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Antibacterial, Antifungal activity of Schiff base and mixed ligand Fe(III),Cr(III) complexes

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ABSTRACT

Antibacterial and antifungal activity were tested on the Schiff base, Schiff base complexes, and Schiff base mixed ligand complexes. It has been noted that mixed ligand Schiff base complexes have effective antibacterial and antifungal properties. This result supported by the docking analysis it reveals that the [Cr(SBL1)2 Cl2]Cl, [Fe(SBL_1)(PPh_3)$_2$$Cl_2$]Cl, and [Fe($SBL_4$) ($PPh_3$)$_2$$Cl_2$]Cl form bonded and non-bonded interactions with the N-myristoyltransferase receptors.

1. Introduction

Schiff bases are chemicals that are more attractive and significant in the pharmaceutical, dye, and plastic industries, as well as in liquid crystal technology and mechanistic investigations of drugs in pharmacology, biochemistry, and physiology [1]. Schiff bases ligands share structural similarities with conventional biological coordination and have implications for describing the process of uprising [2–10]. Schiff base complexes have been used as medications and offer a wide range of antibacterial action against bacteria, fungus, and some types of growths. [11, 12]. Some medicines have increased drive when obtained as metal chelates and cause tumour development [13, 14]. Quinazolinine is a significant heterocyclic chemical having nitrogen as a ring component [15]. Elements such as Co, Cu, Zn, Ni, Mn, Fe, V, and Cr are found in trace amounts in living organisms and perform important roles [16]. Metal complexes of Schiff bases, a ccording to widespread study, are more potent antibacterial agents than their native form [17]. Schiff base ligands function as O, N donor bidentates for Cu(II) and Ni(II) metal ions. When compared to typical medications, both ligands and complexes perform well [18]. Because complexation often boosts activity, knowing the characteristics of both ligands and metals can lead to the development of very active molecules [19-21]. Manganese, iron, cobalt, nickel, copper, and zinc are key metals that have increased biological activity when combined with certain metal protein complexes that participate in oxygen transport, electronic transfer processes, or ion storage [22]. This study focuses on the synthesis and characterisation of Schiff bases formed by the condensation of 2-aminobenzoyl hydrazide with benzaldehyde, 4-chlorobenzaldehyde, 4-methoxybenzaldehyde, and 4-nitrobenzaldehyde, as well as their complexes with Cr (III) and Fe (III). Mixed ligand complexes were synthesised with 1, 10 phenanthroline as a co-ligand. The IR and thermal examinations were used to explore the coordination behaviour of Schif f bases towards transition metal ions. The antibacterial activity of Schiff bases and their metal complexes against the microorganisms Escherichia coli, Bacillus subtilis, and Peudomonas aerginosa has been documented using the well plate diffusion practice. Schiff bases and their metal complexes were tested for antifungal activity against Candida albicans and Aspergillus nigar using agar well plate diffusion. Furthermore, in this work, we

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demonstrated molecular docking of the compounds to correlate them with their antibacterial and antifungal actions.

2. Results and Discussion

2.1 Antibacterial activity: Preliminary antibacterial activity of the ligands (SBL_1-SBL_2) and their respective iron (III) and chromium (III) complexes ($SBLC_1$-$SBLC_{16}$) was performed against Escherichia. Coli, Bacilus Subtilus, Pseudomonas aeruginosa using the agar well diffusion test. Table 1 displays the diameters of the zones of inhibition. The Agar-ditch technique was used to test antibacterial activity [34]. The inhibitory zone generated by these compounds against the specific test bacterial strain determined the synthesised compounds' antibacterial activity. Metal ions play an important part in a wide range of biological activities via co-enzymatic systems. The interface of these ions with physiologically active ligands, such as those found in medications, is of major interest. Some biologically active chemicals act by chelation, although slight is known about how metal coordination affects their activity in the majority of cases. Metal chelates are frequently discovered to have more antibacterial action than free ligands. This is because cell permeability has risen. The lipid membrane that surrounds the cell allows only lipid-soluble materials to get through, and liposolubility is recognised to be a significant factor determining antimicrobial action. However, in this investigation, reduced activity of several metal complexes is seen. The lesser activity of the metal complexes may be attributed to their lower lipophilicity, which reduced their penetration through the lipid barrier and, as a result, they could neither block nor hinder the development of the bacteria. This demonstrates that antibacterial action is determined by the compound's molecular structure, the solvent used, and the bacterial strain under attention. [35]. Such screening of numerous chemical compounds and identification of active agents is critical since early prediction of a lead molecule and drug-like qualities pays dividends later in drug development.Antibacterial activity of SBL1 against Bacilus Subtilus and Peudomonas aeruginosa is excellent. SBL_2 shows good antibacterial activity against Escherichia Coli and Bacilus Subtilus. $SBLC_3$ shows antibacterial activity Escherichia Coli and Peudomonas aeruginosa. $SBLC_4$ shows antibacterial activity against Escherichia Coli. $SBMLC_9$ and $SBMLC_{15}$ shows better antibacterial activity against Escherichia. Coli, Bacilus Subtilus and Pseudomonas aeruginosa.

3.2 Antifungal Activity

Fungi are plant pathogens that cause a range of ailments as well as secondary metabolites such as mycotoxins [36]. Food contamination by fungus and related mycotoxins endangers human and animal health and puts the economy in jeopardy. Physical and biological treatments include heat treatment, washing, and the application of bacteria and enzymes. To prevent fungal proliferation, fungi and mycotoxins are degraded [37]. To reduce fungal infection, inorganic compounds such as silica-based materials, i.e., binders, and their chemical modifications have been utilised [38, 39]. However, their presence in commodities typically has a negative impact on food quality. For these reasons, the ongoing need to find innovative chemicals to avoid microbial resistance to commercially accessible conventional therapies cannot be overstated. SBL_2 has antifungal properties against Candida albican. $SBLC_2$ and $SBMLC_{15}$ are antifungal against Aspergillus nigar. $SBLC_3$ inhibits the growth of Candida albican. Antifungal activity of $SBMLC_9$ and $SBMLC_{11}$ against Candida albican and Aspergillus nigar. Growth inhibition was discovered during a visual assessment of the wells.

3.3 Molecular docking:

3.3.1 Molecular docking of compound $SBMLC_9$ and $SBMLC_{15}$ with anti-bacterial receptors

Molecular docking was achieved to study the binding manner of compound $[Fe(SBL_1)(PPh_3)_2Cl_2]Cl$ and $[Fe(SBL_4)\ (PPh_3)_2Cl_2]Cl$ with anti-bacterial, GyrB receptor (source code: 4URO.pdb) using AutoDock4 software[40]. The compounds $[Fe(SBL_1)(PPh_3)_2Cl_2]Cl$ and $[Fe(SBL_4)\ (PPh_3)_2Cl_2]Cl$ show significant binding affinity and energy with the GyrB receptor protein. The minimum binding energy conformation of $[Fe(SBL_1)(PPh_3)_2Cl_2]Cl$ and $[Fe(SBL_4)\ (PPh_3)_2Cl_2]Cl$ with GyrB receptor was found at -7.66 kcal/mol and -7.99 kcal/mol, respectively as shown in Fig 5. Further, to investigate the bonding and non-bonding interactions of compound $[Fe(SBL_1)(PPh_3)_2Cl_2]Cl$ and $[Fe(SBL_4)\ (PPh_3)_2Cl_2]Cl$ with GyrB receptor, we analyzed the aforementioned least binding energy docked complex as shown in Fig 5.

Table 1. Antimicrobial Activity of Schiff base and their complex with Fe(III),Cr(III) against Escherichia coli, *Bacilus Subtilus, Peudomonas aeruginosa*

Sr. No	Schiff base and complex	Sample code	CONCENTRATION (mg/ml)	ZONE IN DIAMETE(mm) against *Escherichia. Coli*	ZONE IN DIAMETER (mm) against *Bacilus Subtilus*	ZONE IN DIAMETER (mm) against *Peudomonas aeruginosa*

	Control		-	00	00	00
	Standard (Streptomycin)		1	31	31	32
1	SBL_1	SBL_1 (PBADQ)	5mg	00	12	12
2	SBL_2	SBL_2 (CPBADQ)	5mg	16	16	00
3	SBL_3	SBL_3 (NPBAhttps://doi.org/10.1007/BF00207949 DQ)	5mg	00	00	00
4	SBL_4	SBL_4 (MBADQ)	5mg	00	00	00
5	$SBLC_1$	$[Fe(SBL_1)_2\ Cl_2]Cl$	5mg	00	00	00
6	$SBLC_2$	$[Cr(SBL_1)_2\ Cl_2]Cl$	5mg	00	00	00
7	$SBLC_3$	$[Fe(SBL_2)_2\ Cl_2]Cl$	5mg	11	00	10
8	$SBLC_4$	$[Cr(SBL_2)_2\ Cl_2]Cl$	5mg	12	00	10
9	$SBLC_5$	$[Fe(SBL_3)_2\ Cl_2]Cl$	5mg	00	00	00
10	$SBLC_6$	$[Cr(SBL_3)_2\ Cl_2]Cl$	5mg	00	00	00
11	$SBLC_7$	$[Fe(SBL_4)_2Cl_2]Cl$	5mg	00	00	00
12	$SBLC_8$	$[Cr(SBL_4)_2\ Cl_2]Cl$	5mg	00	00	00
13	$SBMLC_9$	$[Fe(SBL_1)(PPh_3)_2Cl_2]Cl$	5mg	10	15	12
14	$SBMLC_{10}$	$[Cr(SBL_1)(PPh_3)_2Cl_2]Cl$	5mg	00	00	00
15	$SBMLC_{11}$	$[Fe(SBL_2)\ (PPh_3)_2Cl_2]Cl$	5mg	00	10	10
16	$SBMLC_{12}$	$[Cr(SBL_2)(PPh_3)_2Cl_2]Cl$	5mg	00	15	00
17	$SBMLC_{13}$	$[Fe(SBL_3)(PPh_3)_2Cl_2]Cl$	5mg	00	00	00
18	$SBMLC_{14}$	$[Cr(SBL_3)(PPh_3)_2Cl_2]Cl$	5mg	00	00	00
19	$SBMLC_{15}$	$[Fe(SBL_4)\ (PPh_3)_2Cl_2]Cl$	5mg	10	11	11
20	$SBMLC_{16}$	$[Cr(SBL_4)(PPh_3)_2Cl_2]Cl$	5mg	00	00	00

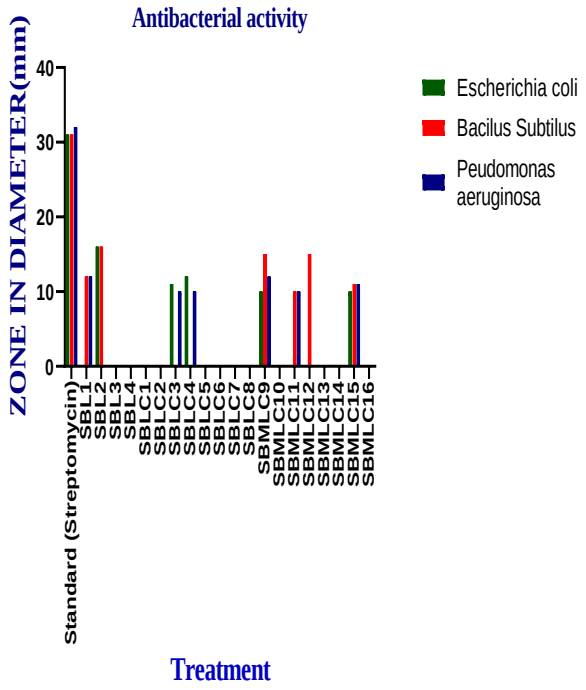

Fig 1. Antibacterial activity of SB and its complexes

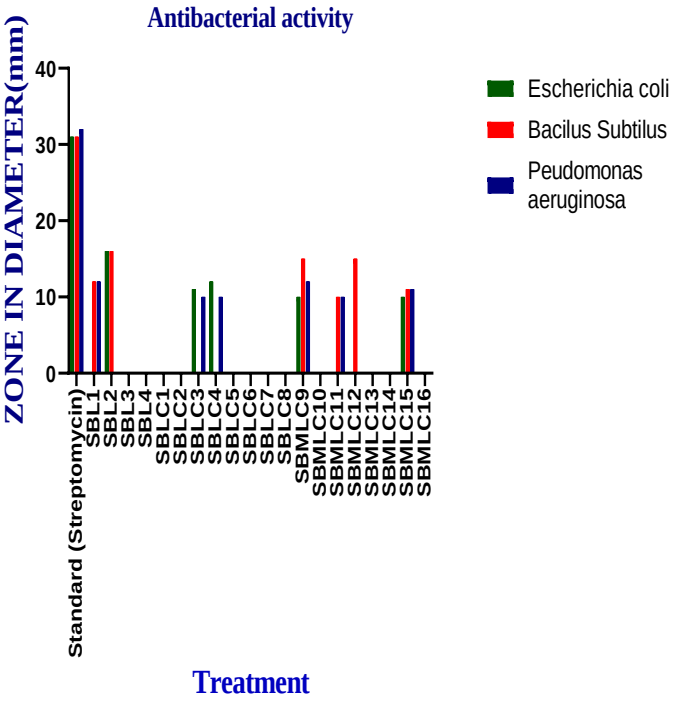

Fig 2. Antifungal activity of SB and its complexes

Table 2. Antifungal Activity of Synthetic compounds against *candida albicans and aspergillus nigar*

Sr.No	Schiff base and Complexes	Sample code	CONC. (mg/ml)	ZONE IN DIAMETER (mm) against *Candida albican*	ZONE IN DIAMETER (mm) against *Aspergillus nigar*
ZONE	Control		-	00	00
	Standard (Streptomycin)		1	16	17
1	SBL_1	SBL_1(PBADQ)	5mg	00	00
2	SBL_2	SBL_2 (CPBADQ)	5mg	17	00
3	SBL_3	SBL_3 (NPBADQ)	5mg	00	00
4	SBL_4	SBL_4 (MBADQ)	5mg	00	10
5	$SBLC_1$	$[Fe(SBL_1)_2\ Cl_2]Cl$	5mg	00	00
6	$SBLC_2$	$[Cr(SBL_1)_2\ Cl_2]Cl$	5mg	00	19
7	$SBLC_3$	$[Fe(SBL_2)_2\ Cl_2]Cl$	5mg	16	00
8	$SBLC_4$	$[Cr(SBL_2)_2\ Cl_2]Cl$	5mg	00	00
9	$SBLC_5$	$[Fe(SBL_3)_2\ Cl_2]Cl$	5mg	00	00
10	$SBLC_6$	$[Cr(SBL_3)_2\ Cl_2]Cl$	5mg	00	00
11	$SBLC_7$	$[Fe(SBL_4)_2Cl_2]Cl$	5mg	00	00
12	$SBLC_8$	$[Cr(SBL_4)_2\ Cl_2]Cl$	5mg	00	00
13	$SBMLC_9$	$[Fe(SBL_1)(PPh_3)_2Cl_2]Cl$	5mg	13	12
14	$SBMLC_{10}$	$[Cr(SBL_1)(PPh_3)_2Cl_2]Cl$	5mg	00	00
15	$SBMLC_{11}$	$[Fe(SBL_2)\ (PPh_3)_2Cl_2]Cl$	5mg	12	12
16	$SBMLC_{12}$	$[Cr(SBL_2)(PPh_3)_2Cl_2]Cl$	5mg	00	00
17	$SBMLC_{13}$	$[Fe(SBL_3)(PPh_3)_2Cl_2]Cl$	5mg	00	00
18	$SBMLC_{14}$	$[Cr(SBL_3)(PPh_3)_2Cl_2]Cl$	5mg	00	00
19	$SBMLC_{15}$	$[Fe(SBL_4)\ (PPh_3)_2Cl_2]Cl$	5mg	00	15
20	$SBMLC_{16}$	$[Cr(SBL_4)(PPh_3)_2Cl_2]Cl$	5mg	00	00

The analysis of docked 4URO-$SBMLC_9$ complex (Fig 5A) reveals that the $SBMLC_9$ is stabilized by the interaction of attractive charges of Lys78, π-cation of Arg214, π-anion of Glu68 types of interactions as shown in Fig 5B. Here, His143, Val174 and Lys170 forms π-π, π-π T shaped interactions with $SBMLC_9$ (Fig 5B and Table 2). Here, the GyrB receptor forms non-bonded interactions only with the $SBMLC_9$ compound. Further, the analysis of docked 4URO- $SBMLC_{15}$ complex (Fig 5C) shows that the $SBMLC_{15}$ is stabilized by hydrogen bonding interactions with Glu68 (2.04 A), as well as $SBMLC_{15}$ forms the Halogen type of interactions with Gln210, Glu68 form π-anion, Lys170, Val174 forms π-alkyl, and His143 forms π-π T shaped interactions with $SBMLC_{15}$ as shown in Fig 5D and Table 3.

3.3.2 Molecular docking of compound $SBMLC_2$, $SBMLC_9$, $SBMLC_{15}$ with anti-fungal receptors:

Molecular docking was employed, to explore the binding manner and interface of compounds $SBMLC_2$, $SBMLC_9$, $SBMLC_{15}$ with anti-fungal, N-myristoyltransferase (1IYL.pdb) receptors using AutoDock4.2 software [41]. The compounds $SBMLC_2$, $SBMLC_9$, $SBMLC_{15}$ show

noteworthy binding affinity with the N-myristoyltransferase receptor, and the least binding energy conformation was originate at -10.38 kcal/mol, -7.67 kcal/mol, and -7.87 kcal/mol as shown in Fig 6. To understand the interactions of compound $SBMLC_2$, $SBMLC_9$, $SBMLC_{15}$ with STAT3 receptors, we analyzed the aforementioned lowest binding energy docked complex (Fig 6).

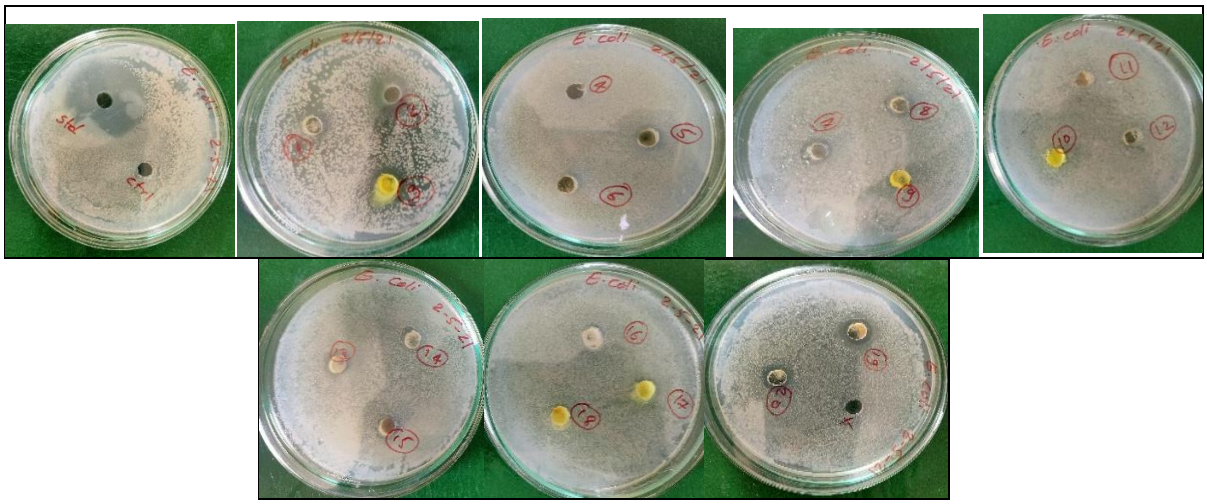

Fig 4. Antimicrobial Activity of 20 compounds against Escherichia coli

Table 3 Interaction of 4URO with $SBMLC_9$ and $SBMLC_{15}$ after molecular docking.

Protein	**Binding energy (kcal/mol)**	**Atoms involved in the interactions**	**Distance (Å)**	**Angle (°)**	**Fig. Ref**
Anti-bacterial (4URO.pdb)	-7.66	LYS78:NZ – LC9:Cl ARG214:NH2 - LC9 GLU68:OE2 - LC9 THR80:CG2 - LC9 HIS143 - LC9 HIS143 - LC9 LC9 - VAL174 LC9 - LYS170	4.61325 3.281 3.16281 3.77897 4.60698 4.31806 4.43528 5.23191	Attractive Charge Pi-Cation Pi-Anion Pi-Sigma Pi-Pi Stacked Pi-Pi T-shaped Pi-Pi T-shaped	12B
	-7.99	LC15:H - D:GLU68:OE1 GLN210:OE1 - :LC15:Cl GLU68:OE2 - LC15 HIS143 - LC15 LC15 - D:LYS170 LC15 - D:VAL174 LC15 - D:VAL174	2.04096 3.21733 3.89742 4.10215 5.22692 5.31211 4.88905	H bond Halogen (Cl, Br, I) Pi-Anion Pi-Pi T-shaped Pi-Alkyl Pi-Alkyl Pi-Alkyl	12D

The analysis of docked N-myristoyltransferase-$SBMLC_2$ complex (Fig 6A) reveals that the $SBMLC_2$ is stabilized by the residues Ile215, Val108, Cys178, Ile179, Arg184 through a π-alkyl type of interactions as shown in Fig 6B. While, Val108, Leu177, and Ala189 form the π-sigma type of interaction (Fig 6B and Table 3). In addition, Arg184 and Asn185 form the π-cation and π-donor hydrogen bonds. These non-bonded interactions could help to stabilize the $SBMLC_2$ with the receptor protein. Next, the analysis of N-myristoyltransferase-$SBMLC_9$ complex (Fig 6C and Table 3) reveals that $SBMLC_9$ forms the Ile179, Arg184, Val108, Ile215, Ala189 form the π-alkyl type of interactions while Ils179 and ala189 also form the π-sigma type of interactions with the $SBMLC_9$ (Fig 6D and Table 3). In addition, Ans185 and ala189, and Arg1984 forms the π-donor and non-conventional carbon-hydrogen bond with $SBMLC_9$ ligand as shown in Fig 6D and Table 3. Lastly, the analysis of N-myristoyltransferase- $SBMLC_{15}$ complex (Fig 6E and Table 3) reveals that the $SBMLC_{15}$ is stabilized by the residue Ile179, Lys181, Ala189, Ile215, Arg184, Val108 through the π-alkyl type of interactions (Fig 6F and Table 3), Gly213, Ile215, Leu177 forms the alkyl type of interactions with $SBMLC_{15}$ and Arg184 forms attractive charges interactions, Lys181, Arg184 forms carbon-hydrogen bonding interactions, Glu109 and Asn185 forms the π-donor type of interactions with the $SBMLC_{15}$ as shown in Fig 6F and Table 3.

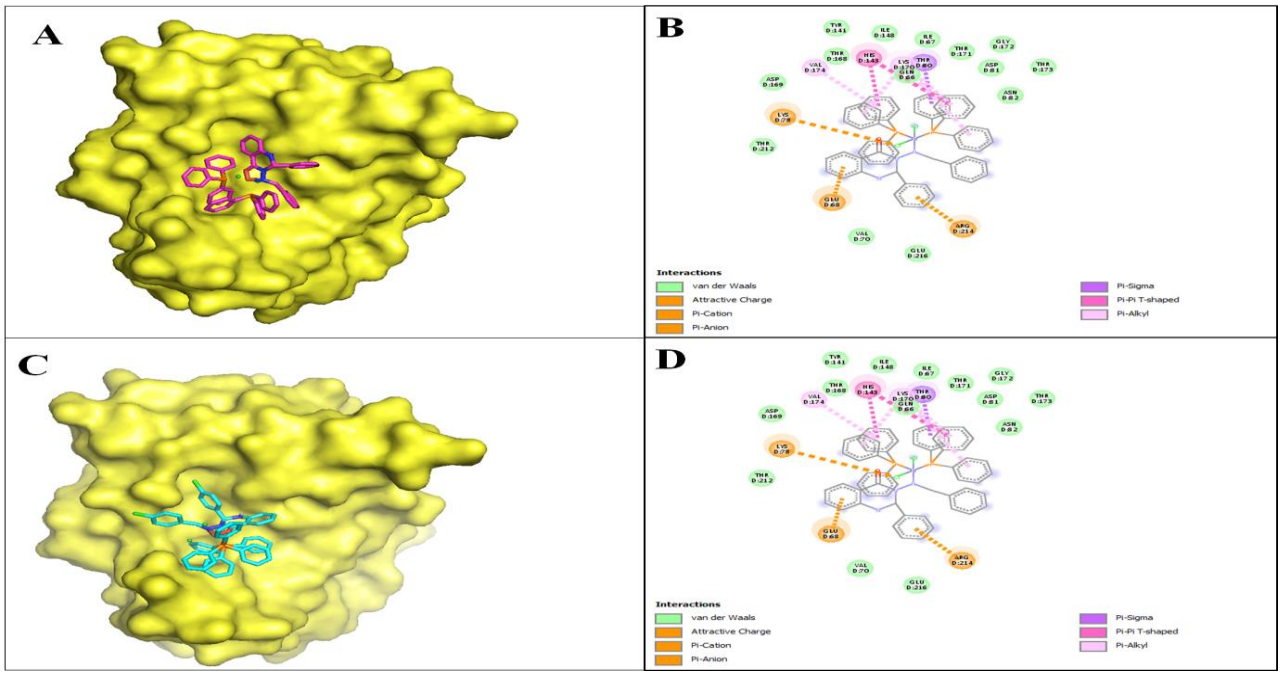

Fig 5. Binding mode of $SBMLC_9$ and $SBMLC_{15}$ with the anti-bacterial GyrB receptor (4URO.pdb). Here a GyrB protein is shown in the surface yellow color model while the $SBMLC_9$ and $SBMLC_{15}$ are shown in the stick model with magenta and cyan color. (A) Shows binding mode of $SBMLC_9$ with GyrB and (B) 2D interaction network of $SBMLC_9$ with GyrB protein. (C) Shows binding mode of SBMLC15 with GyrB and (D) 2D interaction network of $SBMLC_{15}$ with GyrB protein.

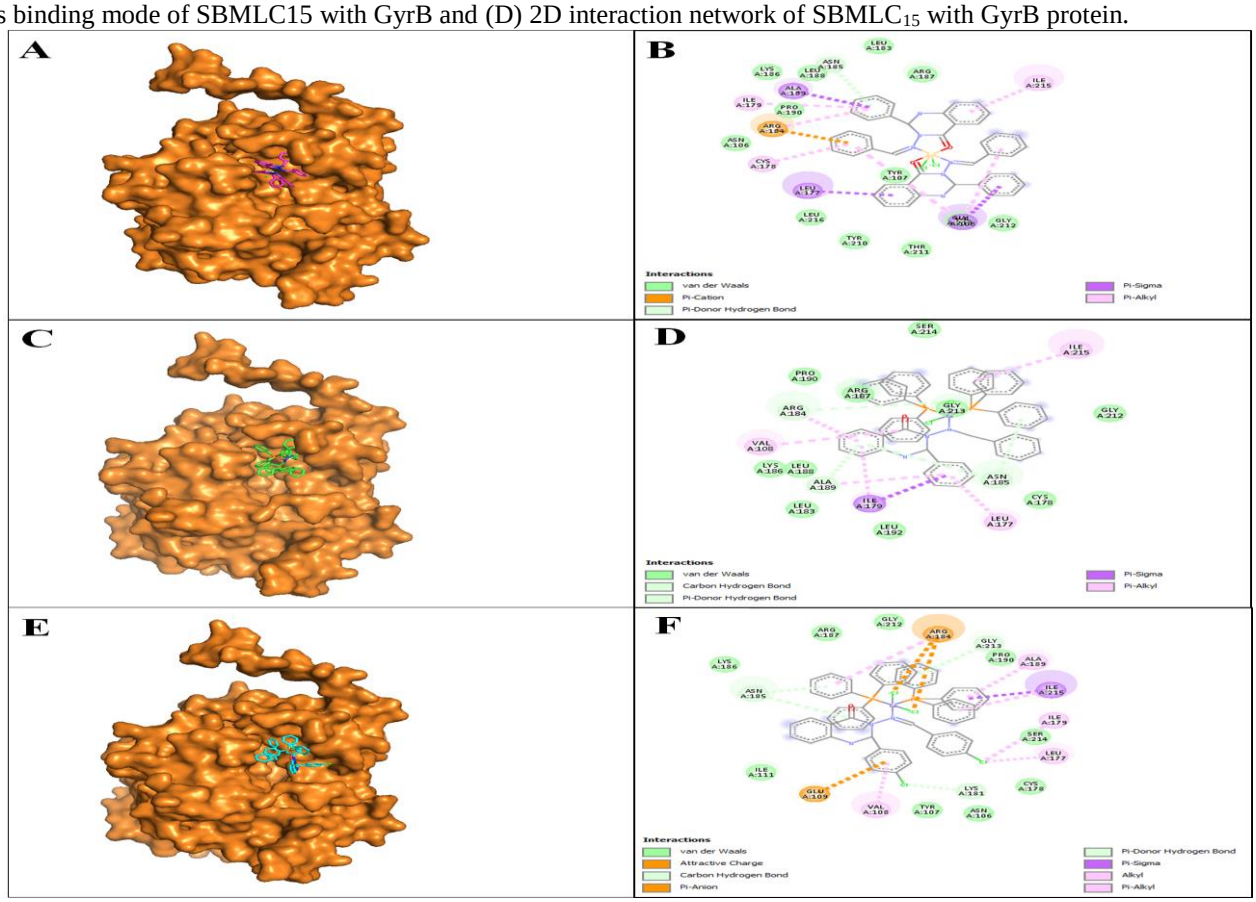

Fig 6. Binding mode of $SBMLC_{12,}$ $SBMLC_{15}$ with the anti-fungal N-myristoyltransferase receptor. Here a N-myristoyltransferase protein is shown on the surface with orange color while the $SBMLC_{2,}$ $SBMLC_{9,}$ $SBMLC_{15}$ are shown in a stick model with magenta, green and cyan color, respectively. (A) Shows binding mode of $SBMLC_2$ with N-myristoyltransferase, (B) 2D interaction network of $SBMLC_{12}$with N-myristoyltransferase protein. (C) Shows binding mode of $SBMLC_9$ with N-myristoyltransferase and (D) 2D interaction network of $SBMLC_9$ with N-myristoyltransferase protein. (E) Shows binding mode of $SBMLC_{15}$ with N-myristoyltransferase and (F) 2D interaction network of $SBMLC_{15}$ with N-myristoyltransferase protein

Table 4. hydrogen bonding interactions of N-myristoyltransferase with $SBMLC_2$, $SBMLC_9$, $SBMLC_{15}$ after molecular docking.

Protein	Binding energy (kcal/mol)	Atoms involved in the interactions	Distance (Å)	Angle (°)	Fig. Ref
Anti-fungal	-10.38	ARG184:NH1 - :UNK1 ASN185:N - :UNK1 VAL108:CG2 - :UNK1 LEU177:CD2 - :UNK1 ALA189:CB - :UNK1 UNK1 - A:ILE215 UNK1 - A:VAL108 UNK1 - A:VAL108 UNK1 - A:CYS178 UNK1 - A:ILE179 UNK1 - A:ARG184	3.68279 3.88795 3.70678 3.73599 3.78395 5.25671 4.80982 5.45664 5.39283 4.7502 4.46075	Pi-Cation Pi-Donor H Bond Pi-Sigma Pi-Sigma Pi-Sigma Pi-Alkyl Pi-Alkyl Pi-Alkyl Pi-Alkyl Pi-Alkyl Pi-Alkyl	13B
	-7.67	ARG184:CD - :UNK1:Cl ASN185:N - :UNK1 ASN185:ND2 - :UNK1 ALA189:N - :UNK1 ILE179:CD1 - :UNK1 ALA189:CB - :UNK1 UNK1 - A:ILE179 UNK1 - A:ARG184 UNK1 - A:VAL108 UNK1 - A:ILE215 UNK1 - A:LEU177 UNK1 - A:ALA189	3.74532 3.50592 3.34658 3.97865 3.9696 3.85555 5.13836 4.90639 5.31388 5.04513 4.73947 5.00696	Carbon H Bond Pi-Donor H Bond Pi-Donor H Bond Pi-Donor H Bond Pi-Sigma Pi-Sigma Pi-Alkyl Pi-Alkyl Pi-Alkyl Pi-Alkyl Pi-Alkyl Pi-Alkyl	13D
	-7.87	ARG184:NH1 - :UNK1:Cl ARG184:NH1 - :UNK1:Cl LYS181:CE - :UNK1:Cl ARG184:CD - :UNK1:Cl GLU109:OE2 - :UNK1 ASN185:ND2 - :UNK1 ASN185:ND2 - :UNK1 GLY213:N - :UNK1 ILE215:CD1 - :UNK1 :UNK1:Cl - A:LEU177 :UNK1:Cl - A:ILE179 :UNK1:Cl - A:LYS181 :UNK1 - A:ALA189 :UNK1 - A:ILE215 :UNK1 - A:ARG184 :UNK1 - A:VAL108	5.38773 4.95073 3.55318 3.19469 4.58804 3.85748 3.73219 3.83193 3.6132 3.49391 3.87 4.40866 4.48505 4.85499 5.37501 4.36402	Attractive Charge Attractive Charge Carbon H Bond Carbon H Bond Pi-Donor H Bond Pi-Donor H Bond Pi-Sigma Alkyl Alkyl Alkyl Pi-Alkyl Pi-Alkyl Pi-Alkyl Pi-Alkyl Pi-Alkyl Pi-Alkyl	13F

Conclusions Promising results of Antibacterial interest shown by mixed ligand complexes. All the compounds additionally studied for antifungal interest, It is found that Schiff bases SBL_2, mixed ligand Schiff base complexes showed good antifungal hobby. These consequences had been supported with the aid of docking study. The docking evaluation well-known shows that the $[Fe(SBL_1)(PPh_3)_2Cl_2]Cl$ and $[Fe(SBL_4)\ (PPh_3)_2Cl_2]Cl$ show a sizeable binding affinity with N-myristoyl transferase receptors, respectively. Here, those complexes suggests bonded and non-bonded interactions with the N-myristoyl transferase receptors. We can right here finish that blended ligand complexes suggests superb Antibacterial activity and Antifungal activity.

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