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Insilico Drug Design and Molecular Docking Studies of Novel 2-Amino Benzothiazole Derivatives for Antiischemic

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ABSTRACT
A series of 2-amino benzothiazole derivatives were designed for their potential as therapeutic agents. This involved the formation of various benzothiazole-based compounds, which were then subjected to molecular docking studies to predict their binding affinities and interaction patterns with target biomolecules. In silico design techniques, including virtual screening and molecular dynamics simulations, were employed to optimize the chemical structure and enhance biological activity. The prediction of biological activity and toxicity profiles was performed using the PASS software, which identified key pharmacological properties, while ADMET analysis (Absorption, Distribution, Metabolism, Excretion, and Toxicity) via ADMETSAR provided insights into the compounds' drug-likeness and safety profiles. The results from these computational approaches suggest that certain derivatives exhibit promising binding affinities and favorable pharmacokinetic properties, indicating their potential as lead candidates for further experimental validation. This study highlights the importance of integrated computational methods in the rational design of bioactive molecules and their potential in drug discovery.

KEYWORDS: 2-Aminobenzothiazole, insilico design, antiischemic activity

I. INTRODUCTION

BENZOTHIAZOLE

Benzothiazoles are an important class of bicyclic hetero cycles that play a key role in the design of biologically active compounds. At the moment, due to the threat of outbreaks of epidemics associated with the emergence and spread of various viruses, modern research and development in medicinal chemistry and pharmacology based on benzothiazole derivatives have become especially relevant. Molecules with a benzothiazole moiety have a pronounced spectrum of biological activity, exhibiting along with antiviral, antimicrobial, anti-inflammatory, antidiabetic, analgesic, antioxidant, anti-depressant, anticonvulsant, antianginal, antitumor, immunomodulatory effects. Benzothiazole derivatives also have anthelmintic, antimalarial, fungicidal, insecticidal and herbicidal effects.

Benzothiazole derivatives play a vital role in biological fields such as antitubercular, antiallergic activities. The benzothiazole derivatives used as painkiller and reduce the muscle spasms and it interact with nerve transfer of glutamate in biochemical and electro-physiological experiments. Benzothiazoles, which have benzene and thiazole rings, are utilized in numerous medicines worldwide. Chemical compounds like benzothiazoles and their heterocyclic derivatives have several biological impacts. Benzothiazole derived drugs wide range of medicinal qualities has inspired medicinal chemists to develop new therapeutic molecules. Anticancer, antibacterial, antidiabetic, anti-inflammatory, antiviral, antioxidant, antitubercular, antimalarial, antiasthmatic, anthelmintic, photosensitizing, diuretic, analgesic, and other properties have been reported in the benzothiazole ring system.

2-Amino benzothiazoles are highly reactive for organic synthesis, including the construction of pharmacologically active heterocycles, due to the facile functionalization of the $_{C2\text{-}NH2}$ group and the benzene ring inside the benzothiazole ring.

Many methods were developed to synthesize 2-amino benzothiazole and its

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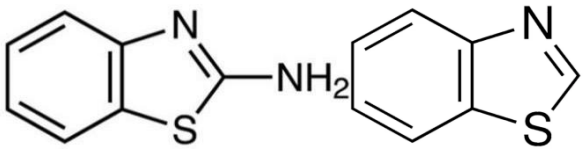
derivatives. 2-Aminobenzothiazole is a key reactant or intermediary in the synthesis of fused heterocycles. The NH2 and endocyclic N groups in 2-aminobenzothiazole are well-positioned to react with electrophilic reagents, forming a variety of fuse compounds.

In the 1950s, a number of 2-aminobenzothiazoles were intensively studied, as the 2- amino benzothiazole scaffold is one of privileged structure in medicinal chemistry and reported cytotoxic on cancer cells 2. It must be emphasized that combination of 2-aminobenzothiazoles with other heterocyclic is a well know approach to design new drug like molecules, which allows achieving new pharmacological profile, action, toxicity lowering.

In last few years it was reported that benzothiazole, its bioisosters and derivatives had antimicrobial activities against Gram-negative, Gram-positive bacteria's aeruginosa, (e.g., E. Enterobacter, coli, and Pseudomonas Staphylococcus epidermidis etc.) and the yeast (e.g., Candida albicans).



2-aminobenzothiazole

Fig 1: Structure of 2-aminobenzothiazole

Benzothizole

Fig 2: Structure of Benzothiazole

II. MATERIALS AND METHODS

SOFTWARES

- ACD Lab Chemsketch
- Molinspiration
- Admet SAR
- PASS
- Autodock

METHODS

IN SILICO DRUG DESIGN

The in silico modeling of all proposed compounds were carried out by using different computational software in order to predict the physico chemical parameters. The softwares used for in silico studies include ACD Lab Chemsketch, Molinspiration, admetSAR and PASS. Molecular docking studies carried out by Discovery studio.

ACD Lab Chemsketch 12.0

ACD Lab Chemsketch is a chemically intelligent drawing interface that allows drawing almost all chemical structure including organics, organometallics, polymers and Markush structures. Use it to produce professional looking structures and diagrams for reports and publications.

Features

- Draw and view structures in 2D, or render in 3D to view from any angle.
- Draw reactions and reaction scheme and calculate reactant quantities.
- Generate structures from InChI and SMILES strings.
- Generate IUPAC systematic names for molecules for molecules upto 50 atoms and 3 ring structures.
- Predict log P for individual structures.
- Search for structures in the built in dictionary of over 165000 systematic, trivial and trade names.

Determination of drug likeness and Lipinski rule of five using Molinspiration software

Determination of drug likeness is an important aspects of the drug design. It is defined as a complex balance of various molecular properties and structural features which determine whether a particular molecule is similar to the known drugs. These properties mainly hydrophobicity, electronic distribution, hydrogen bonding characteristics, molecule size, flexibility and presence of various pharmacophoric features influence the behaviour of molecule in a living organism, including bioavailability, transport properties, affinity to proteins, reactivity, toxicity, metabolic stability and many others. Drug likeness score is calculated by Molinspiration software. The Lipinski Rule of five provides a measure for determining the oral bioavailability of a compound.

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Determination of ADMET profile using admetSAR

In total, 22 highly predictive qualitative classification models were implemented in admetSAR software. These models includes human intestinal absorption, blood-brain barrier penetration, Caco-2 permeability, P-glycoprotein substrate and inhibitor, CYP450 substrate and inhibitor (CYP1A2, 2C9, 2D6, 2C19, and 3A4), hERG inhibitors, AMES mutagenicity, carcinogens, honey bee toxicity, and tetrahymena pyriformis toxicity. In addition, all classification models were given a probability output instead of simple binary output. In scientific community of ADMET prediction, quantitative predictions are more useful. To this a SMILES notation of the compounds taken as input. It determine the ADMET profile of the compound using different models

Prediction of activity spectra for novel molecules using PASS software

PASS software is designed as a tool for the evaluation of general biological potential in the molecule under study. The PASS software, which predicts more than 4000 kinds of biological activity, including pharmacological effects, mechanism of action, toxic and adverse effects, interaction with metabolic enzymes and transporters, mutagenicity etc. PASS uses input files in smiles format and results of predictions can be obtained as text format. A biological spectrum for a substance is a list of biological activity types for which the probability to be revealed (Pa) and not to be revealed (Pi) values are independent and their values ranges from zero to one. The more Pa value, the less is the probability of false positive in the set of compounds selected for study.

Docking methodology

Autodock Vina is an automated docking and virtual screening software for computational drug discovery that can be used to screen libraries of compounds against a potential drug target. The Autodock Vina includes docking wizard with an easy to use use interface which make it a valuable tool for computer aided drug design.The Autodock Vina software finding the best orientation of the molecues such that they have the minimum energy as scored by a predefined scoring function. It is useful in predicting the correct placement of drugs or ligands within the binding pocket of the target receptor.

III. RESULT AND DISCUSSION

The present work revealed the significance of rational designing of 2-aminobenzothiazole derivatives and its anti ischemic cerebral activities.

RESULTS

IN SILICO MOLECULAR STUDIES

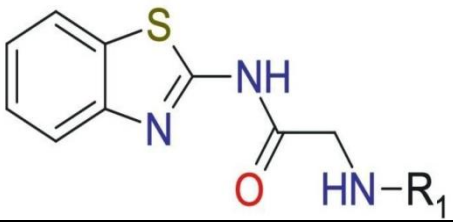
In silico molecular modeling studies were carried out for different ten anologues of 2-aminobenzothiazole derivatives using different software like ACD Lab Chemsketch, Molinspiration, admetSAR, PASS, and Autodock vina software.

Datas from ACD Lab Chemsketch

Structure of novel analogues and their smile notations are shown in Table 1

Various molecular descriptors like molecular volume, surface tension, polarizability, molar refractivity were computed and the result are shown in table 2

Table 1: Novel molecules and their smile notatio

SL.NO.	Compound	Smile Notation
		[*]NCC(=O)Nc1nc2ccccc2s1
C1		

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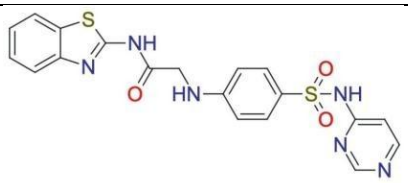
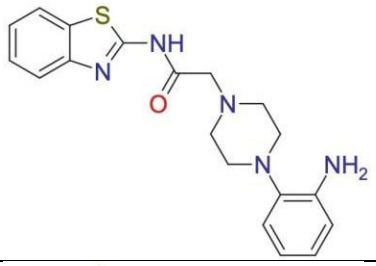
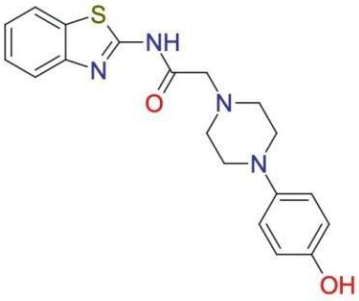
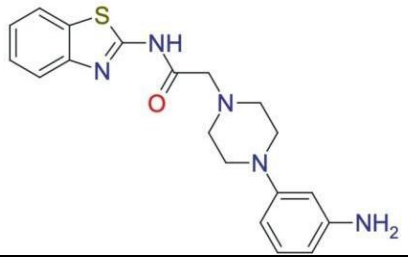
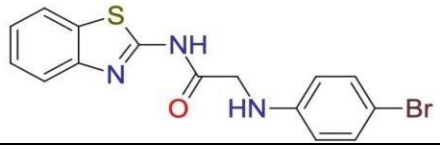
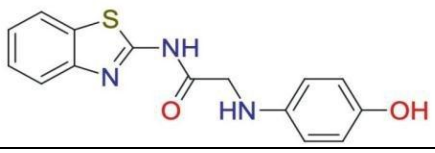
		O=S(=O)(Nc1ccncn1)c1ccc(cc1)NC C(=O)Nc1sc2ccccc2n1
C2		Nc1ccccc1N4CCN(CC(=O)Nc3nc2c cccc2s3)CC4
C3		O=C(CN2CCN(c1ccc(O)cc1)CC2)N c4nc3ccccc3s4
C4		Nc4cccc(N3CCN(CC(=O)Nc2nc1cc ccc1s2)CC3)c4
C5		O=C(CNc1ccc(Br)cc1)Nc3nc2ccccc 2s3

C6		O=C(CNc1ccc(O)cc1)Nc3nc2ccccc2 s3
C7		O=C(CNC1CCCC1)Nc3nc2ccccc2s 3

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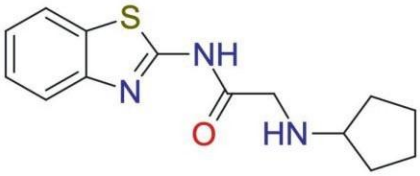
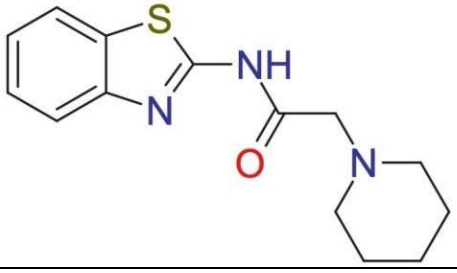
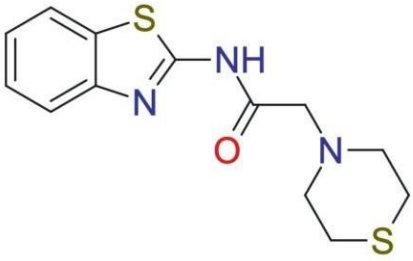
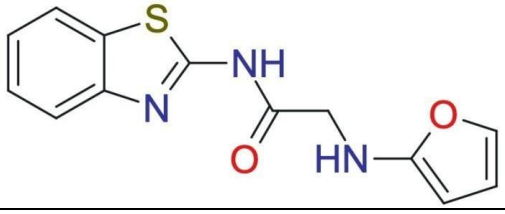
		
C8		O=C(CN1CCCCC1)Nc3nc2ccccc2s 3
C9		O=C(CN1CCSCC1)Nc3nc2ccccc2s 3
C10		O=C(CNc1ccco1)Nc3nc2ccccc2s3

Table 2: Molecular descriptors computed from ACD Lab Chemsketch

Sampe code	MR (cm^3)	MV (cm^3)	Parachor (cm^3)	Surface tension (dyne/cm)	Polarizability (cm^3)
C1	114.41 ±0.4	278.7 ±3.0	875.6 ±6.0	97.3 ±3.0	45.35 ±0.5 10^{-24}
C2	107.11 ±0.3	270.4 ±3.0	787.7 ±6.0	72.0 ±3.0	42.46 ± 0.5 10^{-24}
C3	104.76 ±0.3	104.76 ±0.3	775.0 ±6.0	71.4 ±3.0	41.53 ±0.5 10^{-24}
C4	107.11±0.3	270.4±3.0	787.7±6.0	72.0±3.0	42.46±0.5 10^{-24}

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C5	91.71 ±0.3	219.3 ± 3.0	636.8 ±4.0	71.0 ± 3.0	36.35 ±0.5 10^{-24}
C6	85.90 ±0.3	201.6 ± 3.0	601.3 ±4.0	79.1 ±3.0	34.05 ±0.5 10^{-24}
C7	78.01 ±0.4	215.9 ±5.0	599.5 ±6.0	59.3 ±5.0	30.92 ±0.5 10^{-24}
C8	79.48 ±0.3	212.8 ±3.0	599.6 ±6.0	62.9 ±3.0	31.50 ±0.5 10^{-24}
C9	83.03 ±0.3	212.3 ±3.0	612.0 ±6.0	68.9 ±3.0	32.91 ±0.5 10^{-24}
C10	76.32 ±0.3	185.9 ± 3.0	540.3 ± 4.0	71.2 ± 3.0	30.25 ±0.5 10^{-24}

Datas computed from Molinspiration software:

The drug likeness score and Lipinski rule of five are calculated and analyzed using Molinspiration software as discussed in.

Lipinski Rule of Five

The Lipinski Rule of Five is calculated and analyzed. The results are shown below.

The details of Lipinski Rule of five are shown in Table.

Table 3: Details of Lipinski Rule of Five

Compounds	Log P (<5)	Molecular weight (<500D)	No.of Hydrogen bond acceptors (<10)	No.of Hydrogen bond donors(<5)	nviolation
C1	2.49	440.51	9	3	0
C2	3.10	367.48	6	3	0
C3	3.18	368.46	6	2	0
C4	2.71	367.48	6	3	0
C5	4.33	362.25	4	2	0
C6	3.04	299.36	5	3	0
C7	3.23	275.38	4	2	0
C8	2.98	275.38	4	1	0
C9	2.46	293.42	4	1	0
C10	2.67	273.32	5	2	0

Datas computed from admetSARsoftware

The ADMET profile of novel molecules were determined using admetSAR software as discussed

Table 4: ADMET score of novel molecules obtained from admetSAR software

Sample code	**ADMET prediction**				**Toxicity prediction**	
	Human intestinal absorption	**Sub cellular localization**	**CYP450 1A2**	**Biodegradation**	**AMES Toxicity**	**Carcinogen**
C1	0.9381	0.4755	Inhibitor	NRB	Non AMES toxic	Non-carcinogen

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				(Not ready bio degradable)		
C2	0.9612	0.6095	Inhibitor	NRB (Not ready bio degradable)	Non AMES toxic	Non-carcinogen
C3	0.9722	0.6937	Inhibitor	NRB (Not ready bio degradable)	Non AMES Toxic	Non-Carcinogen
C4	0.9738	0.4814	Non-inhibitor	NRB (Not ready biodegradable	Non AMES toxic	Non-Carcinogen
C5	0.9541	0.4062	Non-inhibitor	NRB (Not ready bio degradable)	Non AMES Toxic	Non-Carcinogen
C6	0.9760	0.5841	Inhibitor	NRB (Not ready bio degradable)	Non AMESToxic	Non-Carcinogen
C7	0.9389	0.4903	Non-inhibitor	NRB (Not ready bio degradable)	Non AMES Toxic	Non-Carcinogen
C8	0.9197	0.4896	Inhibitor	NRB (Not ready bio degradable)	Non AMES Toxic	Non-Carcinogen
C9	0.9197	0.4896	Inhibitor	NRB (Not ready bio degradable)	Non AMES Toxic	Non-Carcinogen
C10	0.9676	0.3892	Inhibitor	NRB (Not ready bio degradable)	Non AMES toxic	Non-Carcinogen

Datas computed from PASS software

The different biological activities were predicted using PASS software as discussed .

Table 5: The bioactivity score of novel molecules obtained PASS software

Compound code	Biological activity	Pa	Pi
C1	Anti ischemic	0.602	0.102
C2	Anti ischemic	0.707	0.027
C3	Anti ischemic	0.473	0.124
C4	Anti ischemic	0.855	0.009
C5	Anti ischemic	0.677	0.033
C6	Anti ischemic	0.461	0.131

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C7	Anti ischemic	0.432	0.159
C8	Anti ischemic	0.506	0.103
C9	Anti ischemic	0.706	0.027
C10	Anti ischemic	0.521	0.022

Molecular Docking using Autodock vina

The docking studies of novel molecules for different biological activities were carried out as discussed .

Docking studies for anti ischemic activity:

Target: Calmodulin channel complex in the Ca2+ bound state PDB ID: 6CNN

Table 6: Docking score for Anti ischemic activity

Name of the ligand	Docking score	Interacting residues
C1	-11.5	Ile, Gly
C2	-11.3	Ile,lys
C3	-11.3	Lys
C4	-11.2	Lys,Gly
C5	-10	Ile,Lys
C6	-9.9	Gly
C7	-8.6	Ile
C8	-8.6	Lys,Gly
C9	-8.2	Gly
C10	-8	Lys
Riluzole	-7.9	TYR, LEU

Fig 3: Docking image of C1

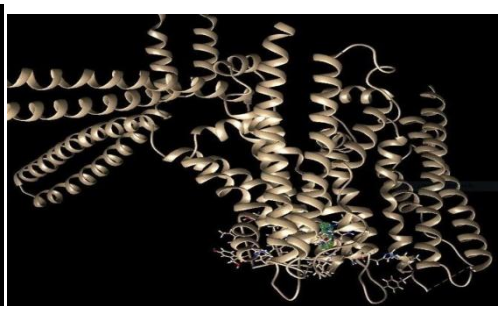

Fig 4: Docking image of C2

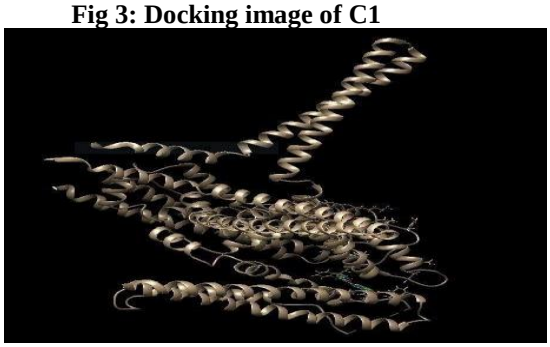

Fig 5: Docking image of C3

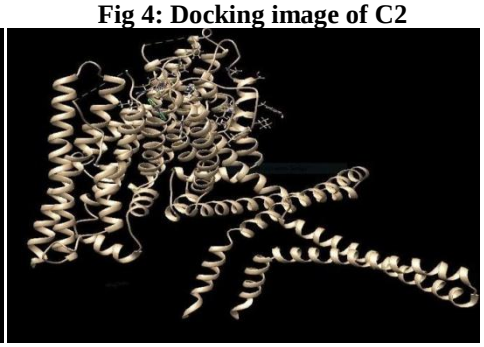

Fig 6: Docking image ofC4

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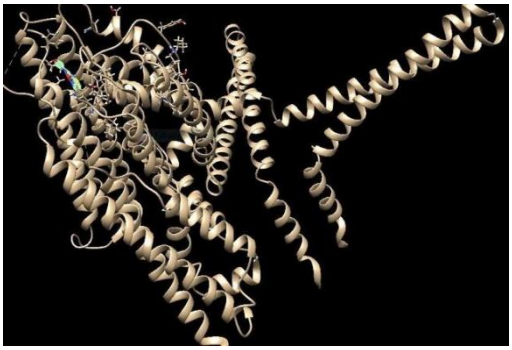

Fig 7: Docking image of C5

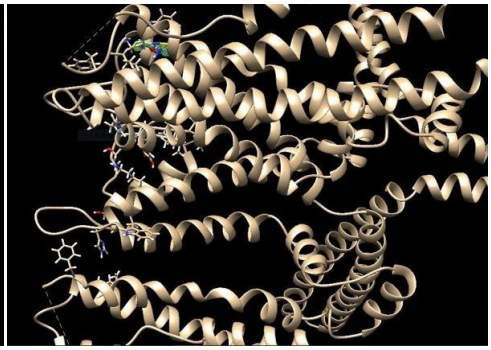

Fig 8: Docking image of C6

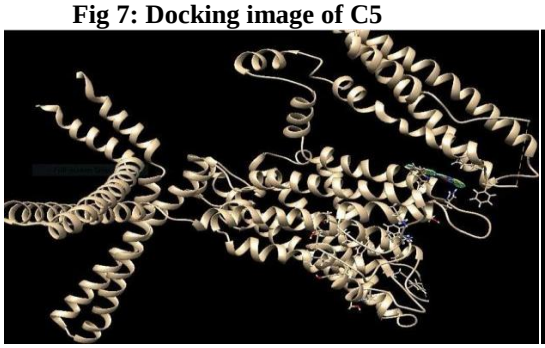

Fig 9: Docking image of C7

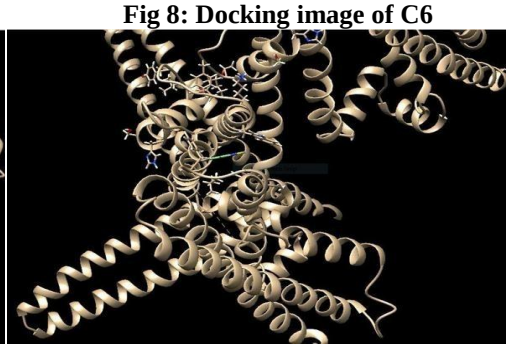

Fig 10: Docking image of C8

Fig 11: Docking image of C9

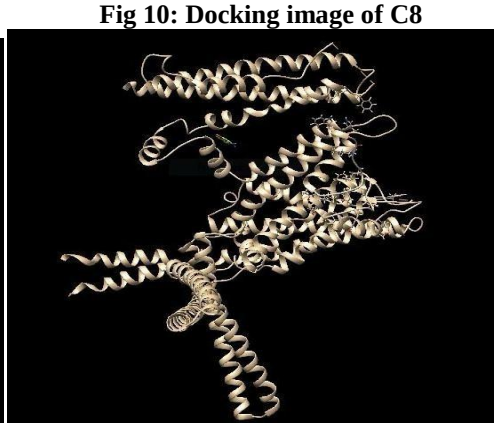

Fig 12: Docking image of C10

IV. CONCLUSION

2-amino benzothiazole derivatives have been studied extensively because of their ready accessibility and diverse chemical activity. The chemistry of 2-amino benzothiazole continues to draw the attention of synthetic organic chemists due to their various biological activities. Encouraged by the above reports and as a part of research, the lead compound N-(1,3-benzothiazol-2-yl)-2-chloroacetamide has been further developed in the present study and investigations are done on their various biological activity.This involves the preliminary insilico screening of various analogues to analyze for their molecular descriptors using computational softwares. Derivatives with desired physicochemical properties, obeying Lipinski Rule of Five and shows good docking score were chosen for wet lab synthesis. The in silico studies highlight the significance of the research, suggesting that these analogues can undergo more comprehensive pharmacological screening for the advancement of a drug candidate.

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