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Review Paper

Molecular Docking of Novel Triazoles Against Pathogens

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ABSTRACT

This review focuses around the use of triazoles as antifungal drugs. Triazole are from the class of azoles which is also one of the most effective antifungal drugs. Fungal infections and their resistance have become a serious issue nowadays. To overcome this issue, we need strong drugs and new techniques such as computational drug design techniques like molecular docking. Molecular docking helps in creating and predict binding interactions for new drug design. This review focuses on computational docking, ADMET evaluations and SAR studies. It also covers recent research and future possibilities in computational based drugs

INTRODUCTION

Over the years the frequency and extent of severe fungal infections have highly increased. Most of the fungal infections are caused by *Candida* and *Aspergillus* species(Pogrebnoi et al., 2022). The most affected patients are those with weak immune system. Despite the powerful existing antimicrobial agents, the resistance to the antimicrobial agent is increasing due to the appearance and broad extension of microbes like gram positive and gram-negative bacteria(Kamoutsis et al., 2021) To overcome this we need more powerful and effective antimicrobial agents. Azoles are selective inhibitors of CYP51 fungal enzyme which is commonly used to treat fungal infections mostly caused due to *Candida albicans* and *Aspergillus fumigatus.* Among azoles triazoles are preferably used for fungal infections probably due to their high therapeutic index. Triazoles act by inhibiting the growth of fungi through interacting with enzymes which are essential for ergosterol biosynthesis. (Akolkar et al., 2023)

Triazole is an important molecule that is widely spread across the nature and found in many important biomolecules. Triazole nuclei plays a vital role in anti-infective therapy, (Kumar et al., 2022) Triazole is an organic heterocycle. it is five-membered ring having two carbon atoms and three nitrogen atoms. The triazole derivatives show different activities like antifungal, antibacterial, anti-tubercular activity.(Toraskar, 2024)

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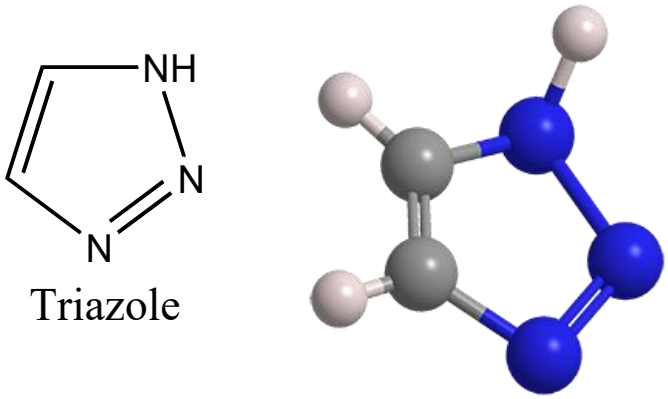

Fig.1: STRUCTURE OF TRIAZOLE

There is various method which are used to create new molecules. One of the widely used method is molecular docking which is a computational method used to predict how two or more molecules or compounds fits together(Raval & Ganatra, 2022). Basically, molecular docking show how a ligand binds to a receptor to form a complex. This helps to predict the binding orientation and strength and stability of complex. (Agarwal & Mehrotra, 2016)

TARGET SELECTION IN MOLECULAR DOCKING

Table no.1

Table 1 sources: (Keniya et al., 2018), (Wacnik et al., 2022), (Bosco-Borgeat et al., 2016), (Joshi & Osheroff, 2025)

PATHOGEN	TARGET PROTEIN	FUNCTION
Candida albicans	Lanosterol 14α- demethylase	Ergosterol biosynthesis (antifungal activity)
Staphylococcus aureus	Penicillin-binding protein	Cell wall synthesis (antibacterial activity)
Escherichia coli	DNA gyrase	DNA replication (antibacterial activity)
Aspergillus fumigatus	CYP15 A (lanosterol 14α-demethylase isoform)	Ergosterol biosynthesis (antifungal activity)
Cryptococcus neoformans	Lanosterol 14α-demethylase	Fungal membrane integrity

TOOLS FOR PREPERATION OF TARGET PROTEIN

Table no.2

Table 2 sources: (Osipov & Strelkov, 2025), (Forli et al., 2016), (Pettersen et al., 2021), (Mateev et al., n.d.), (Webb & Sali, 2016), (Abraham et al., 2015)

TOOLS	PURPOSE
Py MOL	Removing water/ligands
Auto dock tools	Hydrogen addition
Chimera	Removal of heteroatoms
Schrödinger Maestro	Protein preparation
MODELLER	Residue modelling
GROMACS	Molecular docking

LIST OF PROTEIN-LIGAND MOLECULAR MODELING TOOLS **Table no.3**

Table 3 source: (Sahoo et al., n.d.)

SOFTWARE	SCORING FUNCTION
Auto Dock	Predict binding poses and energy
Dock	Helps to match the ligand to the receptors.
Glide	Performs docking and pose prediction.
GOLD	Uses genetic algorithms for scoring of ligand poses.
FRED	Screen Score, PLP, Gaussian shape score

Purpose and objective

Purpose

This review revolves around recent research on triazole compounds a type of chemical that are being studied and used as antifungal and antimicrobial agents mostly against *candida albicans and staphylococcus aureus.* The main goal is to show how molecular help and being used to by researchers to design new medicines that are effective to fight against infections. This study matters due to the more infections becoming resistant to the drugs in use so there is a need for new drugs or compounds for treatment. triazoles are used because they work against a wide range of microbes and also have good absorption and stability. This review combines different research done on how triazoles compound fit into the target enzyme of microbes and their SAR to understand which chemical feature make the compound more powerful.

Objectives:

- Exploring how molecular docking techniques are currently being used to study new triazole compounds in the fight against microbial and fungal infections.
- This study focuses on evaluating how well existing triazole derivatives bind to key microbial enzymes such as CYP51 and DNA gyrase, and how effectively they inhibit their activity.
- It also aims to uncover and synthesize structure-activity relationships (SAR) that link specific chemical modifications in triazole compounds to their antimicrobial potency.

TARGETS

ERGESTEROL

According to (Can et al.,2017) They developed new antifungal agents by synthesizing a series of benzimidazole -triazole hybrid compounds against lanosterol 14*a* demethylase (CYP51) an important enzyme in ergosterol biosynthesis. So, they did work by synthesizing a total 23 novel benzimidazole – triazole derivatives (compounds 5a-5s) by various chemical reactions involving microwave assisted synthesis, hydrazide formation, triazole ring construction, final derivatization with substituted phenyl groups and these compounds were characterized structurally using FTIR, NMR, LC-MS, melting point analysis. Now they selected lanosterol 14*a*-demethylase (CYP51) protein (PDB ID:5EQB) which is cytochrome P450 enzyme essential for ergosterol biosynthesis in fungi. It is targeted because inhibiting CYP51 disrupts fungal growth. The biological evaluation was done by testing all compounds against four *candida* strains names as *candida albicans, candida glabrata, candida krusei, candida parapsilosis.* The results showed that compound 5i and 5s showed strong antifungal activity with MIC_{50} values between 0.78-1.56 µg/ml. These compounds were also found to be

nontoxic to NIH/3T3 cells, with IC_{50} values higher than their $MIC_{50,}$ indicating good selectivity. LC-MS-MS analysis confirmed that 5i and 5s rapidly reduced ergosterol levels in fungal cells and the molecular docking studies simulations showed favourable binding of the synthesized compound at the active site of CYP51 including coordination with heme iron and hydrophobic and hydrogen bonding interactions. The ADME results showed theoretical drug likeness. The study successfully found 5i and 5s as potential antifungal agents targeting CYP51, with strong activity, low toxicity, and good molecular interaction. (Can et al., 2017)

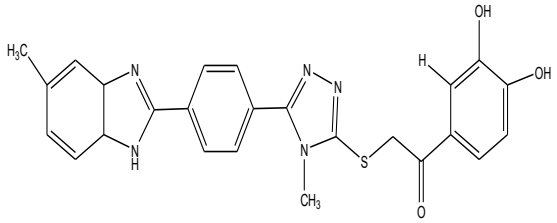

Fig.2.5i compound

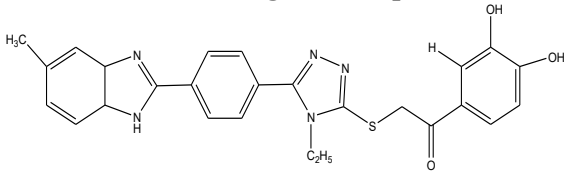

Fig.3. 5s compound

According to (Rather et al.,2022) Their study revolved around evaluating potential of newly synthesized triazole derivatives against *candida albicans* focusing on their ability to inhibit the enzyme lanosterol 14*a*-demethylase (LDM), a main enzyme in ergosterol biosynthesis – one of the important components of fungal cell membranes. They used the three-dimensional crystal structure of enzyme lanosterol 14*a*-demethylase (PDB ID: 5V5Z) from protein data bank (PDB). the structure was essential for molecular docking of triazoles derivatives and simulation studies to assess binding stability and dynamics. They selected six piperidine -based 1,2,3-triazolacetamide derivatives (pta1-pta6) were synthesized to overcome the drug resistance and antifungal activity. so, from this synthesis they selected three most potent compounds that are pta1, pta2, pta3 for further evaluation. the evaluation results of in silico finding showed all three compounds have strong binding affinity to the enzyme, among the three compound pta2 showed the highest docking score and also formed multiple stabilizing interactions and the in vitro finding showed that all three compounds inhibited *C. albicans* also had fluconazole -resistant strains. the compound pta1 was most effective, and also reduce the ergosterol production by over 90%. RT-PCR results showed downregulation of the ERG11 gene, with reduced ergosterol levels. The compounds also inhibited biofilm formation confirmed by XXT assays and confocal microscopy.(Rather et al., 2022)

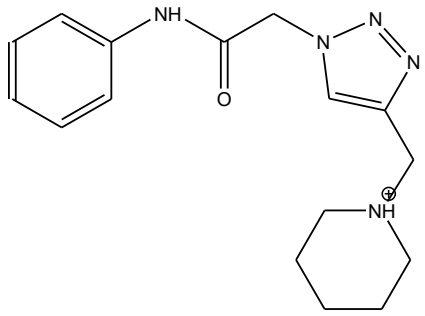

Fig.4. PTA1 compound

According to (Güzel E, et al.,2023) Their study focused on synthesis of new series of benzimidazole-1,2,4-triazole derivatives as antifungal agents against lanosterol 14*a*-demethylase (CYP51). So, they synthesized a total 12 compounds (6a-6l). these compounds were benzimidazole- triazole hybrids which were modified in three different regions that are electron- withdrawing group at substituted at C-5 position in benzimidazole. n-4 of triazole was replaced with a phenyl ring instead of alkyl groups. Phenyl ring was verified with substituents like -Cl, -OCH_3, -NO_2, -F etc. the synthesis of these compounds was done by six -step synthetic route starting from 4-formylbenzoate which were further characterised by ^{1}H NMR, ^{13}C NMR, AND HR-MS. The protein selected for this was lanosterol 14*a*-demethylase (CYP51) having PDB ID :5TZ1. The molecular docking was performed using these molecules which showed strong binding of 6b, 6i, and 6j to the active site of CYP51. In the molecular docking different interaction was seen like aromatic stacking with Tyr118, His377, and HEM601 and hydrogen bonding especially 6i with Tyr132. The cytotoxicity was tested on **L929 fibroblast cell. The compounds were also tested for antifungal activity against four *candida* species *C. albicans, C. glabrata, C. krusei, C. parapsilosis.* the compounds which showed strongest activity are 6b, 6i, 6j which had MIC of 0.97 µg/mL against *C. glabrata* and were seen more potent than the reference drugs voriconazole and fluconazole.(Güzel et al., 2023)

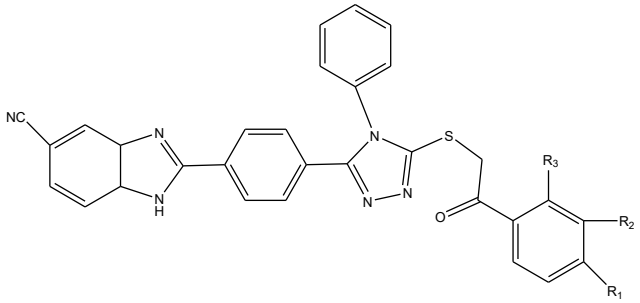

Fig.5. benzimidazole-1,2,4-triazole derivatives

Table no. 4

Compounds	R_1	R_2	R_3
6b	$-OCH_3$	-H	-H
6i	-Cl	-H	-H
6j	-Cl	-H	-Cl

DNA replication

According to **(**Zhang Y et al.,2017) Their study revolved around developing new antifungal agents by modifying the structure of miconazole an imidazole antifungal drug to create new triazole based analogues with improved potency, solubility, safety. They synthesized several types of triazole derivatives as follows: ether triazoles (5a-5h), alkyl triazoles (6a-6e), triazoliums (7a-7e), bis-triazoles (8a-8c), coumarin-triazole hybrids (9a-9c). they synthesized these compounds taking m-difluoro benzene and acylating and reacting it with triazole. they used sodium borohydride for reduction and substituted with various benzyl halides, alkyl chains, and coumarin fragments. Then they were characterized by IR, ^{1}H NMR, MS, HRMS. They used protein (CYP51) lanosterol 14*a*-demethylase (PDB ID:5V5Z). they did molecular docking and the results showed that the compound 5b a hydrogen bond between the triazole nitrogen and His377 in CYP51 with binding energy -7.97 kcal/mol showing strong interaction. Both 5b and 9c showed ability to intercalate into calf thymus DNA, indicating a secondary mechanism of antifungal action by blocking DNA replication. Compound 5b also shown to bind with human serum albumin (HAS) via hydrophobic and electrostatic interactions which suggest good transport and bioavailability potential ability. The compounds were tested against fungal strains like *candida utilis, aspergillus flavus, beer yeast, candida albicans, candida mycoderma* in which the compound 5b (3,4-dichlorobenzyl triazole showed strongest activity with MIC= 0.5-8 µg/mL and also compound 9c (coumarin-triazole hybrid) showed potent activity against *C. albicans,* and *C. mycoderma*.(Zhang et al., 2017)

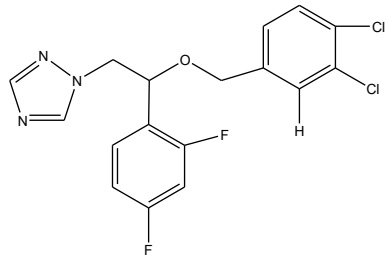

Fig.6. 5b compound

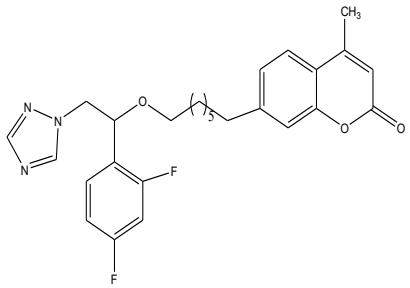

Fig.7. 9c compound

According to (Nehra et al.,2021) They synthesized new series of 1,2,3-triazole hybrid molecules by forming combination of 8-hydroxyquinoline (8-HQ) or 1- naphthol with 2-Hydroxyphenyl benzothiazole (2-HBT) or 4-HBT and all these hybrids were formed by copper-catalysed azide-alkyne cycloaddition reaction, a method known for high selectivity and yield. The protein used for DNA binding study was DNA dodecamer duplex (PDB ID: 1BNA) with target herring sperm DNA (hs-DNA) using UV-vis absorption titration, molecular docking and for antifungal activity they used lanosterol 14*a*-demethylase enzyme (PDB ID: 1EA1). The compounds 6a-6l were formed with different linker lengths (n = 2,3,4) and substitutions (X = N or C) and among these compound 6a seen as the most potent in multiple assays. In DNA binding it was seen that 6a showed highest affinity having binding constant (Kb) 3.90 × 10^5 $L.mol^{-1}$ with groove binding in CG-rich regions and it interacted with H-bonds, hydrophobic contacts, electrostatic forces. The antimicrobial activity of these compounds was tested and they see effective against *candida tropicalis and aspergillus terreus* and the compound 6a showed superior inhibition comparatively to fluconazole. the antibacterial activity also tested against *S. aureus, B. subtilis, E. coli, P. aeruginosa* having the compound 6a inhibition zones of 15.5-17.6 mm also 6a compound had the highest binding energy to DNA: -8.7 kcal/mol and lanosterol 14*a*-demethylase: -9.7kcal/mol and it also showed favourable molecular weight, Log P (lipophilicity), TPSA (polarity) in ADME. (Nehra et al., 2021)

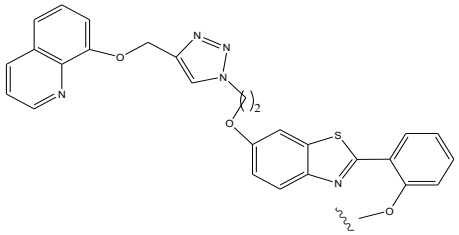

Fig.8. 6a compound

According to (Agarwal et al.,2025) Their study revolved around the design, and synthesis of new triazole-tethered tetrazole hybrids as potent antimicrobial agents. So, they synthesized a series of triazole-tethered derivatives (6a-6o) using click chemistry. These compounds were evaluated by NMR and HRMS techniques. They used the protein DNA gyrase B (PDB ID: 4ZVI) which is essential for DNA replication. they synthesized these compounds and performed molecular docking which showed that the compounds 6g and 6e had good docking score (-5.9 and -5.4 kcal / mol) compared to ciprofloxacin (-4.8 kcal / mol) showing stronger binding to DNA gyrase. The molecular docking simulation result showed that compound 6g had stable binding over 100 ns, making it an essential lead molecule. the antibacterial activity was tested against *Staphylococcus epidermidis* and other Gram-positive and Gram-negative strains which showed that the compounds 6g,6e,6h, and 6m had strong activity against the bacterial strains. (Agarwal et al., 2025)

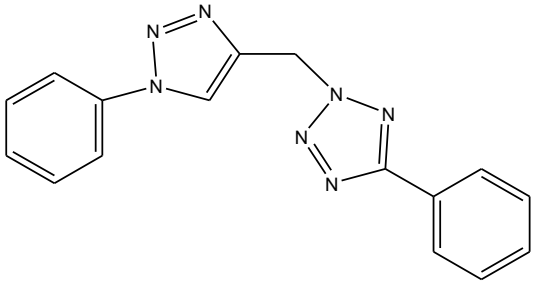

Fig.9. Triazole-tethered tetrazole hybrids

Table no. 5

-COMPOUNDS	-X
6e	2-Cl, 4-F
6g	2,4-Cl_2
6h	4-phenoxyphenyl
6m	4-trifluromethoxy

Methodology of literature selection

- It focuses on molecular docking studies of new triazole compounds against the microbial and fungal pathogens.
- It is aimed to show the effectiveness of triazole derivatives against resistant towards the drugs using molecular docking and SAR.
- It revolves around how triazole compounds act as an inhibitor of resistance in microbes and fungi by docking method.

Clinical trials:

Table no. 6

Title	Disease	Treatment
Study to evaluate the efficacy and safety of ibrexafungerp in patients with fungal diseases that are refractory to or intolerant of standard antifungal treatment.	Fungal infection	Ibrexafungerp – it is a novel antifungal which is designed with structure-based insights to specifically target glucan synthase.
Voriconazole vs. fluconazole in allogenic bone marrow transplant patients	Fungal infection in immunocompromised patients	Fluconazole vs. voriconazole – a triazole antifungals.
Azole – echinocandin combination therapy for invasion aspergillosis	Invasion aspergillus	Combination of triazole antifungals with echinocandin.
Olorofim aspergillus infection study	Invasion aspergillosis (lower respiratory tract disease)	Olorofim with AmBisome
Efficacy and safety of efinaconazole 10% solution in onychomycosis	Onychomycosis	Efinaconazole a new triazole derivative

Source: ClinicalTrials.gov

Table no. 7

Patents:

Patent number	Title	Disease	Treatment
WO2024258316A1	Novel potential antifungal agents based on thiazolidine -2,4-dione and triazole	Fungal strain resistant	Hybrid scaffold combining triazole
WO202115636A1	Triazole derivatives with antifungal activity	Fungal infection resistant to all azoles	New triazole derivatives
WO2014117318A1	Novel triazole antifungal compounds and pharmaceutical composition	Broad fungal infections	Novel triazole antifungal compounds with improved binding to CYP51

US11,789,456	Novel triazole derivatives as antifungal agents	*Candida aspergillus* infections	New triazole scaffold targeting CYP51
US11,755,892	Triazole – based antimicrobial compositions	Broad spectrum bacterial and fungal infections	Hybrid triazole molecules with antibacterial and antifungal activity
US11,645,210	Combination therapy of triazoles and echinocandins	Invasion *Aspergillosis*	Voriconazole and caspofungin synergistic formulation
US11,702,314	Topical triazole formulation for Onychomycosis	Nail fungal infections	Eficonazole improved formulation
US11,590,112	Novel triazole derivatives for resistant fungal strains	Azole resistant *candida auris*	Modified triazole scaffold with enhanced binding

Source: Google Patents, USPTO Patent Public Search

CONCLUSION

The research and study on molecular docking of triazole compounds show a strong various different approaches of computational modelling, chemical synthesis, and biological activity. Molecular docking helps to show or predict how these compounds bind to essential enzymes like CYP51 and DNA gyrase through the azole-heme coordination, hydrogen bonds, and hydrophobic interactions. All these predictions are tested and confirmed by lab based antimicrobial tests, confirming that docking is useful tool for designing effective antifungal and antimicrobial drugs.

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