



Synthesis, characterization, biological activity and molecular docking studies of (E)-2-(((3 aminophenyl) imino)methyl) phenol and its complexes.

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Abstract

A new Schiff base ligand (E)-2-(((3-aminophenyl)imino)methyl)phenol (HL) has been synthesized by the reaction between *m*-phenylenediamine and 2-hydroxybenzaldehyde in 1:1 molar ratio. The structure of the ligand was characterized using different spectroscopic techniques. A new series of metal complexes of (HL) with La(III), Er(III) and Yb(III) have been synthesized. The structural features of the complexes have been obtained from their elemental analyses, molar conductivity, ESI-Mass, FT-IR, UV-VIS spectra, magnetic susceptibility, and thermogravimetric analysis (TG). The complexes were found to have 1:1 [M:L] stoichiometry. The infrared spectral studies reveal that HL behaves as a neutral tridentate ligand and coordinated to the metal ions via the azomethine nitrogen, protonated phenolic oxygen and nitrogen atom of the amine group. The presence of coordinated and hydrated water molecules in the complexes was confirmed by thermogravimetric analysis. All complexes possessed an octahedral geometrical structure as suggested from all the above techniques. The calculated binding energy values of the receptors of the colon cancer (PDB code: 2hq6) and the lung cancer (PDB code: 1x2j) were discussed. The ligand and the complexes were evaluated for their antibacterial and antifungal activity against *Gram-positive bacteria*, *Gram-negative bacteria* and fungi. The compounds showed effective antifungal and antibacterial activities against different microorganisms. Yb(III) complex showed the highest biological activity against most tested bacteria organisms.

Keywords: Schiff base metal (III) complexes; Molecular docking; Thermal analysis; Spectroscopic analyses; Biological activity.

Introduction

Schiff base ligands can be easily synthesized by the condensation reactions of primary amines and carbonyl compounds in which the azomethine bond is formed and they can be used as complex formation reactions. Schiff bases have played an important role in the development of coordination chemistry, as they can form stable complexes with most of the transition metals. One of the oldest known classes of Schiff base ligands used in organic synthesis is the salen derivatives. The chemistry and the biological potential of Schiff base ligands and their metal complexes have been investigated extensively. Schiff bases are reported to possess various biological activities, such as antibacterial [1, 2] and antitumor activities [3, 4]. Metal complexes with Schiff bases as ligands have played important role in the development of coordination chemistry due to their

preparative accessibility, structural variety, and biological properties [5–7]. Interest is still high as few have found their way into application as therapeutic drugs, health, skin care products and in paint dye manufacturing [8]. There is also increasing interest in the preparation, reactivity, and structure of Schiff bases, because of their widespread and potential applications in catalysis, ligand modelling, and material chemistry, and because of their biological activity [9]. Schiff bases are also widely used as ligands in coordination with metal ions because of their electron-donor and chelating ability [10]. Moreover, in the developing of new DNA-interacting transition metal based coordination compounds, it has been realized that multi-mode binding would provide advantages in terms of administration, lowering of toxicity, etc. [11, 12]. Due to their distinctive structures and prospective uses in cutting-edge materials including Ln doped

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semiconductors, magnetic, catalytic, fluorescent, and nonlinear optical materials, lanthanides coordination compounds are the focus of significant research. Due to the inclusion of these molecules in both basic and applied research in a number of scientific fields, including chemistry, material science, and life science [4, 13, 14], the coordination chemistry of lanthanide (III) ions is of utmost relevance.

In view of these points above, the new Schiff base ligand (E)-2-((3-aminophenyl)imino)methyl)phenol (HL) is synthesized by condensation of *m*-phenylenediamine with

2-hydroxybenzaldehyde. As an extension of our previous work on metal complexes with bulky Schiff bases, three metal complexes are prepared by reaction of HL with La(III), Er(III) and Yb(III) chloride salts. The ligand and its complexes are characterized by different physicochemical techniques and evaluated for their biological activities against different Gram-positive and Gram-negative bacteria and fungi. The calculated binding energy values of the receptors of the structure of the Cyclophilin-CeCYP16-Like Domain of the serologically defined colon cancer Antigen 10 from Homo Sapiens (PDB code: 2hq6) and the structural basis for the defects of human lung cancer somatic mutations in the repression activity of Keap1 on Nrf 2 (PDB code: 1x2j) are discussed.

Experimental

Materials and reagents

Analytical reagent grade (AR) with highest purity were used. They included 2-hydroxybenzaldehyde (Merck), *m*-phenylenediamine (Merck), $\text{LaCl}_3 \cdot 7\text{H}_2\text{O}$, $\text{ErCl}_3 \cdot 6\text{H}_2\text{O}$ and $\text{YbCl}_3 \cdot 6\text{H}_2\text{O}$ were bought from Sigma - Aldrich.

Absolute ethyl alcohol and dimethylformamide (DMF) were either spectroscopic pure from BDH or purified by the recommended methods [9] and tested for their spectral purity.

Fresh stock solution of HLLigand was prepared by dissolving the accurately weighed amount of HL (0.4 g/L) in the appropriate volume of a mixture of ethanol and DMF (2:1 v/v). Stock solutions of the metal salts (La(III), 0.70 g/L; Er(III), 0.72 g/L and Yb(III), 0.73 g/L) were prepared by dissolving the accurately weighed amounts of the metal salts in the appropriate volume of ethanol. 1×10^{-3} M solutions of the synthesized metal complexes were prepared by dissolving in DMF for measuring the molar conductivity of these metal complexes.

Instruments

Carbon, hydrogen and nitrogen percentages were carried out at the Microanalytical Center, Cairo University, Egypt, using CHNS-932 (LECO) Vario Elemental Analyzer. A Perkin-Elmer 1650 spectrometer ($4000\text{--}400\text{ cm}^{-1}$) was used for the FT-

IR spectra in the form of KBr pellets. Electronic spectra were recorded at room temperature on a Shimadzu 3101pc spectrophotometer as solutions in DMF. ^1H NMR spectrum of the ligand was recorded on a 300 MHz Varian-Oxford Mercury at room temperature, as a solution in DMSO- *d*₆ using TMS as an internal standard. Mass spectra were recorded by the EI technique at 70 eV using MS-5988 GS-MS Hewlett-Packard instrument at the Microanalytical Unit, National Research Center, Egypt. The diamagnetic corrections were made by Pascal's constant and $\text{Hg}[\text{Co}(\text{SCN})_4]$ was used as a calibrant. Molar conductivities of 10^{-3} M solutions of the solid complexes in DMF were measured by using Jenway 4010 conductivity meter. The thermogravimetric analyses (TG) of the solid complexes were carried out from room temperature to 1000 °C using a Shimadzu TG-50H thermal analyzer. Docking calculations were carried out on receptors of the structure of the Cyclophilin-CeCYP16-Like Domain of the serologically defined colon cancer Antigen 10 from Homo Sapiens (PDB code: 2hq6) and the structural basis for the defects of human lung cancer somatic mutations in the repression activity of Keap1 on Nrf2 (PDB code: 1x2j). The MMFF94 Force field was used for energy minimization of molecules using Docking Server [13-20].

Fresh stock solution of HLLigand was prepared by dissolving the accurately weighed amount of HL (0.4 g/L) in the appropriate volume of a mixture of ethanol and DMF (2:1 v/v). Stock solutions of the metal salts (La(III), 0.70 g/L; Er(III), 0.72 g/L and Yb(III), 0.73 g/L) were prepared by dissolving the accurately weighed amounts of the metal salts in the appropriate volume of ethanol. 1×10^{-3} M solutions of the synthesized metal complexes were prepared by dissolving in DMF for measuring the electrical conductance of these metal complexes. The absorption spectra of (1×10^{-4} M) solutions of the Schiff base ligand HL under study and its metal complexes were prepared by accurate dilution from the previously prepared stock solutions (1×10^{-3} M) were recorded for measuring their UV-Vis spectra in the wavelength range from 200 to 700 nm.

Biological activity

A modified Kirby-Bauer disc diffusion method was used for the determination of antimicrobial activity of the tested complexes [9]. 100 μl of the tested bacteria or fungi were grown in 10 ml of fresh media until they reached a count of approximately 10⁸ and 10⁵ cells/ml for bacteria and fungi, respectively. 100 μl of microbial suspension was spread onto agar plates corresponding to the broth in which they were maintained. Isolated colonies of each organism that might be playing a pathogenic role should be selected

from primary agar plates and tested for susceptibility by disc diffusion method [13].

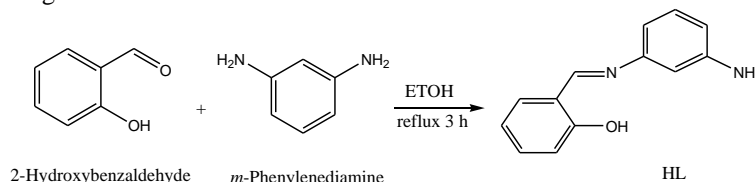
Plates inoculated with Gram (+) bacteria as *Bacillus subtilis* and *Staphylococcus aureus*; Gram (-) bacteria as *Salmonella SP*, *Pseudomonas aeruginosa*, and *Escherichia coli*. They were incubated at 37 °C for ~ 28 hours and yeast fungus as *Aspergillus fumigatus* and *Candida albicans* incubated at 30 °C for ~ 28 hours and the diameters of the inhibition zones were measured in millimeters [9]. Standard discs of Ampicillin and Gentamycin (antibacterial agents), and Amphotericin B (antifungal agent) served as positive controls for antimicrobial activity but filter discs impregnated with 10 µl of solvent (distilled water, chloroform, DMSO) were used as a negative control. The agar used is Mueller-Hinton agar is rigorously tested for composition and pH. Further the depth of the agar in the plate is a factor to be considered in the disc diffusion method. This method is well documented and standard zones of inhibition have been determined for susceptible and resistant values. Blank paper discs (Schleicher and Schuell, Spain) with a diameter of 8.0 mm were impregnated with 10 µl of tested concentration of the stock solutions. When a filter paper disc impregnated with a tested chemical is placed on agar, the chemical will diffuse from the disc into the agar. This diffusion will place the chemical in the agar only around the disc. The solubility of the chemical and its molecular size will determine the size of the area of chemical infiltration around the disc. If an organism is placed on the agar, it will not grow in the area around the

disc if it is susceptible to the chemical. This area of no growth around the disc is known as zone of inhibition or clear zone. For the disc diffusion, the zone diameters were measured with slipping calipers of the national committee for clinical laboratory standards [9]. Agar based methods such E-test and disc diffusion can be good alternatives because they are simpler and faster than broth-based methods [21].

Synthesis of ligand (HL)

Novel Schiff base ligand (HL) was synthesized by the condensation reaction of *m*-phenylenediamine with 2-hydroxybenzaldehyde. An ethenolic solution of 2-hydroxybenzaldehyde (129.4 mmol, 15.8 g, 13.5 ml) was added dropwise to *m*-phenylenediamine (129.4 mmol, 14 g) dissolved in ethanol. The resulting mixture was stirred under reflux for about 3 h during which an orange solid compound was separated. It was filtered, recrystallized and washed with diethylether and dried in vacuum (Scheme 1).

HL: Yield 50.70 %; m.p. 130 °C; yellowish green solid. Microanalysis for C₁₃H₁₂N₂O, Calcd. (%): C, 73.59; H, 5.66; N, 13.21. Found (%): C, 73.57; H, 5.65; N, 13.20. FT-IR spectrum (cm⁻¹): phenolic ν(OH) 3431, azomethine ν(C=N) 1613, ν(C-N) 1396, ν(C-O) phenolic 1274. ¹H NMR (300 MHz, DMSO-d₆, δ, ppm): 9.1 (s, H, OH phenolic), 8.86 (s, H, CH=N), 6.54-7.69 (m, 8H, Ar H), 4.23 (s, 2H, NH₂). λ_{max} (cm⁻¹): 46083 and 40650 π-π*, 30030 n-π*.



Scheme 1. Preparation of Schiff base ligand (HL).

Synthesis of complexes

The metal complexes were prepared by the addition of hot solution of the appropriate metal chlorides (1.887 mmol) in ethanol to the hot solution of the ligand (0.4g, 1.887 mmol) in a mixture of ethanol and DMF by ratio (2:1 v/v). The resulting mixture was stirred under reflux for two hours whereupon the complexes were precipitated. They were collected by filtration, washed with hot ethanol and purified by washing several times with diethyl ether. The analytical data for C, H and N were repeated twice.

[La(HL)(H₂O)Cl₂].H₂O.Cl (1)

Yield 80.65 %; yellowish green solid, m.p. 90°C. Microanalysis for La(C₁₃H₁₆Cl₃N₂O₃), Calcd. (%): C, 31.62; H, 3.24; N, 5.68; La, 28.15. Found (%): C, 31.60; H, 3.25; N, 5.69; La, 28.14. FT-IR spectrum (cm⁻¹): phenolic ν(OH) 3408, azomethine ν(C=N) 1649, ν(C-N) 1385, phenolic ν(C-O) 1238, ν(H₂O) stretching bands of coordinated water 840 and 735,

ν(M-O) stretching bands of coordinated water 520, metal-oxygen bond ν(M-O) 540, metal-nitrogen bond ν(M-N) 465. Molar conductivity (10⁻³ M, DMF): 99.90. Λ_mΩ⁻¹ mol⁻¹ cm². λ_{max} (cm⁻¹): 46083 and 243 π-π*, 29850 n-π*.

[Er(HL)(H₂O)₂Cl].H₂O.Cl₂ (2)

Yield 49.16 %; black solid, m.p. 121°C. Microanalysis for Er(C₁₃H₁₈Cl₃N₂O₄), Calcd. (%): C, 28.91; H, 3.34; N, 5.19; Er, 31.00. Found (%): C, 28.90; H, 3.35; N, 5.20; Er, 31.01. FT-IR (cm⁻¹): phenolic ν(OH) 3423, azomethine ν(C=N) 1641, ν(C-N) 1386, phenolic ν(C-O) 1255, ν(H₂O) stretching bands of coordinated water 846 and 753, ν(M-O) stretching bands of coordinated water 523, metal-oxygen bond ν(M-O) 542, metal-nitrogen bond ν(M-N) 459. Molar conductivity (10⁻³ M, DMF) : 117.50 Λ_m Ω⁻¹ mol⁻¹ cm². λ_{max} (cm⁻¹): 46083 and 41152 π-π*, 29850 n-π*.

[Yb(HL)(H₂O)Cl₂].H₂O.Cl (3)

Yield 80.47 %; blue solid, m.p. 120°C. Microanalysis for Yb(C₁₃H₁₆Cl₃N₂O₃), Calcd. (%): C, 29.58; H, 3.03; N, 5.31; Yb, 32.81. Found (%): C, 29.57; H, 3.02; N, 5.30; Yb, 32.80. FT-IR (cm⁻¹): phenolic $\nu(\text{OH})$ 3412, azomethine $\nu(\text{C}=\text{N})$ 1655, $\nu(\text{C}-\text{N})$ 1382, phenolic $\nu(\text{C}-\text{O})$ 1246, $\nu(\text{H}_2\text{O})$ stretching bands of coordinated water 867 and 754, $\nu(\text{M}-\text{O})$ stretching bands of coordinated water 566, metal-oxygen bond $\nu(\text{M}-\text{O})$ 589, metal-nitrogen bond $\nu(\text{M}-\text{N})$ 466. Molar conductivity (10⁻³ M, DMF): 93.50. $\Lambda_m \Omega^{-1} \text{ mol}^{-1} \text{ cm}^2 \lambda_{\text{max}}$ (cm⁻¹): 46083 and 41152 $\pi-\pi^*$, 29850 $n-\pi^*$.

Results and discussion

Characterization of the ligand (HL)

The symmetric Schiff base ligand was prepared by stirring an appropriate amount of 2-hydroxybenzaldehyde with the corresponding *m*-phenylenediamine (1:1) in ethanol. The new Schiff base ligand formed was characterized with respect to its composition using elemental and spectral analyses. The results of elemental analysis of the ligand (C, H, and N) with molecular formula and the melting point are presented in experimental part. The obtained results are in good agreement with those calculated for the suggested formula, and the melting point is sharp indicating the purity of the prepared ligand. The ligand is soluble in DMF and DMSO.

Mass Spectrum of the ligand

The mass spectral decomposition modes of the Schiff base ligand (HL) have been investigated. The mass spectrum of HL shows the molecular ion peak at $m/z = 212$ amu (Calcd. 212 amu) corresponding to its molecular formula C₁₃H₁₂N₂O. The peaks at $m/z = 164, 149, 143, 122, 105$ and 78 are due to different fragments.

FT-IR Spectrum of the ligand

Fundamental IR spectral bands for the ligand are given in Table 1. The IR spectrum of the free ligand is characterized mainly by the strong bands at 3431, 1396, 1274 and 685 cm⁻¹ attributed to the stretching frequencies of $\nu(\text{OH})$ phenolic, $\nu(\text{C}-\text{N})$ stretching, $\nu(\text{C}-\text{O})$ phenolic and $\nu(\text{NH}_2)$ bending, respectively. Also a band for the azomethine $\nu(\text{C}=\text{N})$ stretching vibration was recorded due to the condensation reaction between *m*-phenylenediamine and 2-hydroxybenzaldehyde at 1613 cm⁻¹ confirming the formation of the Schiff base ligand [22,23].

¹H NMR spectral study

The ¹H NMR data of the newly synthesized Schiff base ligand is featured by the peaks appeared at 6.54-7.69 ppm which may be assigned to the aromatic ring protons. Sharp band at 8.86 ppm may be assigned to the proton of azomethine (-CH=N-)

group which confirms the formation of Schiff base ligand [16,24-26]. A singlet peak at lower field 9.10 ppm can be assigned to the proton of OH phenolic group [27, 28]. A peak at 4.23 ppm is attributed to protons of amine NH₂ group.

Molecular docking study of Schiff base ligand (HL)

Exploration of molecular docking interaction of the Schiff base ligand (HL) was performed through molecular docking studies using Docking Server [29-32]. The Schiff base ligand (HL) was evaluated for their inhibitory effect on receptors of the colon cancer (PDB code: 2hq6) and the lung cancer (PDB code: 1x2j) [31-37]. The data showed a favorable arrangement between the Schiff base ligand (HL) and the receptors of the colon cancer (PDB code: 2hq6) and the lung cancer (PDB code: 1x2j) and the interaction curves are shown in Fig. 1 and the calculated energy as well as some parameters with the selected anticancer receptors are listed in Table 2. The 2D plot curves of binding for Schiff base ligand (HL) with the receptors of colon cancer (PDB code: 2hq6) and lung cancer (PDB code: 1x2j) are shown in Fig. 2. The HB plot curves explain the interactions between Schiff base ligand (HL) and receptors of the colon cancer (PDB code: 2hq6) and the lung cancer (PDB code: 1x2j) as shown in Figure 3.

Compositions and structures of the complexes

The results of elemental analyses (C, H, and N) with molecular formula and the melting points are presented in Experimental part. The prepared complexes are colored, air stable complexes. They are soluble in DMF and partially soluble in ethanol but they are insoluble in water. The elemental analysis results for the metal complexes are in good agreement with the calculated values. The elemental analyses data of the complexes show the formation of the complexes in the ratio 1:1 and correspond to a composition of [MHL] type for all complexes.

Molar conductivity measurements

Molar conductivity measurements provide a method of testing the degree of ionization of the complexes. The measured molar conductance values of 10⁻³ M solutions metal complexes in DMF are present in experimental part. The La(III) and Yb(III) complexes have molar conductivity values of 99.9 and 93.5 $\Omega^{-1} \text{ mol}^{-1} \text{ cm}^2$, respectively. It is obvious from these data that, these chelates are ionic in nature and considered as 1:1 electrolytes [38, 39]. On the other hand the Er(III) complex showed 1:2 electrolytic nature with the molar conductance value of 117.5 $\Omega^{-1} \text{ mol}^{-1} \text{ cm}^2$ indicating that the chloride ions are outside the coordination sphere, and the complex has the general formula [MHL]Cl₂ [40].

Mass spectra

The electron impact mass spectrum of the $[\text{Er}(\text{HL})(\text{H}_2\text{O})_2\text{Cl}]\cdot\text{H}_2\text{O}\cdot\text{Cl}_2$ complex showed the molecular ion peaks at $m/z = 539$ amu (Calcd. 539.61 amu) which confirm the stoichiometry as being of the type MHL. The proposed formula was confirmed also by appearance of a peak at 212 amu corresponding to the Schiff base ligand moiety of ($\text{C}_{13}\text{H}_{12}\text{N}_2\text{O}$). The observed peaks were in good agreement with its proposed formula as indicated by the microanalytical data. Thus, the mass spectral data support the conclusions drawn from the analytical and molar conductivity values.

FT-IR spectral study

The IR band in the region of 1641-1655 cm^{-1} in the complexes are assigned to the $-\text{CH}=\text{N}-$ imine bond appears at higher wave numbers as compared with the free ligands (1613 cm^{-1}) due to the involvement of the nitrogen atom in coordination with the metal ions. Another band appearing in the spectrum of the ligand in 1274 cm^{-1} region assigned to the $\nu(\text{C}-\text{O})$ phenolic mode [41-46]. This band is shifted to lower wavenumber in the complexes at 1238-1255 cm^{-1} region indicating the coordination of the ligand with the metal ions through phenolic oxygen atom. New bands appearing in the 1382-1386 cm^{-1} region in the spectra of complexes, were assigned to the $\nu(\text{C}-\text{N})$ vibrations. This band appeared at 1396 cm^{-1} in the spectrum of the ligand and shifted to lower wavenumber in complexes due to coordination through nitrogen atom. A broad band in the region 3408-3423 cm^{-1} in all complexes is attributed to OH stretching vibrations of coordinated water molecules [9]. The chelates also show the presence of water molecules, which can be inferred from the bands at 735-754 and 840-867 cm^{-1} , and may be due to the wagging and rocking modes of vibrations of the coordinated and lattice water, respectively.

An important feature is the presence of new intense bands are observed in the far-IR region (540-589 and 457-465 cm^{-1}) in the complexes assigned to (M-O) and (M-N) stretching vibrations, respectively, which confirms the coordination of oxygen and nitrogen atoms of the ligand to the metal atom. Additional support for the formation of the complexes was provided by presence of the weak-intensity bands at 520-566 cm^{-1} region which were attributed to the formation of M-O of coordinated water in the complexes [47-49].

From IR spectra it is concluded that, the ligand acts as a neutral tridentate ligand coordinated to the metal ions through azomethine nitrogen, protonated phenolic oxygen and nitrogen of amine group.

Thermal studies

Thermogravimetric studies (TG) for the La(III), Er(III) and Yb(III) complexes were carried out from room temperature to 1000°C. The stages of decomposition, temperature range, decomposition products as well as the observed and calculated mass loss percentages of all complexes are illustrated in Table 3. The results show a good agreement with the theoretical formula as suggested from the analytical data.

The Schiff base ligand with the molecular formula [$\text{C}_{13}\text{H}_{12}\text{N}_2\text{O}$] decomposed at a temperature range from 45 to 1000°C with four steps as follows. The first and second steps were within the temperature range of 45-395°C representing the loss of H_2O and C_4H_2 molecules with a found mass loss of 32.07 % (Calcd. 32.08 %). The third step represented the loss of $\text{C}_2\text{H}_4\text{N}_2$ molecule with a mass loss of 26.38 % (Calcd. 26.41 %) within the temperature range 395-675°C. The last step represented the loss of C_7H_4 molecule with a mass loss of 41.50 % (Calcd. 41.51 %) within the temperature range 675-1000 °C. At the end of the thermogram, the total estimated mass loss amounted to 99.95 % (Calcd. 100 %).

In case of complex (1), the decomposition occurs within four steps. The first step at 35-160 °C temperature range occurred with an estimated mass loss of 17.28% (Calcd. 17.73%), may be attributed to the loss of $1.5\text{H}_2\text{O}$ and C_2HCl molecules. The second decomposition step occurs within temperature range of 160-390°C with an estimated mass loss of 14.20% (Calcd. 14.37%) accounting for the removal of Cl_2 gas. The third decomposition step occurs within temperature range of 390-750 °C with an estimated mass loss of 15.39% (Calcd. 15.41%) accounting for the removal of C_6H_4 organic fragment. The last step is due to the removal of the organic molecule $\text{C}_3\text{H}_8\text{N}_2$ and occurs within the temperature range of 750-1000 °C with an estimated mass loss of 14.57% (Calcd. 14.59%) leaving the metal oxide ($\frac{1}{2}\text{La}_2\text{O}_3$) contaminated with carbon as a final product. The overall weight loss amounts to 61.44% (Calcd. 62.10%).

The TG curve of complex (2), decomposed in three stages. The first estimated mass loss of 19.45% (Calcd. mass loss 19.54%) observed in the temperature range of 30-205 °C is due to the loss of $2.5\text{H}_2\text{O}$ and C_2HCl molecules. The second step is found in the temperature range of 205-400 °C with an estimated mass loss of 13.42% (Calcd. mass loss 13.51%) corresponding to the loss of 2HCl molecules. The third step occurs within the temperature range of 400-1000°C with an estimated mass loss of 13.66% (Calcd. mass loss 13.72%) is due to the removal of $\text{C}_3\text{H}_{10}\text{N}_2$ organic fragment leaving the metal oxide ($\frac{1}{2}\text{Er}_2\text{O}_3$) contaminated with

carbon as a residue. The overall weight loss amounts to 46.53% (Calcd. 46.77%).

The complex (**3**) is thermally decomposed in three stages. The first stage corresponds to a mass loss of 20.31% (Calcd. 20.37%) within the temperature range 15-150 °C represents the loss of 1.5H₂O, HCl, CH₄ molecules and N₂ gas molecule. The second stage corresponds to a mass loss of 19.47% (Calcd. 19.34%) within the temperature range 150-565 °C and represents the loss of C₈H₆ organic molecule. The third stage of decomposition occurs within the temperature range 565-1000 °C, with a found mass loss of 15.87% (Calcd. 16.10%) which is reasonably accounted for decomposition of the remaining organic part of the complex through the removal of CH₂Cl₂ molecule leaving out ½Yb₂O₃ contaminated with carbon as a residue. The overall weight loss amounts to 55.65% (Calcd. 55.81%).

Structural interpretation

The structure of HL complexes of La(III), Er(III) and Yb(III) ions was confirmed based on spectroscopic techniques as elemental analyses, IR, molar conductance, mass, UV-vis and thermal analysis. Therefore, from the IR spectral studies, it is concluded that HL ligand behaves as a neutral tridentate ligand with ONN coordination sites and coordinated to the metal ions via the azomethine nitrogen, protonated phenolic oxygen and nitrogen atom of amine group. From conductance measurements, the La(III) and Yb(III) complexes were found to be 1:1 electrolytes but Er(III) complex was found to be 1:2 (L:M) electrolyte. Based on the above techniques, an octahedral geometry was suggested for the complexes and their structures are proposed as follows in Fig. 4.

Table 1. IR spectra data of HL ligand and its metal complexes*

HL	1	2	3	Assignment
3431	3408	3423	3412	OH stretching
1613	1649	1641	1655	CH=N stretching
1396	1385	1386	1382	C-N stretching
1274	1238	1255	1246	C-O phenolic
-----	840w, 735w	846w, 753w	867s, 754s	H ₂ O stretching of coordinated water
685	672	676	684	NH ₂ bending
-----	540	542	589	M-O
-----	520	523	566	M-O stretching of coordinated water
-----	465	459	457	M-N

*Numbers are given in Experimental part

Table 2. Energy values and parameters obtained in docking calculations for Schiff base ligand (HL) with receptors of the colon cancer (PDB code:2hq6) and the lung cancer (PDB code:1x2j)

Receptors	Estimated free energy of binding (kcal/mol)	Estimated inhibition constant (K _i) (µM)	vdW+ bond+ desolv energy (kcal/mol)	Electrostatic Energy (kcal/mol)	Total intercooled Energy (kcal/mol)	Interact surface (Å)
2hq6	-4.94	238.20	-6.06	-0.09	-6.16	557.059
1x2j	-6.41	20.01	-7.48	-0.16	-7.65	653.362

Biological activity

The antimicrobial activity of the Schiff base ligand and its complexes against human pathogenic Gram-positive (*Staphylococcus aureus* and *Bacillus subtilis*), Gram-negative (*Salmonella SP.*, *Escherichia coli* and *Pseudomonas aeruginosa*) bacteria and *Aspergillus fumigatus* and *Candida albicans* fungi was measured by measuring the zone of inhibition in disc diffusion method (Table 3). The compounds showed less activity against Gram-positive bacteria than the activities against Gram negative and *Candida albicans* fungi.

Coordination structure of complexes plays an important role in their biological activity mechanisms. Complexation may be reducing the polarity of the metal ion due to the strong overlap in

between the d_{x²-y²} orbital of metal ion and donor orbital of the ligand. Thus, the lipophilic character of the central metal atom is enhanced, which results in a higher capability to penetrate the microorganisms through the lipid layer of the cell membrane. The lipophilic nature of the central metal atom can be increased by these factors and hence increasing the liposolubility and hydrophobic character of the molecule favoring its permeation through the lipid layer of the bacterial membrane. This enhances the rate of uptake/entrance and thus the antibacterial activity of the testing compounds [50-52]. The involvement of the azomethine (C=N) group, which was crucial in elucidating the mechanism of transamination and re-transamination processes in biological systems [26, 36, 42, 45, 50-

52], may also be used to explain this improvement. Additionally, the reduced polarity of the ligand resulting from the overlap of the ligand orbitals and the partial sharing of the positive charge of the metal ion with electron-releasing groups can be used to explain the higher activity of the metal chelates. It goes without saying that lowering the total electron density on free ligands speeds up transport across bacterial cells [50–52].

The activity of the prepared complexes is quite comparable with the reference free ligand. From the results, it is observed that the investigated compound's antimicrobial activity values in this research were higher than that reported for the Schiff base free ligand.

Of the three complexes, Yb(III) complex has a significant biological activity against most of the tested organisms compared with other

complexes and the free ligand (Figure 5). Er(III) complex has the highest biological activity against *Escherichia coli* and *Aspergillus fumigatus* microorganisms. La(III) complex has the lowest biological activity against *Escherichia coli* and *Pseudomonas aeruginosa*.

The results of the antifungal evaluation are represented in Table 3. Amphotericin B was used as standard drug. All the complexes expressed antifungal activity against *C. albicans* and *Aspergillus fumigatus*. The antifungal activity of the complexes followed the order: amphotericin B > complex 2 > complex 3 > complex 1 > HL for *Aspergillus fumigatus* and amphotericin B > complex 3 > complex 2 > complex 1 > HL for *Candida albicans*.

Table 3. Thermoanalytical results (TG) of HL ligand and its metal complexes

Complex*	TG range (°C)	DTG _{max} (°C)	n*	Mass loss loss Estim (Calcd) %	Total mass	Assignment	Residues
HL	45-395 395-675 675-1000	93, 253 537 740	2 1 1	32.07 (32.08) 26.38 (26.41) 41.50 (41.51)	99.95 (100)	- Loss of H ₂ O and C ₄ H ₂ . - Loss of C ₂ H ₄ N ₂ . - Loss of C ₇ H ₄ .	-----
[La(HL)(H ₂ O)Cl ₂].H ₂ O.Cl	35-160 160-390 390-750 750-1000	85 279 523 870	1 1 1 1	17.72 (17.73) 14.20 (14.37) 15.39 (15.41) 14.57 (14.60)	61.88 (62.11)	- Loss of 1.5H ₂ O and C ₂ HCl. - Loss of Cl ₂ . - Loss of C ₆ H ₄ . - Loss of C ₃ H ₈ N ₂ .	½La ₂ O ₃ +2C
[Er(HL)(H ₂ O) ₂ Cl].H ₂ O.Cl ₂	30-205 205-400 400-1000	85 302 650	1 1 1	19.45 (19.54) 13.42 (13.51) 13.69 (13.72)	46.56 (46.77)	- Loss of 2.5H ₂ O and C ₂ HCl. - Loss of 2HCl. - Loss of C ₃ H ₁₀ N ₂ .	½Er ₂ O ₃ +8C
[Yb(HL)(H ₂ O)Cl ₂].H ₂ O.Cl	15-150 150-565 565-1000	83 265 765	1 1 1	20.31 (20.37) 19.47 (19.34) 15.87 (16.10)	55.65 (55.81)	- Loss of 1.5H ₂ O, CH ₄ , N ₂ and HCl. - Loss of C ₈ H ₆ . - Loss of CH ₂ Cl ₂ .	½Yb ₂ O ₃ +3C

*Numbers are given in Experimental part

Table 4. Biological activity of HL ligand and its metal complexes*

Sample	Inhibition zone diameter (mm / mg sample)						
	<i>Staphylococcus aureus</i> (G ⁺)	<i>Bacillus subtilis</i> (G ⁺)	<i>Salmonella</i> SP. (G ⁻)	<i>Escherichia coli</i> (G ⁻)	<i>Pseudomonas aeruginosa</i> (G ⁻)	<i>Aspergillus fumigatus</i>	<i>Candida albicans</i>
Control: DMSO	0	0	0	0	0	0	0
HL	10	11	13	15	16	11	12
1	13	13	15	14	13	16	14
2	14	15	17	19	15	18	16

3	15	19	18	16	16	17	18
Ampicillin	23	32	-	-	-	-	-
Gentamycin	-	-	17	19	16	-	-
Amphotericin B	-	-	-	-	-	23	25

*Numbers are given in Experimental part

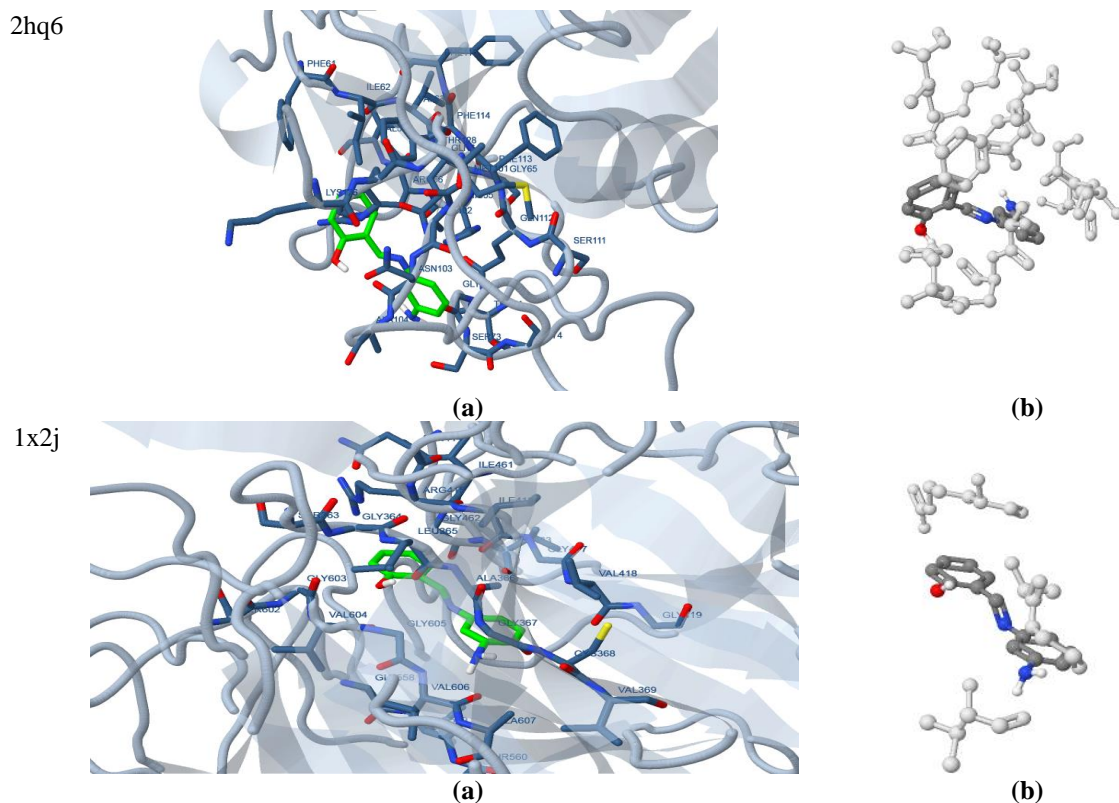


Fig. 1. The Schiff base ligand (HL)(green in (a) and gray in (b)) in interaction with receptors of colon cancer (PDB code: 2hq6) and lung cancer (PDB code: 1x2j).

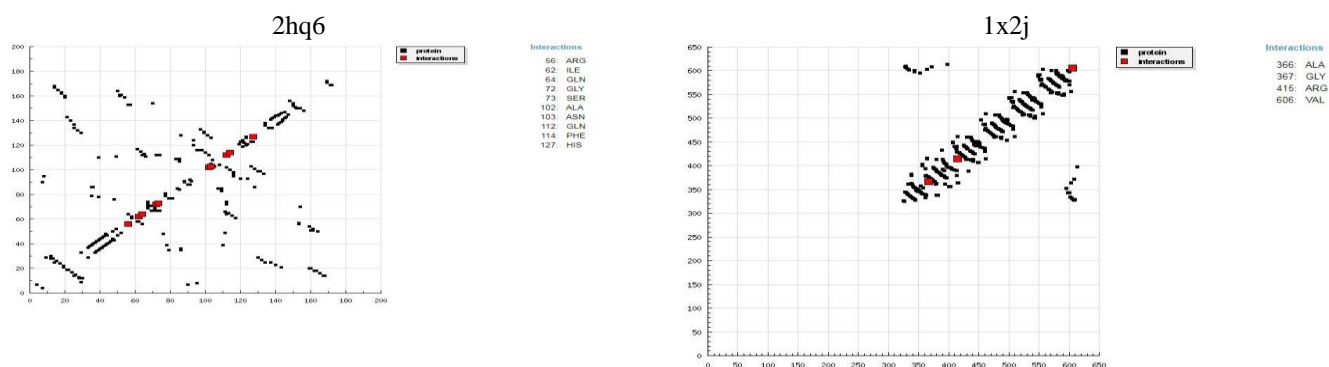


Fig.2. HB plot of interaction between Schiff base ligand (HL) and receptors of colon cancer (PDB code: 2hq6) and lung cancer (PDB code: 1x2j).

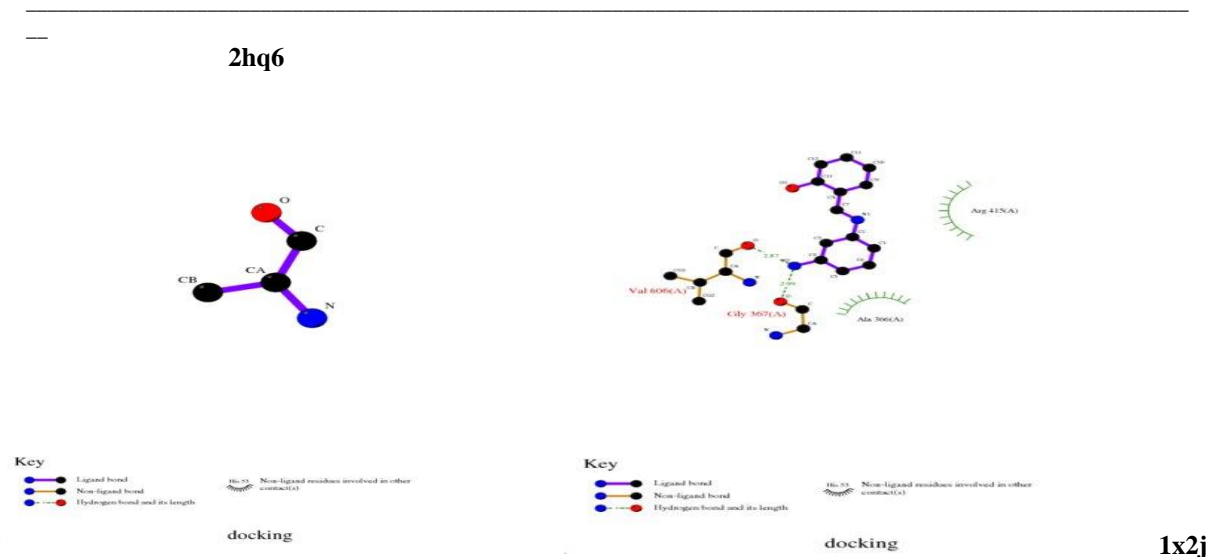


Fig. 3. 2D plot of interaction between Schiff base ligand (HL) and receptors of colon cancer (PDB code: 2hq6) and lung cancer (PDB code: 1x2j).

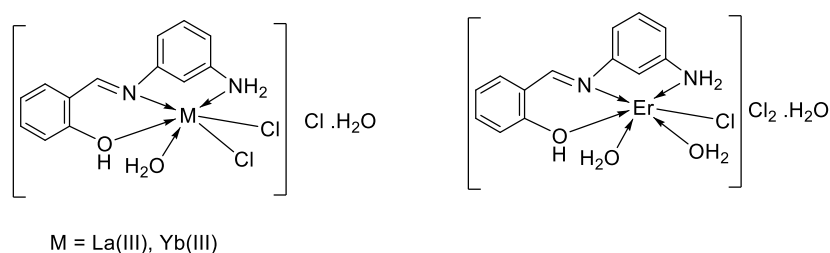


Fig. 4. The structures metal complexes of the Schiff base ligand (HL).

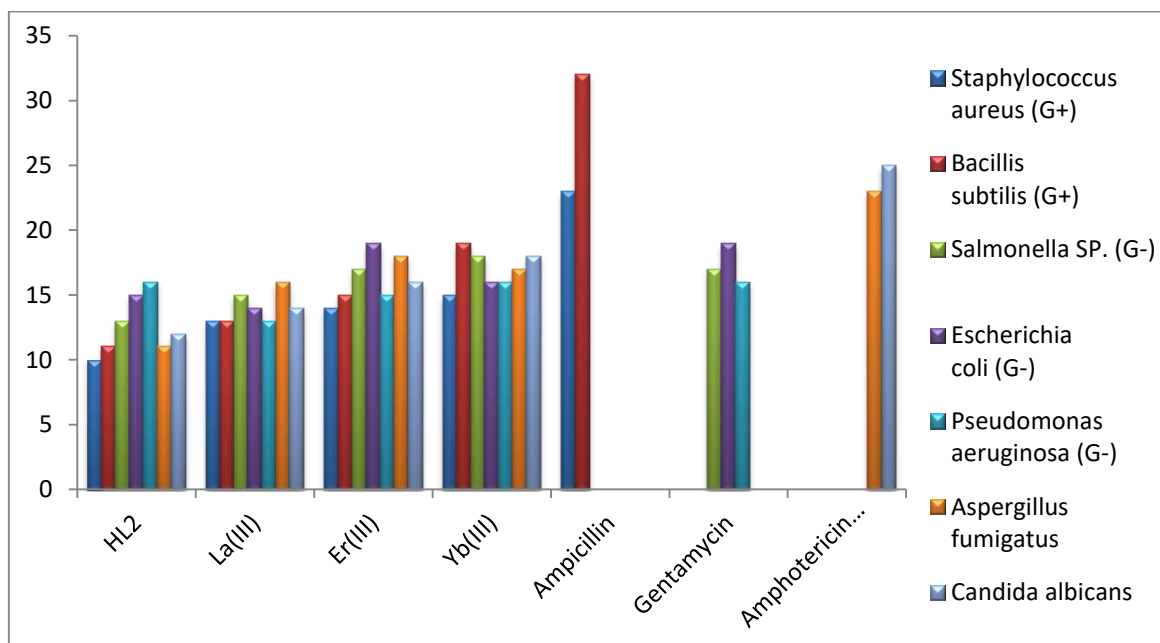


Fig. 5. Biological activity of the Schiff base ligand (HL) and its metal complexes.

4. Conclusion

The metal complexes of La(III), Er(III) and Yb(III) with (E)-2-(((3-aminophenyl)imino)methyl)phenol (HL) Schiff base ligand derived from the reaction of *m*-phenylenediamine and 2-hydroxybenzaldehyde in 1:1 molar ratio were synthesized and characterized. From IR spectral data, the Schiff base is found to be neutral tridentate ligand coordinated through the azomethine nitrogen, protonated phenolic oxygen and nitrogen atom of amine group, confirmed by analytical, spectral and thermal studies. From elemental analysis, the complexes have composition of the MHL type with general formulae $[M(HL)(H_2O)Cl_2] \cdot H_2O \cdot Cl$ ($M = La(III)$ and $Yb(III)$) and $[M(HL)(H_2O)_2Cl] \cdot H_2O \cdot Cl_2$ ($M = Er(III)$). From conductance values of the complexes, La(III) and Yb(III) complexes are found 1:1 electrolytes but Er(III) complex is 1:2 (L:M) electrolyte. The geometrical structure can be described as octahedral for all complexes. From thermal analyses, the structure of complexes was confirmed and all complexes were found to have coordinated and hydrated water molecules. The newly synthesized ligand and its complexes were evaluated for their antibacterial and antifungal activities against different microorganisms. The complexes were found to have higher activity than the ligand.

References

- [1] S. Matin, R. Khojasteh, Synthesis, characterization, and antibacterial activities of Cr (III), Co (III), Ni (II), and Mn (III) complexes of heptadentate Schiff base ligand derived from tris (2-aminoethyl) amine, Russian Journal of General Chemistry 85 (2015) 1763-1767.
- [2] W.M. Hassan, E.M. Zayed, A.K. Elkholy, H. Moustafa, G.G. Mohamed, Spectroscopic and density functional theory investigation of novel Schiff base complexes, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 103 (2013) 378-387.
- [3] E.M. Zayed, G.G. Mohamed, A.M. Hindy, Transition metal complexes of novel Schiff base: Synthesis, spectroscopic characterization, and in vitro antimicrobial activity of complexes, Journal of Thermal Analysis and Calorimetry 120 (2015) 893-903.
- [4] R.M. Ramadan, A.K.A. Al-Nasr, A.F. Noureldeen, Synthesis, spectroscopic studies, antimicrobial activities and antitumor of a new monodentate V-shaped Schiff base and its transition metal complexes, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 132 (2014) 417-422.
- [5] C. Chang, W. Chen, Y. Chen, Y. Chen, Y. Chen, F. Ding, C. Fan, H.J. Fan, Z. Fan, C. Gong, Recent progress on two-dimensional materials, Acta Phys.-Chim. Sin 37(12) (2021) 2108017.
- [6] G.G. Mohamed, E.M. Zayed, A.M. Hindy, Coordination behavior of new bis Schiff base ligand derived from 2-furan carboxaldehyde and propane-1, 3-diamine. Spectroscopic, thermal, anticancer and antibacterial activity studies, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 145 (2015) 76-84.
- [7] H. Moustafa, G.G. Mohamed, S. Elramly, Spectroscopic studies, Density Functional Theory calculations, and non-linear optical properties of binuclear Fe (III), Co (II), Ni (II), Cu (II), and Zn (II) complexes of OONN Schiff base ligand, Journal of the Chinese Chemical Society 67(10) (2020) 1783-1793.
- [8] T. Khoo, bin Break MK, Crouse KA, Tahir MIM, Ali AM, et al.(2014) Synthesis, characterization and biological activity of two Schiff base ligands and their nickel (II), copper (II), zinc (II) and cadmium (II) complexes derived from S-4-picolylidithiocarbamate and X-ray crystal structure of cadmium (II) complex derived from pyridine-2-carboxaldehyde, Inorg Chim Acta 413 68-76.
- [9] E.M. Zayed, G.G. Mohamed, W.M. Hassan, A.K. Elkholy, H. Moustafa, Spectroscopic, thermal, biological activity, molecular docking and density functional theoretical investigation of novel bis Schiff base complexes, Applied Organometallic Chemistry 32(7) (2018) e4375.
- [10] E.A.J. Al-Mulla, Lipase-catalyzed synthesis of fattythioic acids from palm oil, Journal of Oleo Science 60(1) (2011) 41-45.
- [11] E. Wong, C.M. Giandomenico, Current status of platinum-based antitumor drugs, Chemical reviews 99(9) (1999) 2451-2466.
- [12] E.M. Zayed, A.M. Hindy, G.G. Mohamed, Molecular structure, molecular docking, thermal, spectroscopic and biological activity studies of bis-Schiff base ligand and its metal complexes, Applied Organometallic Chemistry 32(1) (2018) e3952.
- [13] M.I. Abou-Dobara, N.F. Omar, M.A. Diab, A.Z. El-Sonbati, S.M. Morgan, M.A. El-Mogazy, Allyl rhodanine azo dye derivatives: Potential antimicrobials target d-alanyl carrier protein ligase and nucleoside diphosphate kinase, Journal of Cellular Biochemistry 120(2) (2019) 1667-1678.

- [14] S.M. Morgan, A. El-Sonbati, M. El-Mogazy, Polymer complexes. LXX. Synthesis, spectroscopic studies, thermal properties and antimicrobial activity of metal (II) polymer complexes, *Applied Organometallic Chemistry* 32(4) (2018) e4264.
- [15] A. El-Sonbati, M. Diab, S.M. Morgan, A. Eldesoky, M. Balboula, Polymer complexes. LXIX. Some divalent metal (II) polymer complexes of potentially bidentate monomer N-[4-(5-methyl-isoxazol-3-ylsulfamoyl)-phenyl]-acrylamide: Synthesis, spectroscopic characterization, thermal properties, antimicrobial agents and DNA studies, *Applied Organometallic Chemistry* 32(3) (2018) e4207.
- [16] A. El-Sonbati, M. Diab, S.M. Morgan, H. Seyam, Supramolecular structures for determination and identification of the bond lengths in novel uranyl complexes from their infrared spectra, *Journal of Molecular Structure* 1154 (2018) 354-365.
- [17] A. El-Sonbati, M. Diab, S.M. Morgan, M. El-Mogazy, Polymer complexes. LXXIII. Synthesis, characterization, thermal properties, electron spin resonance study and antimicrobial activity of Cu (II) polymer complexes: Relation between representative Pascal constants and thermal activation energy of decomposition, *Applied Organometallic Chemistry* 32(11) (2018) e4530.
- [18] A. El-Sonbati, M. Diab, S.M. Morgan, M. Balboula, Polymer complexes. LXVIII. Spectroscopic studies of supramolecular copper (II) polymeric complexes of biologically active monomer derived from novel sulfa drug, *Applied Organometallic Chemistry* 32(2) (2018) e4059.
- [19] S.M. Morgan, M. Diab, A. El-Sonbati, Synthesis, spectroscopic, thermal properties, Calf thymus DNA binding and quantum chemical studies of M (II) complexes, *Applied Organometallic Chemistry* 32(5) (2018) e4281.
- [20] M.M. Khalaf, H.M. Abd El-Lateef, M. Gouda, F.N. Sayed, G.G. Mohamed, A.M. Abu-Dief, Design, Structural Inspection and Bio-Medicinal Applications of Some Novel Imine Metal Complexes Based on Acetylferrocene, *Materials* 15(14) (2022) 4842.
- [21] M. Diab, G.G. Mohamed, W. Mahmoud, A. El-Sonbati, S.M. Morgan, S. Abbas, Inner metal complexes of tetradentate Schiff base: Synthesis, characterization, biological activity and molecular docking studies, *Applied Organometallic Chemistry* 33(7) (2019) e4945.
- [22] A.Z. El-Sonbati, M.A. Diab, G.G. Mohamed, S.M. Morgan, Preparation, Characterization and Biological Activity Screening on Some Metal Complexes Based of Schiff Base Ligand, *Egyptian Journal of Chemistry* 64(8) (2021) 4125-4136.
- [23] E.M. Zayed, M.A. Zayed, A.M. Hindy, G.G. Mohamed, Coordination behaviour and biological activity studies involving theoretical docking of bis-Schiff base ligand and some of its transition metal complexes, *Applied Organometallic Chemistry* 32(12) (2018) e4603.
- [24] R. Anbazhagan, K. Sankaran, Syntheses, spectral characterization, single crystal X-ray diffraction and DFT computational studies of novel thiazole derivatives, *Journal of Molecular Structure* 1050 (2013) 73-80.
- [25] M. Abou-Dobara, N. Omar, M. Diab, A. El-Sonbati, S.M. Morgan, O. Salem, A. Eldesoky, Polymer complexes. LXXV. Characterization of quinoline polymer complexes as potential bio-active and anti-corrosion agents, *Materials Science and Engineering: C* 103 (2019) 109727.
- [26] S.M. Morgan, A. El-Sonbati, H. Eissa, Geometrical structures, thermal properties and spectroscopic studies of Schiff base complexes: Correlation between ionic radius of metal complexes and DNA binding, *Journal of Molecular Liquids* 240 (2017) 752-776.
- [27] E.M. Zayed, F.A. El-Samahy, G.G. Mohamed, Structural, spectroscopic, molecular docking, thermal and DFT studies on metal complexes of bidentate orthoquinone ligand, *Applied Organometallic Chemistry* 33(9) (2019) e5065.
- [28] A. El-Sonbati, M. Diab, S.M. Morgan, M. Abou-Dobara, A. El-Ghettany, Synthesis, characterization, theoretical and molecular docking studies of mixed-ligand complexes of Cu (II), Ni (II), Co (II), Mn (II), Cr (III), UO₂ (II) and Cd (II), *Journal of Molecular Structure* 1200 (2020) 127065.
- [29] G.G. Mohamed, A.A. El-Sherif, M.A. Saad, S.E. El-Sawy, S.M. Morgan, Mixed-ligand complex formation of tenoxicam drug with some transition metal ions in presence of valine: Synthesis, characterization, molecular docking, potentiometric and evaluation of the humeral immune response of calves, *Journal of Molecular Liquids* 223 (2016) 1311-1332.
- [30] Y.M. Ahmed, G.G. Mohamed, New Tin (IV) Schiff base complexes: synthesis, characterization and antibacterial investigation, docking and theoretical studies, *Inorganic Chemistry Communications* 144 (2022) 109864.
- [31] E.M. Zayed, G.G. Mohamed, H.A. Abd El Salam, Ni (II), Co (II), Fe (III), and Zn (II)

- mixed ligand complexes of indoline-dione and naphthalene-dione: Synthesis, characterization, thermal, antimicrobial, and molecular modeling studies, *Inorganic Chemistry Communications* 147 (2023) 110276.
- [32] E.M. Zayed, G. Mohamed, Synthesis, spectroscopic, DFT and docking studies, molecular structure of new Schiff base metal complexes, *Egyptian Journal of Chemistry* 65(1) (2022) 633-644.
- [33] E.M. Zayed, M.A. Zayed, H.A. Abd El Salam, G.A. Nawwar, Synthesis, structural characterization, density functional theory (B3LYP) calculations, thermal behaviour, docking and antimicrobial activity of 4-amino-5-(heptadec-8-en-1-yl)-4H-1, 2, 4-triazole-3-thiol and its metal chelates, *Applied Organometallic Chemistry* 32(12) (2018) e4535.
- [34] E.M. Zayed, M. Zayed, H.A. Abd El Salam, M.A. Noamaan, Novel Triazole Thiole ligand and some of its metal chelates: Synthesis, structure characterization, thermal behavior in comparison with computational calculations and biological activities, *Computational biology and chemistry* 78 (2019) 260-272.
- [35] L.M. Aroua, S.K. Alhag, L.A. Al-Shuraym, S. Messaoudi, J.A. Mahyoub, M.Y. Alfaifi, W.M. Al-Otaibi, Synthesis and characterization of different complexes derived from Schiff base and evaluation as a potential anticancer, antimicrobial, and insecticide agent, *Saudi Journal of Biological Sciences* 30(3) (2023) 103598.
- [36] N. Hassan, A. El-Sonbati, M. El-Desouky, Synthesis, characterization, molecular docking and DNA binding studies of Cu (II), Ni (II), Zn (II) and Mn (II) complexes, *Journal of Molecular Liquids* 242 (2017) 293-307.
- [37] M. Diab, S. Nozha, A. El-Sonbati, M. El-Mogazy, S.M. Morgan, Polymer complexes. LXXVIII. Synthesis and characterization of supramolecular uranyl polymer complexes: Determination of the bond lengths of uranyl ion in polymer complexes, *Applied Organometallic Chemistry* 33(10) (2019) e5153.
- [38] A. El-Sonbati, M. Diab, G. Mohamed, M. Saad, S.M. Morgan, S. El-Sawy, Polymer complexes. LXXVII. Synthesis, characterization, spectroscopic studies and immune response in cattle of quinoline polymer complexes, *Applied Organometallic Chemistry* 33(8) (2019) e4973.
- [39] G. Moustafa, E. Sabry, E.M. Zayed, G.G. Mohamed, Structural characterization, spectroscopic studies, and molecular docking studies on metal complexes of new hexadentate cyclic peptide ligand, *Applied Organometallic Chemistry* 36(2) (2022) e6515.
- [40] B.V. Kumar, H.B. Naik, D. Girija, N. Sharath, S. Pradeepa, H.J. Hoskeri, M. Prabhakara, Synthesis, DNA-binding, DNA-photocleavage profiling and antimicrobial activity of novel tetra-aza macrocyclic Ni (II), Co (II) and Cu (II) complexes constrained by thiadiazole, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 94 (2012) 192-199.
- [41] M. Diab, A. El-Sonbati, N. El-Ghamaz, S.M. Morgan, O. El-Shahat, Conducting polymers X: Dielectric constant, conduction mechanism and correlation between theoretical parameters and electrical conductivity of poly (N, N'-bis-sulphinyl p-phenylenediamine-2, 6-diaminopyridine) and poly (N, N'-bis-sulphinyl p-phenylenediamine-3, 5-diamine-1, 2, 4-triazole), *European Polymer Journal* 115 (2019) 268-281.
- [42] S.M. Morgan, S. Nozha, M. El-Mogazy, Supramolecular structures and applications of azo rhodanine complexes, LAP LAMBERT Academic Publishing Sunnyvale 2019.
- [43] H.A. Abd El Salam, G.G. Mohamed, E.M. Zayed, Synthesis, spectroscopic characterization, biological application and molecular docking studies of some transition metal complexes of isophthalamide ligand, *Journal of Molecular Structure* 1273 (2023) 134231.
- [44] M. Abou-Dobara, A. El-Sonbati, S.M. Morgan, Influence of substituent effects on spectroscopic properties and antimicrobial activity of 5-(4'-substituted phenylazo)-2-thioxothiazolidinone derivatives, *World Journal of Microbiology and Biotechnology* 29 (2013) 119-126.
- [45] A. El-Sonbati, A. Belal, M. El-Gharib, S.M. Morgan, Supramolecular structure, mixed ligands and substituents effect on the spectral studies of oxovanadium (IV) complexes of bioinorganic and medicinal relevance, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 95 (2012) 627-636.
- [46] N. El-Ghamaz, A. El-Sonbati, S.M. Morgan, Optical properties of some synthesized azo thin films, *Journal of Molecular Structure* 1027 (2012) 92-98.
- [47] S.M. Morgan, N. El-Ghamaz, M. Diab, Effect of the type of metal on the electrical conductivity and thermal properties of metal complexes: The relation between ionic radius of metal complexes and electrical conductivity, *Journal of Molecular Structure* 1160 (2018) 227-241.

-
- [48] H.A. Abd El Salam, G. Moustafa, E.M. Zayed, G.G. Mohamed, Isophthaloylbis (Azanediyl) Dipeptide Ligand and Its Complexes: Structural Study, Spectroscopic, Molecular Orbital, Molecular Docking, and Biological Activity Properties, Polycyclic Aromatic Compounds (2022) 1-23.
- [49] B. Shafaatian, Z. Ozbakzaei, B. Notash, S.A. Rezvani, Synthesis, characterization, single crystal X-ray determination, fluorescence and electrochemical studies of new dinuclear nickel (II) and oxovanadium (IV) complexes containing double Schiff base ligands, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 140 (2015) 248-255.
- [50] E.M. Zayed, M. Zayed, Synthesis of novel Schiff's bases of highly potential biological activities and their structure investigation, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 143 (2015) 81-90.