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Review Paper

Recent Advances in 2-Aminothiazole Derivatives: Molecular Docking and Anti-Inflammatory Potential

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ABSTRACT

Inflammation is a fundamental biological defence mechanism triggered dine Esposito infection, Injury, or exposure to harmful stimuli. Although acute inflammation is protective, its persistence Can progress into chronic inflammation, contributing to the' such as development of major Diseases such as cancer and cardiovascular disorders, arthritis, diabetes, and neurode generative Conditions. Due to the limit actions and adverse effects associated with existing anti-Inflammatory drugs, there is a continuous need for after and more effective therapeutic agents. Thiazole and its derivatives present antiport ant classify heterocyclic compounds exhibiting diverse pharmacological activities, particularly anti-inflammatory and antioxidant effects. In This study, novel2-aminothiazole derivatives were designed, synthesized, and evaluated using Molecular docking techniques. Protein–ligand interactions were assessed during the crystal Structure of DNA gyrase (PDBID: 4PS8). The binding affinity values ranged between−9.6to−7.0kcal/mol, with several derivatives showing strong interaction with a key Amino acid residue. Structure-activity relationship (SAR) is analysis highlighted the importance of substituent position, electronic effects, and as the ring modifications in enhancing biological Activity. Overall, the results confirm that thiazole derivatives at possess significant potential as anti-Inflammatory agents. The molecular docking outcomes and SAR findings support further Optimization and biological evaluation to develop promising drug candidates for inflammation-Related disorders

INTRODUCTION

Inflammation is an ancient medical term initially referring to classic signs and symptoms, including edema, erythema (redness), warmness, pain, and loss of function (stiffness and immobility). Currently, inflammation is recognized as a set of changing responses to tissue injury primarily caused by factors such as toxic chemicals, environmental agents, trauma, overuse, or infection. Some of these responses can facilitate wound healing and infection control or pathology,

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as in many chronic disease states. Inflammation is a second-line defence against infectious agents. The responses evoked by inflammation are a keystone of pathology. Diseases where inflammation plays a dominant pathological role have the suffix -itis. Both cell-mediated and humoral responses of the immune system are central to inflammation. This activity summarizes how inflammation is can cause to cardiovascular disease and cancer, two global causes of mortality and morbidity.

1.1 Pathogenesis

Chronic inflammation is the root cause of so many diseases. The origin of all pain is due to inflammation and the inflammatory response. Pathogens (bacteria, viruses or fungi), external injuries (scrapes or damage through foreign objects), effects of chemicals or radiation, etc. are the causative factors of inflammation the initial inflammation phase consists of three subphases: acute, subacute, and chronic (or proliferative). The special cells that take part in inflammation are called inflammatory cells and they are part of the body's immune system. The acute phase typically lasts 1-3 days and is characterized by the five classic clinical signs: heat, redness, swelling, pain, and loss of function. Inflammation results from activation of the immune system in response to a broad range of different stimuli. Shifts in the inflammatory response from short- to long-lived can cause a breakdown of immune tolerance and lead to major alterations in all tissues and organs, as well as normal cellular physiology, which can increase the risk for various non-communicable diseases in both young and older individuals. When living with chronic inflammation, animal body's inflammatory response can eventually start damaging healthy cells, tissues, and organs. Over time, this can lead to DNA damage, tissue death, and internal scarring. Indeed, chronic inflammatory diseases are the most significant cause of death in the world today, with more than 50 percent of all deaths being attributable to inflammation-related diseases (12-14) Pathogen

1.2 Types of Inflammation

A. Acute inflammation: This is a type of short-term inflammation that the body produces to address injuries,
illnesses, and infections. When there is an injury or contract a virus, the white blood cells begin to flood the area to provide protection and healing. Symptoms of acute inflammation include redness, warmth, and swelling Depending on the severity of the infliction, the inflammatory response will slowly fade away over hours or days.

B. Chronic inflammation: The body's response is the same as with acute inflammation, although there isn't always an injury that needs healing. Instead, the body wrongly signals that there is an issue of some kind, leading to inflammation that is persistent.
Chronic inflammation has a more heterogeneous histological appearance than acute inflammation. In general, chronic inflammation is characterized by the presence of macrophages, monocytes, and lymphocytes, with the proliferation of blood vessels and connective tissue Chronic inflammation is typically less painful than acute inflammation and lasts for a longer amount of time. Chronic inflammation

1.3 Treatment:

Better understanding of inflammatory response pathways and molecular mechanisms will undoubtedly contribute to improved prevention and treatment inflammatory diseases. in domesticated and pet animals' doctor will have to suspect inflammation by himself. Medications for an inflammatory disease may include:
Corticosteroids. This is a type of drug that releases an anti-inflammatory hormone that works to offset

tissue inflammation.it is usually prescribed in lung infections.

Immuno-suppressants. This is a type of drug that works to decrease immune system's response to perceived threats

1.4 Diagnosis: Serum protein electrophoresis (SPEP) Professionals consider SPEP to be one-way Trusted Source that may confirm chronic inflammation. It measures a certain protein in the blood to identify any issues. Too a much little of these

proteins can point to inflammation and markers for other conditions.

B.C-reactive protein (CRP)

CRP is naturally produced in the liver in response to act inflammation. A high level of CRP in your blood will occur due to several inflammatory conditions.

While this test is sensitive to inflammation occur, it does can help differentiate between acute and chronic inflammation to since CRP will be elevated during both. High amount combined with certain symptoms can help doctor make a diagnosis.

C. Erythrocyte sedimentation rate (ESR)

The ESR test Trusted Source as sometimes called a sedimentation rate test. This test indirectly measures inflammation by measuring the rate at which red blood cells dip in the tube of blood. The quicker they dip the more likely experiencing inflammation.

D.Other blood tests

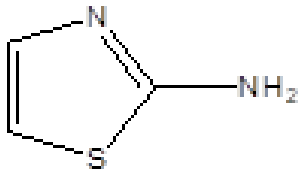
Doctor believes the inflammation is due to a viruses or bacteria, they may perform other a specific test. In this case, doctor can discuss what to expect with you.

E.Other diagnostic tests

You have certain symptoms, such as chronic diarrhoea or numbness on one side of your face, doctor may request an imaging test to check certain parts of the body or brain.

To diagnose inflammatory gastrointestinal conditions, doctor may perform a procedure to see inside the digestive tract. These tests can include: Colonoscopy, Sigmoidoscopy, Upper endoscopy

2.1 2-Aminothiazole and its derivatives



thiazol-2-amine

2.1. Basic structure and properties of 2-aminothiazole :2-Aminothiazole is a heterocyclic amine featuring a thiazole core. It can also be considered a cyclic is thiourea. It possesses an Odor similar to a pyridine and is soluble in water, alcohols and diethyl ether. 2-Aminothiazole itself is mainly of academic interest, with few anther exceptions**.**

2.2 Structure-Activity Relationship (SAR) :2-aminothiazole derivatives is highly dependent on the specific biological target (e.g., antitubercular, anticancer, antiproton). Generally, the central **thiazole ring and its 4-position substituent are crucial** for activity and often intolerant to modification, while the **N-2 amino position offers significant flexibility** for chemical modification to optimize potency and pharmacokinetic properties.

2.3 Central Thiazole Ring: The fundamental **2-aminothiazole core is essential** for activity and generally cannot be replaced by other heterocycles (e.g., thiophene, oxazole) without significant loss

of potency. The 2-amino group is crucial and often participates in key interactions, such as hydrogen bonding within the target protein's binding site.

2.4Substituent at the 4-Position (C-4): The nature of the substituent at C-4 is a critical determinant of activity. For many targets (e.g., antitubercular, antiproton, Src/Abl kinase inhibitors), a **2-pyridyl ring at the**

2.5 C-4 position is required Ring: for potent activity. Other aromatic or heteroaromatic rings can be tolerated, but often result in reduced potency compared to the 2-pyridyl group. Alkyl groups at this position are generally less effective or inactive. The co-planar arrangement of the C-4 aryl/heteroaryl ring and the thiazole ring often appears important for activity.

2.6 Substituent at the 2-Amino Position (N-2): This position exhibits high flexibility and is a primary site for structural modification to improve activity, selectivity, and pharmacokinetic profiles (e.g., metabolic stability, brain penetration).

2.7Acylation (forming an amide): Of the N-2 amine is a common and effective modification that can dramatically increase potency. The nature of the acyl group (aliphatic vs. aromatic, size, electronic properties) influences activity, with specific groups being optimal for different targets. For antitubercular activity, *m*-chlorobenzyl groups were highly effective.

For anticancer activity (e.g., as PI3K inhibitors), the linker length and specific substituents (e.g., certain proline amides or acyclic chains) are critical for binding affinity and selectivity.

Modifications at this position can also influence the molecule's interaction with metabolizing enzymes, allowing for the tuning of metabolic stability and reduction of potential toxicity.

2.8 Substituent at the 5-Position (C-5): The C-5 position can be modified, though its impact varies. In some cases (e.g., certain anticancer agents), lipophilic or specific functional groups (like isothiocyanatomethyl) at C-5 are important for activity.

In other instances, substitution at the C-5 position can lead to a loss of activity or altered activity profiles.

3. Molecular docking: - The Suitable orientation of ligand molecule ovens the receptor molecule to build a stable complex is called as molecular docking. This orientation is used for binding affinity Prediction and strength of ligand binding and proteins using a scoring function. Medicine Receptor interaction predicts affinity and activity of the molecule.

3.1 Types of molecular docking: -

A. Rigid Docking: In this docking the receptor and ligand molecule both are fixed.

B. **Flexible Docking**: In this docking the ligand and the receptor are movable. It is conformational flexible. Each rotation the energy is calculated. Each conformation surface cell occupancy is calculated. After that the most optimum binding pose is selected

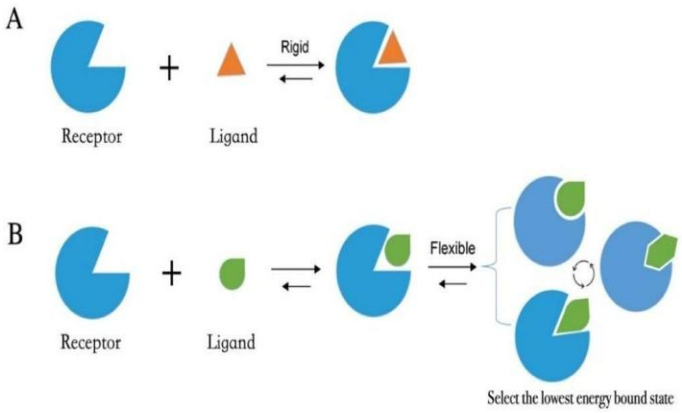


Fig.1.Rigid and Flexible Docking

3.2 Molecular docking mechanics steps: - In-Silico method studied the intermolecular interaction between 2 drug molecules. The protein receptor is Macromolecule. It acted as an inhibitor. The following steps involved in docking process are as

Step I - Preparation of protein and Ligand: From Research Collaboratory Structural Bioinformatics Protein data bank (PDB) downloading the 3D-structure of the Protein. After that downloaded structure should be pre-processed. From removal of the water molecules, the charges stabilization, missing residues filling, add hydrogen atom side chains generation.

Step II - Ligand Preparation: By using different databases similar as a ZINC, Pub Chem Ligands patch can be downloaded. It can be drawing structure in Chem sketch tool in the spook train. also structure an employed LIPINSKY'S RULE OF 5 for this ligand patch. It is used for the medicines like and like molecules. It increases the high chance of success rate and decreases the failure due to a drug likeness property for molecules.

Step III - Grid Generation: In this site, rotatable group, excluded volumes, constraints kept constant. The number operations performed (crossover, migration, mutation) is the key parameter in determining. Binding Cavity Prediction are to be done.

Step IV - The active site of protein molecule should be predicted. After that Preparation of protein, the water molecules and hetero atoms if present they are removed from cavity.

Step V- Docking: Ligand and protein interactions are analysed. Best docking score should be selected.

3.3 PyRx Software: - PyRx virtual screening tool software was used in the molecular docking studies along with the Graphical User Interface (GUI) to build a grid, create a dock score and evaluate conformers. PyRx is a virtual a screening tool for computational drug discovers and property that can be used to check compound libraries against desired target for drugs. This software helps to decrease time and resources which are required to test the whole database experimental by selecting most promising ones only. Docking based virtual screening (DBVS) method helps to find out the binding behaviour of small molecules to targets and also helps in selection of best interaction of molecule for testing.

3.4 pKCSM Analysis: pkCSM is a computational method that uses graph-based signatures to predict the pharmacokinetic and toxicity characteristics of small molecules. By training predictive models on

molecular features, such as atomic pharmacophores and molecular properties like lipophilicity and molecular weight, it covers important ADMET (absorption, distribution, metabolism, excretion, and toxicity) properties. In drug discovery, pkCSM is used to minimize late-stage failures and quickly screen compounds for favorable ADMET profiles.

3.5 Swiss ADME Analysis: Swiss ADME is a free online tool that estimates multiple ADME properties, drug-likeness and medicinal chemistry friendliness of a compound. It provides estimates on physiochemical properties, lipophilicity, water solubility, pharmacokinetics (including P-)

MATERIALS AND METHOD

Table No. 1. Software's used in Docking Study and their Company names.

Softwares	Company Name
ChemDraw	Cheminformatics
ChemSketch	ACD/Labs
BIOVIA Discovery Studio	Dassault Systems
PyRx 0.8 program	Source Forge

Method: -

Ligand preparation: The designed compounds' chemical structures and SMILES were produced using ACD/Chemdraw software. BIOVIA Discovery Studio was used to protonate the generated structures in order to correct the tautomeric and ionization states. The Avogadro program was used to reduce the energy in the chemical structures that were produced. The chem 3D ultra was applied to the developed compounds in order to minimize their energy. The newly created ligands' structure was illustrated (Table 1).

Protein preparation: The previously published crystal form structure of Extremely 'open' clamp structure of DNA gyrase(PDB ID:4PS8)with a resolution of 2.6 Å, was made available by the RCSB Protein Data Bank and all of the hetero atoms and water molecules were removed. Polar hydrogen atoms were added in order to protonate the amino acid residues in a pure protein crystal structure. BIOVIA Discovery Studio was used to carry out the protein structure improvement protocol.

Molecular Docking: - PyRx 0.8 program was used to carry out the docking protocol. Prepared protein and ligand structures were imported and selected using PyRx 0.8's Autodocking wizard unit. The ability of docked molecules to bind to the full protein surface was investigated using the blind docking protocol. The grid box's centre coordinates were X: 96.8294, Y: -10.041, Z: 308.5555, and its dimensions were chosen to be X: 103.8633, Y: 113.4580, and Z: 146.6926. The exhaustiveness was set to 8 by default. The pdb format of each compound's docked pose with the highest negative binding affinity was saved, and other binding interactions were investigated using BIOVIA Discovery Studio.

RESULT AND DISCUSSION

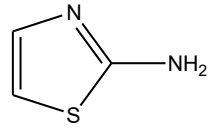
Result and Discussion: -

Molecular docking studies were conducted to evaluate the binding affinity of the synthesized 2-Aminothiazole thiazole derivatives against the DNA gyrase receptor (PDB ID: 4PS8). All eight designed compounds successfully interacted with the active site of the protein, exhibiting docking scores ranging from –9.6 to –7.0 kcal/mol. Among these, Compound 7 showed the highest binding affinity (–8.6 kcal/mol), followed by Compounds 1 (–8.4 kcal/mol), 5 (–8.2 kcal/mol), and 3 (–8.1

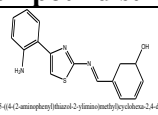
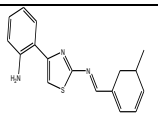
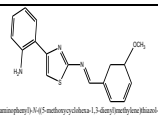
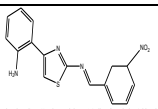
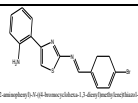
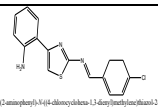
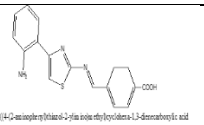
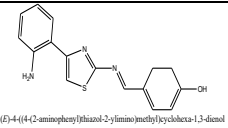
kcal/mol), indicating strong and stable binding. The docking interactions involved multiple key residues, including ARG550, ASP348, TYR297, TYR867, and VAL882, through hydrogen bonds, carbon–hydrogen bonds, and π-alkyl interactions. Some compounds also displayed significant interactions such as π–π T-shaped stacking (Compound 7) and halogen bonding (Compound 5). These results collectively demonstrate that the designed thiazole derivatives exhibit favourable binding orientations and strong molecular interactions within the active site of DNA gyrase, highlighting their potential as promising lead molecules for anti-inflammatory drug development

Table No-2: Newly designed 2- Aminothiazole

General structure

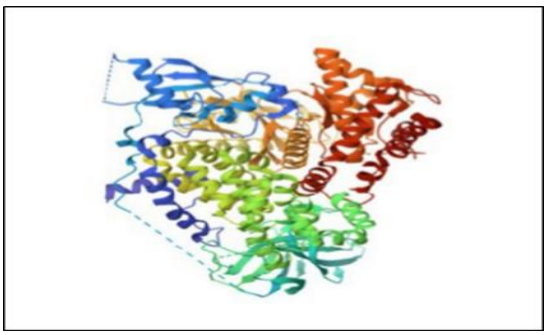


thiazol-2-amine

Compound code	Compound structure
1	
2	
3	
4	
5	
6	
7	
8	

TableNo.3. Binding affinity along with binding interactions of designed compounds against PDB 4PSD

Comp.Code	PDBID	Binding affinity	Interacting residues	Type of interaction	Distance
1	4PS8	**-8.4**	ASP841 TYR867	Carbon Hydrogen bond	3.29 5.15
			LYS833 ILE881	Pi alkyl	4.72 5.05
2	4PS8	-7.9	VAL882	Conventional Hydrogen bond	4.38
			LEU838 LYS833	Pi alkyl	4.68
			ARG634	Pisigma	3.84
3	4PS8	**-8.1**	ARG550 TYR297 ASP348	Conventional hydrogen bond	3.19
			TYR867 ASP841	Carbon-Hydrogen bond	3.29 5.15
4	4PS8	**-7.9**	TYR845	Carbon Hydrogen bond	3.55
			ILS963	Pi-alkyl	4.60
5	4PS8	**-8.2**	VAL882	Conventional Hydrogen bond	2.92
			LYS833	Carbon Hydrogen bond	4.72
			HIS1052	Pisigma	3.77
			MET812 TRP812	Pi-sulfur	3.65 5.32
6	4PS8	**-8.0**	VAL882	Conventional hydrogen bond	3.19
7	4PS8	**-8.6**	TYR867 ASP842	Carbon Hydrogen bond	3.28 4.71
			LYS833 ILE881	Pi alkyl	5.04 5.32
8	4PS8	**-8.3**	VAL882	Conventional Hydrogen bond	3.19
			LEU838	Pi alkyl	3.80



FigNo.2:PDB4PS8

Classification:
TRANSFERASE/TRANSFERASE INHIBITOR
Organism(s): Homo sapiens

Table -4 : Predicated ADMET Properties of the identified by using pkCSM Server

Comp. Code	Absorption	Distribution			Metabolism					Excretion	Toxicity	
	Intestinal Absorption (%Abs)	Vds Permeability (Log L/Kg)	BBB Permeability (LogBB)	CNS Permeability (LogPS)	Substrate (Yes/No)		Inhibitor(Yes/No)			Total Clearance Log ml/min/kg	AMES Toxicity (Yes/No)	Hepatotoxicity
					2D6	3A4	1A2	2c19	3A4			
1	90.89	1.067	-0.22	-3.415	Yes	No	No	No	No	0.656	No	No
2	71.50	-0.366	-1.434	-3.715	No	No	No	No	No	0.142	No	NO
3	73.29	1.166	-0.820	-3.093	No	No	No	No	No	0.88	No	No
4	95.89	0.047	0.25	-2.493	No	No	Yes	No	No	0.171	No	No
5	93.88	0.594	0.44	-2.234	No	No	Yes	No	No	0.27	No	No
6	94.45	0.129	0.356	-2.047	No	No	Yes	No	No	0.036	No	No
7	91.59	0.619	0.308	-3.302	No	No	No	No	No	1.00	No	No
8	90.89	1.067	0.845	-2.036	No	Yes	Yes	Yes	No	0.217	No	No

TABLE NO 5: Predicated physiochemical properties lipophilicity, solubility and drug likness of identified compounds

Comp. No	MW (g/mol)	nRot	mlog P	HB A	HB D	MR	TPSA	Lipinski's Violations	Ghose Violations	Veber 's Violations
1	362.22	4	0.65	2	1	94.79	52.65	0	0	0
2	297.65	3	-3.36	6	4	67.27	123.93	0	0	0
3	279.2	3	-4.42	7	5	64.05	144.16	0	0	0
4	340.17	4	-0.22	5	2	72.64	92.7	0	0	0
5	341.28	2	0.86	7	2	82.02	77.84	0	0	0
6	323.69	5	-2.36	6	2	74.51	109.77	0	0	0
7	413.81	6	-1.78	6	3	104.74	120.77	0	0	0
8	387.77	5	-1.88	6	4	96.57	123.93	0	0	0

CONCLUSION

Inflammation plays a significant role in the development and progression of various chronic diseases, including arthritis, cardiovascular disorders, diabetes, and cancer. Therefore, the discovery of new and effective anti-inflammatory agents remains an important area of research. Thiazole derivatives, particularly 2-aminothiazole compounds, have gained considerable attention due to their diverse pharmacological properties and promising anti-inflammatory activity.

This review highlights recent advances in the synthesis, structure-activity relationship, molecular docking studies, and pharmacological evaluation of 2-aminothiazole derivatives. The findings indicate that structural modifications at different positions of the thiazole ring significantly influence biological activity and binding affinity. Molecular docking studies further confirmed the strong interaction of these compounds with target proteins, supporting their potential as therapeutic agents.

Overall, 2-aminothiazole derivatives represent a promising class of compounds for the development of novel anti-inflammatory drugs. However, further studies including in vitro, in vivo, and clinical evaluations are necessary to confirm their safety and therapeutic efficacy. Future research should focus on optimization of these derivatives to develop potent and selective anti-inflammatory agents.

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