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A Novel Naphthalene-Based Schiff Base as a Colorimetric Probe for Fe(III) Ion Detection

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ABSTRACT

A novel naphthalene based Schiff base ligand (SBL) was synthesized by the condensation of naphthalene-1,8-diamine with 4-dimethylamino benzaldehyde as a colorimetric probe for the detection of Fe(III) ions selectively in ethanol solution. UV-visible spectroscopic technique was employed to study the sensing ability of probe SBL for Fe(III) ions and monitored in ethanol solution (pH 4). The Jobs plot confirmed 1:1 SBL to Fe(III) molar complex formation. DFT computation was also supported the binding framework between SBL and Fe(III). The binding constant for this complex is with detection limit of 6.925×10^{-4} M. Cyclic voltammetry study shows that there is no change in electrochemical structure of SBL after complex formation of SBL with Fe(III). The core finding of this research is that both the SBL and the SBL:Fe complex exhibited significant antibacterial activity, specifically effective against gram-negative bacterial strains. These results highlight the potential of this synthesized Schiff base framework as a novel, dual purpose compound with applications not only in metal ion sensing but also as a promising candidate for antimicrobial agent in biological system.

1. Introduction

Schiff base ligands represent a vital category of organic compounds widely recognized for their versatile biological and pharmacological properties. These molecules are synthesized through a straightforward condensation reaction between primary amines and carbonyl compounds, resulting in the characteristic C=N (imine) group. This specific functional group, along with the presence of electronegative donor atoms like nitrogen and oxygen, provides these ligands with significant coordination potential and biological efficacy [1-3]. A major area of interest for Schiff bases lies in their inherent antimicrobial activity. Research has consistently demonstrated that these compounds can exhibit potent inhibitory effects against various pathogens, including bacteria and fungi, making them essential candidates for new drug development. Furthermore, their pharmacological profile often includes significant cytotoxicity, which is increasingly explored in anti-cancer research. Naphthalene-based derivatives, in particular, are highly valued for these medicinal applications [1-5]. Beyond their direct biological effects, these ligands play a crucial role in monitoring essential biological metal ions, such as iron. Iron is the most abundant heavy metal in the human body and is fundamental to life, being a central component of haemoglobin for oxygen transport and a key factor in enzymatic catalysis. However, maintaining iron balance is critical; while deficiency leads to anaemia, excessive accumulation is linked to severe neurodegenerative disorders, including Alzheimer's and Parkinson's diseases [6-10]. Traditional methods for monitoring these ions often rely on expensive and complex equipment, such as atomic absorption spectroscopy or inductively coupled plasma mass spectrometry. In contrast, colorimetric Schiff base probes offer a more accessible and cost-effective alternative for biological monitoring [11-17]. In this study, we report the synthesis and characterization of a novel naphthalene-based Schiff base, bis(4-(dimethylamino)benzylidene)naphthalene-1,8-diamine (SBL). In addition to its potential as a bioactive agent, SBL serves as a highly sensitive and selective colorimetric sensor for Fe(III) ions. This dual-purpose ligand enables the detection of critical metal ions through a simple visual colour change, facilitating advanced monitoring in both environmental and biological systems.

2. Experimental Methods

2.1 Chemicals and Characterization

4-methylamino benzaldehyde, 1,8-diaminonaphthalene and ethanol were obtained from Sigma Aldrich and are used as it is without further purification. Nitrate salts of Fe³⁺, Co²⁺, Ni²⁺, Zn²⁺, Al³⁺, Mg²⁺, Ca²⁺, Ba²⁺, Pb²⁺, Cd²⁺ and Hg²⁺ and sulphate salts of Fe²⁺ and Cu²⁺ were purchased from CDH and used as procured without further purification. ¹H NMR spectrum (TMS as internal standard) was recorded from Bruker Avance III 400 MHz instrument using DMSO-d₆ as solvent with chemical shift in ppm. FT-IR spectrum was obtained from Parkin Elmer Spectrophotometer (Bruker Avance II 400 MHz) over a range of 4000 to 400 cm⁻¹ with KBr pellets. The UV-Vis absorption spectrum was recorded on Shimadzu UV 2450 spectrophotometer at room temperature (200-800 nm region). Whenever necessary all the experiments were carried out in distilled water. The electrochemical behaviour of SBL with various metal ions is studied by cyclic voltammetry (K-Lyte12 series electrochemical analyzer).

2.2 Synthesis of the Schiff Base Ligand (SBL)

The ligand, [4-(dimethylamino)benzylidene] naphthalene-1,8-diamine (SBL), was prepared via a previously unreported synthetic pathway. A solution of 4-dimethylaminobenzaldehyde was added to 1,8-diaminonaphthalene dissolved in 10 mL of ethanol. This mixture was maintained under reflux for duration of 5 hours. Upon cooling the solution to ambient temperature, a brown precipitate formed. The resulting solid was isolated through filtration and subjected to vacuum drying. After allowing the product to sit undisturbed for 24 hours, high-quality crystals were obtained. The final structure of the SBL was verified through comprehensive spectroscopic analysis. Yield: 90%.

¹H NMR (400MHz, DMSO-d₆): δ 7.48-7.20 (add, J = 1.8/8.0 Hz, 6H), 7.5 (s, 2H), 7.18-6.91 (dd, J = 1.8/8.0 Hz, 4H), 6.71-6.50 (dd, J = 1.8/8.0 Hz, 4H), 2.99 (s, 6Hx2) (Fig. 1).

¹³C NMR (125 MHz, DMSO-d₆): 2 (190), 2 (154), 2 (151), 2 (142), 136, 4 (131), 2 (127), 2 (126), 120, 2 (117), 4(111), 4 (40) (Fig. 2).

IR Spectra: Fig. 3 shows IR spectra of a) SBL and b) SBL-Fe (III) complex. SBL: 1600–1650 cm⁻¹ → Strong peak, C=N (azomethine group) → confirms Schiff base, 3000–3100 cm⁻¹ → weak/medium peaks, aromatic or aliphatic C–H stretching, ~1500–1400 cm⁻¹, Aromatic C=C stretching, ~1200–1000 cm⁻¹, C–N stretching / fingerprint region.

SBL-Fe (III) complex: C=N peak shifts (from ~1600 cm⁻¹ to lower value), Indicates coordination through nitrogen to metal, broadening in 1500–1600 cm⁻¹ region, suggests interaction with metal ion, new peaks in ~500–600 cm⁻¹ region, M–N or M–O bonds (metal–ligand coordination),

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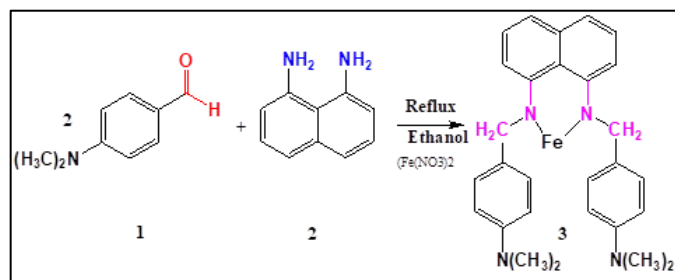
changes in fingerprint region (1000–1200 cm^{-1}) and hence observed structural modification due to complex formation.

2.3 Procedure for Fe(III) Detection in Ethanol

For the analytical studies, 1 mmol stock solutions of various metal salts of Fe^{3+} , Co^{2+} , Fe^{2+} , Cu^{2+} , Ni^{2+} , Zn^{2+} , Al^{3+} , Mg^{2+} , Ca^{2+} , Ba^{2+} , Pb^{2+} , Cd^{2+} and Hg^{2+} were prepared using ethanol as the primary solvent. Similarly, a 10 mmol stock solution of the SBL ligand was prepared in ethanol and subsequently diluted to reach the required experimental concentrations. All prepared solutions were maintained at ambient temperature throughout the study. To investigate the influence of acidity and alkalinity on the sensor's performance, the pH of the solutions was adjusted using hydrochloric acid (HCl) and sodium hydroxide (NaOH). During the sensing experiments, a 2 mL aliquot of the SBL solution (50.0 μmol) was transferred into a quartz cuvette with a 1 cm path length. The metal ion solutions were then introduced into the cuvette incrementally using a precision pipette. For spectroscopic measurements, the excitation and emission slit widths were maintained at 3.0 nm and 5.0 nm, respectively. The proposed coordination framework illustrating the interaction between Fe^{3+} ions and the SBL ligand is detailed in Scheme 1.

2.4 DFT Calculations

Quantum mechanical calculation to understand binding behaviour of Fe(III) with SBL were performed using density functional theory (DFT) calculation by using computer program Gaussian 03W [18]. All DFT calculations were evaluated by applying B3LYP (Becke's three parameter hybrid functional using the LYP correlation function) in the gas phase by using the 6-314(d, p) basic set for ligand SBL



Scheme 1 Interaction between Fe(III) ions and the SBL ligand

2.5 Binding Constant Calculations

K_a , the binding constant was evaluated by UV-Vis method for SBL- Fe^{3+} . Bensi-Hildebrand equation was applied to determine the binding constant, K_a and equation used is as follows.

$$\frac{1}{(A-A_0)} = \frac{1}{\{K(A_{\text{max}}-A_0)[M] + A_0\}} + \frac{1}{[A_{\text{max}}-A_0]} \quad (1)$$

where, A_0 - Absorbance of host in absence of metal ions, A - Absorbance recorded in the presence of added metal ions, A_{max} - Absorbance in presence of added $[M]_{\text{max}}$, K - binding constant (M^{-1}). The graph between $1/[A-A_0]$ versus $1/[M]$ is straight line and the slope obtained gives the value of the association constant (K_a).

3. Results and Discussion

3.1 UV-Visible Spectral Studies of SBL

The chemosensing behaviour of SBL with various 11 metal ions Fe^{3+} , Co^{2+} , Fe^{2+} , Cu^{2+} , Ni^{2+} , Zn^{2+} , Al^{3+} , Mg^{2+} , Ba^{2+} , Pb^{2+} and Cd^{2+} was primarily investigated by applying UV-Visible absorption in ethanol solvent. SBL showed intense absorption peak at 350 nm in absence of metal ions and corresponds to $n-\pi^*$ and $\pi-\pi^*$ transition. Fig. 4 depicts after addition of 1 equivalent of every metal ion, only Fe^{3+} ions show sudden rise in absorbance near 400 nm.

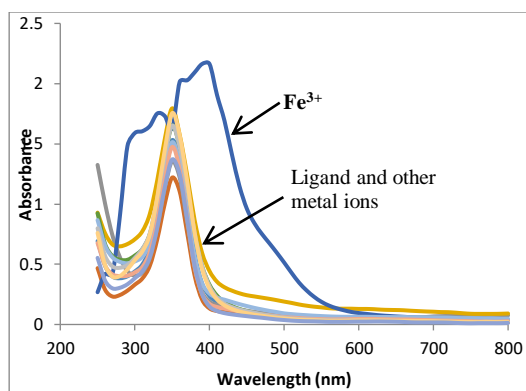


Fig. 4 UV-visible absorption spectra of SBL for various cations in ethanol solution at room temperature

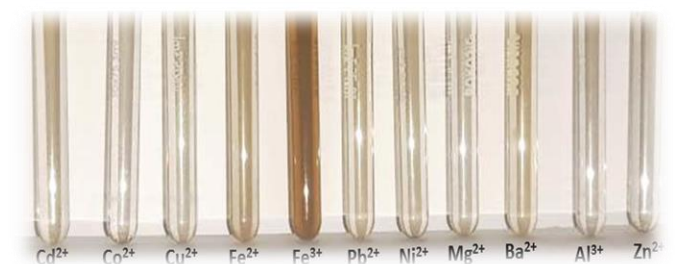


Fig. 5 Colour change observed after the addition of various metal ions (1.0 equiv) to a solution of SBL ($1 \times 10^{-4} \text{M}$) in ethanol showing only Fe^{3+} shows colour change

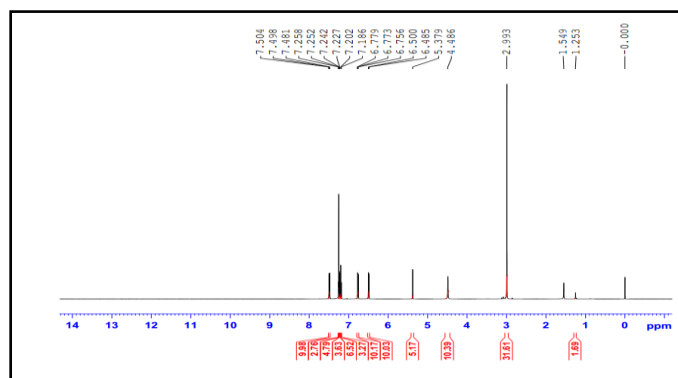


Fig. 1 ^1H NMR spectrum of SBL

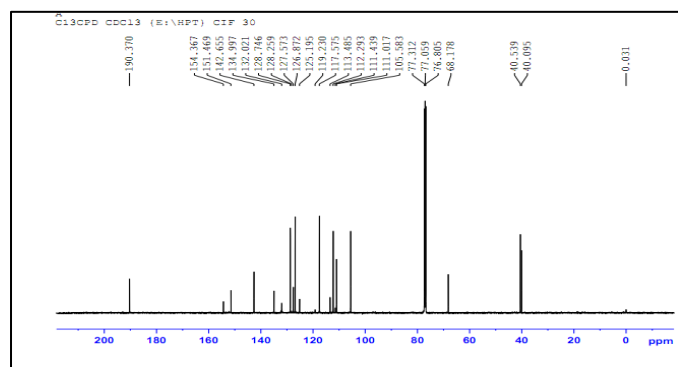


Fig. 2 ^{13}C NMR of SBL

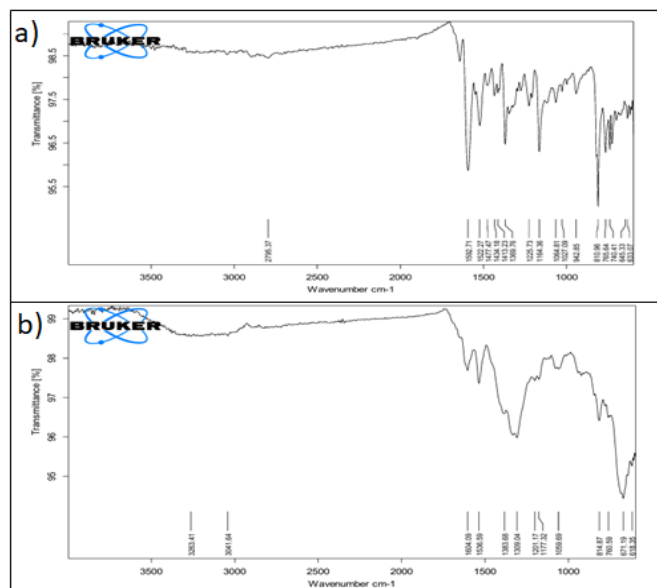


Fig. 3 IR spectrum of a) SBL and b) SBL-Fe (III) complex
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In comparison with SBL this shows red shift of 50 nm in visible region for Fe^{3+} . With the same condition other metal ions including Co^{2+} , Fe^{2+} , Cu^{2+} , Ni^{2+} , Zn^{2+} , Al^{3+} , Mg^{2+} , Ba^{2+} and Cd^{2+} showed very small and unremarkable change in the UV-Vis spectra. This result indicates that SBL is highly sensitive and selective towards Fe^{3+} (0-100 equiv.) in ethanol. The SBL represented change in colour only in the presence of Fe^{3+} , while other metals do not show any change in colour (Fig. 5).

Considering the same conditions, other metal ions including Fe^{3+} , Co^{2+} , Fe^{2+} , Cu^{2+} , Ni^{2+} , Zn^{2+} , Al^{3+} , Mg^{2+} , Ba^{2+} , Pb^{2+} and Cd^{2+} showed small and inconsiderable changes in the UV-spectra (Fig. 6). This confirms synthesized SBL is highly sensitive for Fe^{3+} in ethanol. To understand the interaction between SBL and Fe^{3+} , it was examined by UV-Visible absorption spectra of SBL in ethanol with addition of various concentration of Fe^{3+} from 1 to 100 equivalents. The addition of increasing concentration of Fe^{3+} induced gradual increase in absorbance at 400 nm. This confirms formation of highly stable complex of SBL with Fe^{3+} . Binding constant was evaluated by using Benesi-Hilderbrand equation and found to be 6.925×10^4 (Fig. 7).

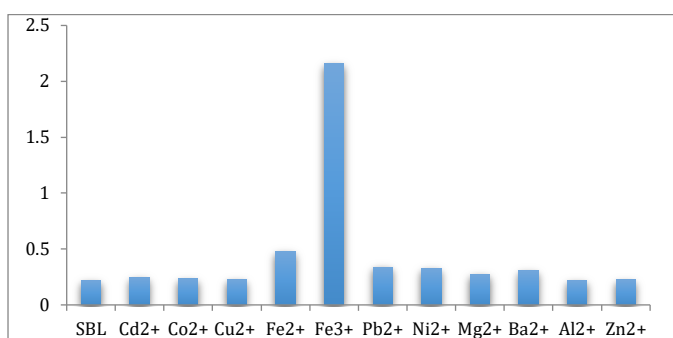


Fig. 6 Bar diagram showing absorbance of SBL after addition of 1 equiv. of various metal ions at 400 nm

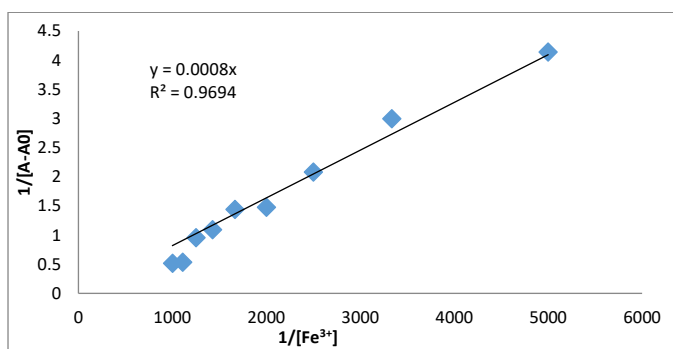


Fig. 7 Benesi-Hilderbrand plot for determination of binding constant

3.2 Selectivity and Competition Studies

The practical utility of a chemosensor depends heavily on its selectivity. To validate this, the sensing performance of the naphthalene-1,8-diamine-based ligand (SBL) was tested against a variety of metal ions, including Fe^{3+} , Co^{2+} , Fe^{2+} , Cu^{2+} , Ni^{2+} , Zn^{2+} , Al^{3+} , Mg^{2+} , Ba^{2+} and Cd^{2+} . Competition experiments were conducted by treating a 1×10^{-4} M solution of SBL with 10 equivalents of Fe^{3+} in the presence of 10 equivalents of interfering ions. As shown in Fig. 8, the absorbance response for Fe^{3+} remained consistent regardless of the presence of other competing metals. The lack of spectral interference confirms that SBL possesses exceptional selectivity, making it a highly effective colorimetric chemosensor for the precise detection of Fe^{3+} .

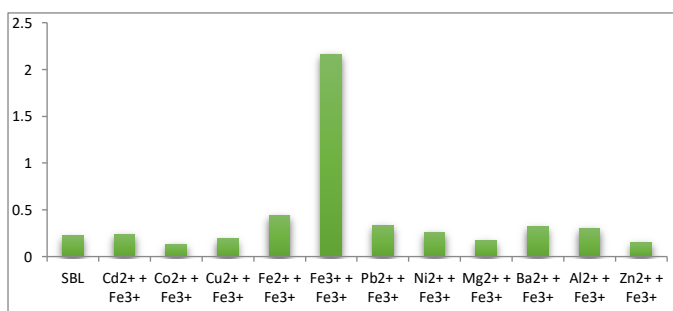


Fig. 8 Absorbance of SBL in ethanol solution in the presence of Fe^{3+} (10 equiv.) and miscellaneous cations at 400nm

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3.3 Electrochemical Stability of the SBL- Fe^{3+} Complex

The electrochemical properties and reversibility of the SBL ligand upon interaction with Fe^{3+} were investigated using cyclic voltammetry. As shown in Fig. 9, the complex exhibits distinct cathodic and anodic peaks in ethanol. Upon the addition of 2.0 equivalents of Fe^{3+} , the oxidation potential shifted slightly from 1.4967 V to 1.487 V, while the reduction potential shifted from -0.600 V to -0.007 V. These minimal variations indicate that the fundamental electrochemical framework of SBL remains intact during coordination. The results confirm the formation of a highly stable SBL- Fe^{3+} complex without any significant structural degradation of the ligand under redox conditions.

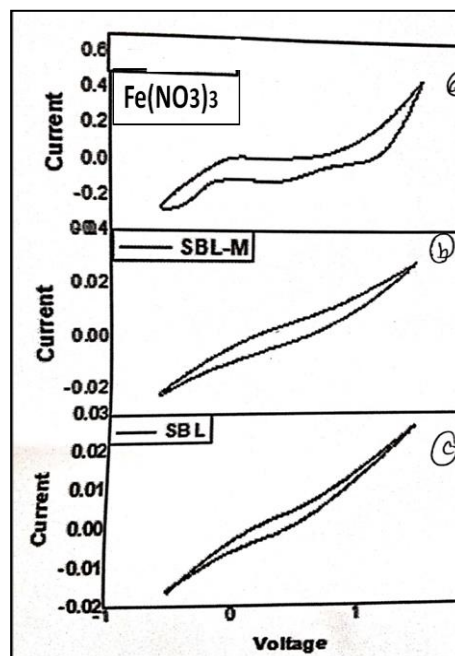


Fig. 9 Titration of SBL with Fe^{3+} using cyclic voltammetry (a) $\text{Fe}(\text{NO}_3)_3$ (b) SBL- Fe^{3+} (c) SBL

3.4 DFT Calculations

The supporting information about coordination mode is provided by molecular modelling studies. The binding behaviour was studied by full geometrical optimization of ligand SBL and its $\text{Fe}(\text{III})$ complex was investigated by density functional theory (DFT) using computer program Gaussian 03 W [19]. All the DFT calculations were carried out at the B3LYP level (Becke's three parameter hybrid functional using the LYP correlation function) in the gas phase by using 6-31G (d,p) basic set (for C, N, H atoms of SBL).

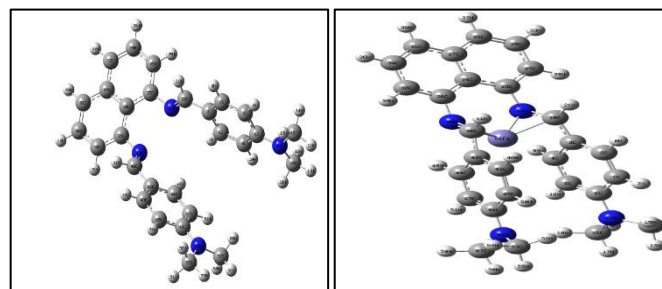


Fig. 10 Geometrical optimization structure of a) Ligand (SBL) and b) SBL and its complex with $\text{Fe}(\text{III})$ calculated at B3LYP/6-31G level. The dark gray, faint gray, dark blue and faint blue C,H,N,Fe atoms respectively

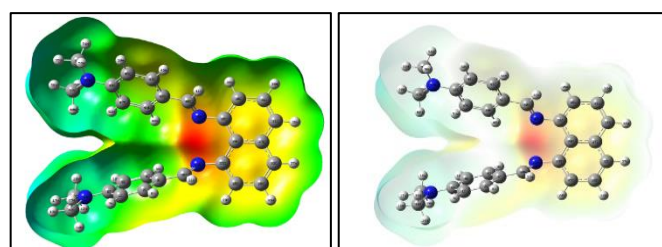


Fig. 11 The HOMO-LUMO gap of a) SBL and b) SBL and its complex with $\text{Fe}(\text{III})$ calculated at the B3LYP/6-31G (d,p) level

Full geometrical optimization of structure of SBL and its complex with Fe(III) in the ground state are shown in Figs. 10(a) and 10(b). The SBL show's non planar geometry in which other atoms are in different plane. The formation of complex indicated that increase in stability confirmed by energy optimization. Fig. 11 gives the frontier molecule orbital (FMO) plot of SBL and Fe (III) ion complex and it was analyzed, which shows the photo induced electron transfer take place between SBL after the addition of Fe(III) ion. The energy gap between HOMO-LUMO of Ligand SBL and SBL-Fe (III) complex was measured to be 0.13263 eV and 0.07188 eV respectively. The decrease in energy gap of Fe(III) complex with ligand SBL indicate easy electron transfer mechanisms and gives intense colour of the complex.

3.5 Biological Screening

The antibacterial and antifungal activity [20] of SBL and SBL-Fe(III) was evaluated using the bacteria *Escherichia coli* (ATCC 8739), *Staphylococcus aureus* (NCIB 9308) and the fungus *Aspergillus niger* (MCIM10281).

The antibacterial activity of the chemical was evaluated using the paper disc diffusion method. The Mcfarland standard was used to determine the inoculum size, which was set at 10^8 cfu/mL for bacterial cultures and 10^8 cfu/mL for fungal spores as per CLSI recommendations. For both bacterial and fungal cultures 0.1 mL of the given inoculum was spread on sterile MH agar plates.

The SBL and SBL-Fe(III) was diluted to 0.01 mg/mL in DMSO. As a control, DMSO and common antibiotic compounds have been used. The sterile filter paper disc was dipped in the solution of SBL and SBL-Fe(III) at previously stated concentrations. Petri dishes were kept in the fridge for a half-hour, the bacterial culture plates were kept at 37 °C in an incubator for 24 hrs. The fungal plates were incubated for 48 hrs at 30 °C. After incubation results were recorded in terms of zone of inhibition in mm. The experiments were carried out in triplicates [21]. Petri plates containing SBL and SBL-Fe(III) for antibacterial and antifungal activity is shown in Fig. 12.

The antimicrobial activity of the SBL and SBL-Fe(III) series of compounds was screened using the paper disc diffusion method against Gram positive bacteria (*Staphylococcus aureus*), Gram negative benenia (*E. coli*) and Fungs (*Aspergillus niger*). A series of compounds shows antibacterial activity against gram negative bacteria (*staphylococcus aureus*). In the case of SBL-Fe(III) series compounds zone of inhibition was observed against gram- positive bacteria (*Staphylococcus aureus*) with no zone I inhibition against gram-negative bacteria (*E. coli*). Both SBL and SBL-Fe (III) compounds are lacks of antifungal properties. The results obtained are shown in Table 1.

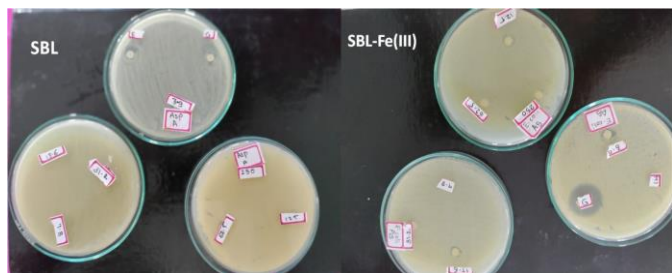


Fig. 12 Petri plates containing SBL and SBL-Fe(III) for antibacterial and antifungal activity

Table 1 The antimicrobial activity of the SBL and SBL-Fe(III) series of compounds was Screened using the paper disc diffusion method

| S. No. | Compound | Zone of inhibition (mm) (s. aureus) | Zone of inhibition (mm) (E. coli) | Zone of inhibition (mm) (A. niger) |
|--------|---------------|-------------------------------------|-------------------------------------|-------------------------------------|
| 1 | SBL | No zone of inhibition was observed. | 19 mm | No zone of inhibition was observed. |
| 2 | SBL-Fe(III) | 24 mm | No zone of inhibition was observed. | No zone of inhibition was observed. |
| 3 | Solvent: DMSO | No zone of inhibition was observed. | No zone of inhibition was observed. | No zone of inhibition was observed. |

4. Conclusion

In the present work, novel synthesis route is investigated for SBL and characterized by means of different spectral advanced techniques including FTIR, ^1H NMR, and ^{13}C NMR. The ligand SBL confirmed selective recognition of Fe(III) ions over other ions including Fe^{3+} , Co^{2+} , Fe^{2+} , Cu^{2+} , Ni^{2+} , Zn^{2+} , Al^{3+} , Mg^{2+} , Ca^{2+} , Ba^{2+} and Cd^{2+} showed very minor and unremarkable changes in through colorimetric response. In visible region for Fe (III) at 400 nm a new peak is appeared with red shift of 50 nm. Binding constant calculated by Benesi- Hildebrand method 6.925×10^4 M. Density functional theory (DFT) computational data also certify that, the binding stoichiometry among SBL and Fe (III) ions. After detailed study, it has been concluded that SBL is an excellent colorimetric and selective probe to sense Fe (III) ions for environmental and biological monitoring.

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