015; 2: 6-10.
5. Sharma D, Bhatt SA Comprehensive review on ulcer healing potential of medicinal plants. Int J Pharm Pharm Sci, 2014; 6: 10.
6. KOUITCHEU MABEKU, L. B.; NANFACK NANA, B.; EYOUM BILLE, B.; TCHUENTEU TCHUENGUEM, R.; & NGUEPI, E. Anti-Helicobacter pylori and antiulcerogenic activity of Aframomum pruinosum seeds on indomethacin-induced gastric ulcer in rats. Pharmaceutical biology, 2017; 55: 929-936.
7. Rajesh, R.; Manikandan, A.; Sivakumar, A.; Ramasubbu, C.; & Nagaraju, N. Substituted methoxybenzyl-sulfonyl-1H-benzo [d]imidazoles evaluated as effective H+/K+- ATPase inhibitors and anti-ulcer therapeutics. European journal of medicinal chemistry, 2017; 139: 454- 460.
8. Adam J, Singer MD, Richard AF, Clark MD. Cutaneous wound healing. N Engl J Med, 1999; 341: 738-746.
9. Yousuke Katsura,. Studies on Anti-ulcer drugs. V. Synthesis and Antiulcer Activity of Aralkylbenzazoles.
10. Ferreira L.G., Dos Santos R.N., Oliva G., Andricopulo A.D. Molecular docking and structure-based drug design strategies. Molecules, 2015; 20(7): 13384-13421. [DOI] [PMC free article] [PubMed] [Google Scholar].
11. Morris GM, Huey R, Lindstrom W, Sanner MF, Belew RK, Goodsell DS, Olson AJ. Auto Dock Tools4: automated docking with selective receptor flexibility. J Computer Chem,

2009; 30: 2785-2791.

12. Iqbal Azad. Molecular docking in the study of ligand-protein recognition: An Overview. DOI: 10.5772/intechopen.106583.
13. Vishwajit S. Patil*, Prithviraj A. Patil. Molecular Docking: A useful approach of Drug Discovery on the Basis of their Structure. https://asianjpr.com/HTML_Papers/Asian Journal of Pharmaceutical. Research PID 2023-13-3-10.html.
14. Abdulfatai, U.; Uzairu, A.; & Uba, S. Molecular docking and quantitative structure-activity relationship study of anticonvulsant activity of aminobenzothiazole derivatives. Beni-Suef University Journal of Basic and Applied Sciences, 2017.
15. Daina A., Michielin O., Zoete V. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Sci. Rep, 2017; 7: 42717. [DOI] [PMC free article] [PubMed] [Google Scholar].