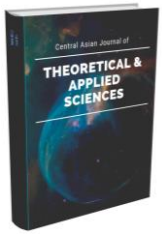

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Article

Synthesis, Characterization & Biological Survey of Novel 1,2,4-Triazole Schiff Base Derivatives

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Abstract: In the present study, a new ligand, 4-{[(1E)-1-(2-hydroxy-5-methyl-3 nitrophenyl) ethylidene]amino}-5-phenyl-2,4-dihydro-3H-1,2,4-triazole-3-thione (L) and synthesis of iron (III), copper (II) and red copper (III) complexes. By using techniques including FT-IR, 1H-NMR, mass, molar conductivity, and magnetic susceptibility, the ligand and its complexes were verified to be real. Researchers looked into the compounds' antibacterial activities against the Gram-positive and Gram-negative bacterial strains of Staphylococcus aureus and Pseudomonas aeruginosa. The ligand's bioavailability investigations and its complexes showed good results compared to a standard antibiotic (ampicillin). Theoretical calculations were performed using the Hyperchem program and the electrostatic potential was studied using a semiempirical approach, which provided good information about the location of the complex. In addition, the stabilization energies of the complexes were studied. Based on the magnetic susceptibility and molar conductivity results, for the Cr(III) and Fe(III) complexes, we suggest an octahedral geometry, and for the Cu(II) complex, a tetrahedral geometry.

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1. Introduction

Triazole derivatives are a significant class of heterocyclic systems that are nitrogen-rich and have been the focus of much research recently [1-4]. Many promising and important structures are used in the synthesis and design of pharmaceutical compounds Triazole nuclei only exist in two isomeric states and contain three nitrogen atoms. 1,2,3-triazole and 1,2,4-triazole. Triazole compounds were first prepared by Fisher in 1878. Triazole derivatives' all-encompassing qualities have piqued interest [5-7]. 1,2,4-Triazole has a variety of different biological activities, such as antidepressants [8], antibacterial drugs [9], antiasthmatic drugs [10], antituberculosis drugs [11], antiviral drugs [12], and anticancer drugs [13]. Anti-inflammatory [14], antispasmodic [15], analgesic [16], insecticide and plant growth regulator [17]. Antioxidants [18] 1,2,4-Triazole is basic structure for a variety of interesting things of therapeutic drugs, such as etizolam [19], alprazolam [20], anastrozole [21], etrozole, voriconazole [22], voriconazole, and cycloconazole [23]. 1,2,4-Triazole derivatives also play an important role in synthetic

chemistry. For example, they are used to synthesize biologically active compounds of heterocyclic rings In addition to Schiff bases [24], Mannich bases [25], triazolothiadiazoles [26], thioureas [11, 27], thioethers [24, 28], etc. Triazole has two isomers: 1H-1,2,3-triazole and 1H-1,2,4-triazole. The two tautomeric forms of 1,2,4-triazole, 4H-1,2,4-triazole and 1H-1,2,4-triazole, are important pharmaceutical nucleophiles, as shown in Figures [28, 29]. 1) Fungal and bacterial infections have become serious medical challenges for humans because nitrogen donor compounds have biological activities such as anticancer and antifungal effects [30]. It has been observed that triazole derivatives exhibit excellent antibacterial activity in vitro [31].

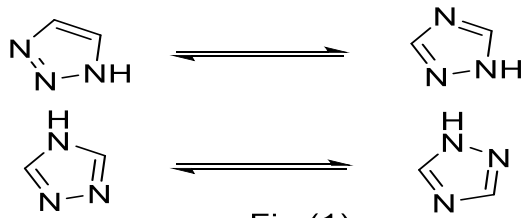


Fig (1)

2. Materials and Methods

1. Experimental

Both the chemical substance and its solvents were completely free of any impurities. before use. All metal salts were used in the form of chlorides.

1.1. Physical measurements

The melting points of the synthesized ligands and their complex compounds of metal which specified using the capillary method in an electrothermal melting point apparatus. FTIR spectra in the range of (4000-200) cm-1 were recorded as CsI slices using a Shimadzu spectrophotometer. NMR spectra acquired with a Bruker spectrometer DXR system AL500 (500 MHz) of ligand and Shimadzu DXR system AL250 (250 MHz) of coplexes. (Network Mass Selective Detector 5973) was used to obtained Mass spectra.

1.2. Synthesis of ligands

The ligand was prepared as 4-{[(1E)-1-(2-hydroxy-5- methyl-3-nitrophenyl) ethylidene] amino}-5 phenyl-2,4-dihydro-3H-1,2,4-triazole 3-phosphothioate. was ready in the manner described below.

1.2.1. 2-hydroxybenzoylhydrazide (A) synthesis

Hydrazine monohydrate (0.1 mol, 5 mL) and methyl 2-hydroxybenzoate (0.1 mol, 16.6 mL) were combined in 100 mL of anhydrous ethanol. For ten hours, the mixture was refluxed. The resultant substance partially evaporated. The final chemical, compound (A) 2-hydroxybenzoylhydrazide, white, melting point 118 °C, yield 90%, was obtained by cooling, filtering, and washing with ethanol [32].

1.2.2. Synthesis of [2-(2-hydroxybenzoyl)hydrazine] disulfide potassium (B)

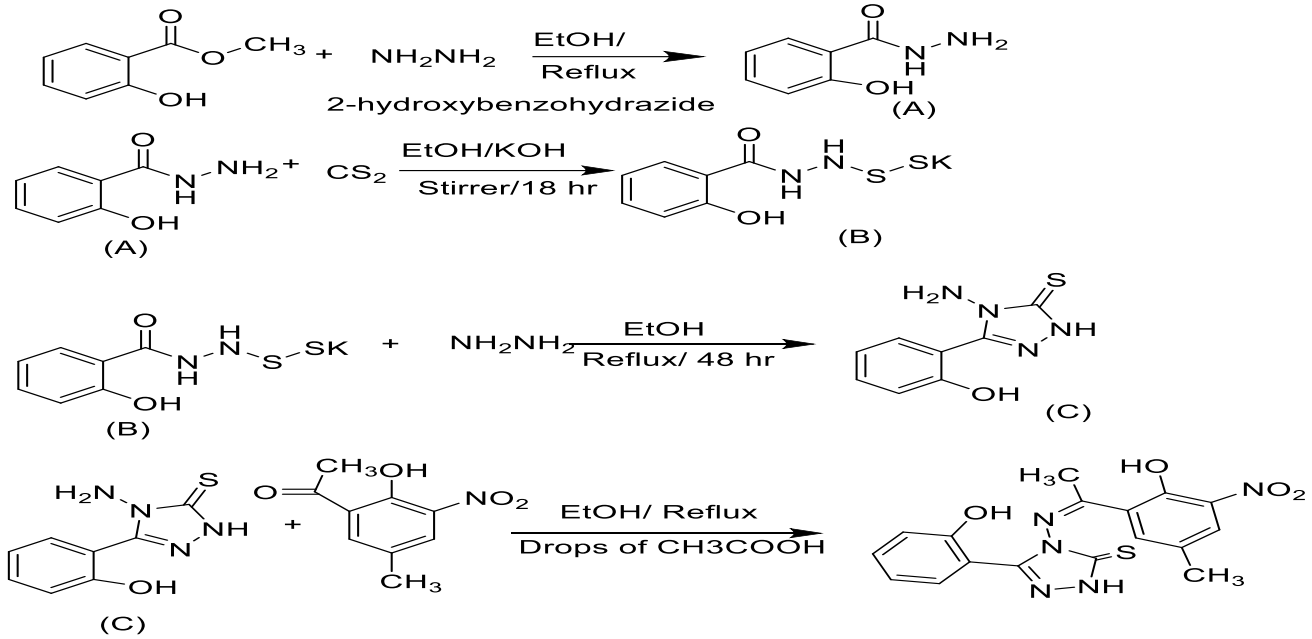
Mix 2-hydroxybenzoylhydrazide (A) (0.01 mol, 15.2 g) with (0.1 mol, 5.6 g) potassium hydroxide (KOH), dissolved in (50 ml) ethanol, and then add carbon disulfide (CS2) (0.1 mol, 7.5 mL) and cool the mixture to 0°C before adding. The mixture was stirred at 25° C. for 18 hours. The resultant was dried to obtain a yellowwhite product, potassium [2-(2-hydroxybenzoyl)hydrazino]disulfide (B).

1.2.3. Synthesis of 2-(4-amino-5-sulfanyl-4H-1,2,4-triazol-3-yl) Phenol (C)

Potassium [2-(2-hydroxybenzoyl)hydrazinyl]disulfanide (B) (2.54 g, 0.01 mol), hydrazine monohydrate (0.01 mol, 0.5 ml), and water (50 ml) were combined, and the mixture was refluxed for 46 hours, then cooled and filtered. Add (50) of water to the product, which is acidified with HCl (10%) to produce white crystals that are 2-(4-amino-5-sulfanyl-4H-1,2,4-triazol-3-yl) Phenol. The product's melting point is 83% of the product's melting point, which is 215 degrees Celsius.

1.2.4. Synthesis (Z)-4-((1-(2-hydroxy-5-methyl-3 nitrophenyl) ethylidene) amino)-5-(2-hydroxyphenyl)-2,4- dihydro-3H-1,2,4-triazole-3-thione (L)

The ligand was created by combining (4,6 g, 0.012 mol) of 2-(4- amino-5-sulfanyl-4H-1,2,4-triazol-3-yl) Phenol (C) and (1)-(2- hydroxy-5-methyl-3-nitrophenyl) (2.5 g, 0.012 mol) in absolute alcohol (50 ml). The mixture was heated under reflux for (3 hours). The yellowish precipitate of the ligand was formed, it was then filtered, washed with cold alcohol, and re-purposed in cold alcohol. (solid, yellow, melting point 248 °C, yield 80%) [33]. Fig. (2).



Fig(2)

1.3. The preparation of complexes

The salts of the transition elements $FeCl_3.6H_2O$, $CrCl_3.6H_2O$ and $CuCl_2.6H_2O$) (0.001 mol) were incorporated separately with the ligand (0.385 g, 0.001 mol) in ethanol the mixture was heated for three hours while refluxed. After filtering, the product was cleaned with pure ethanol as shown in figure (3).

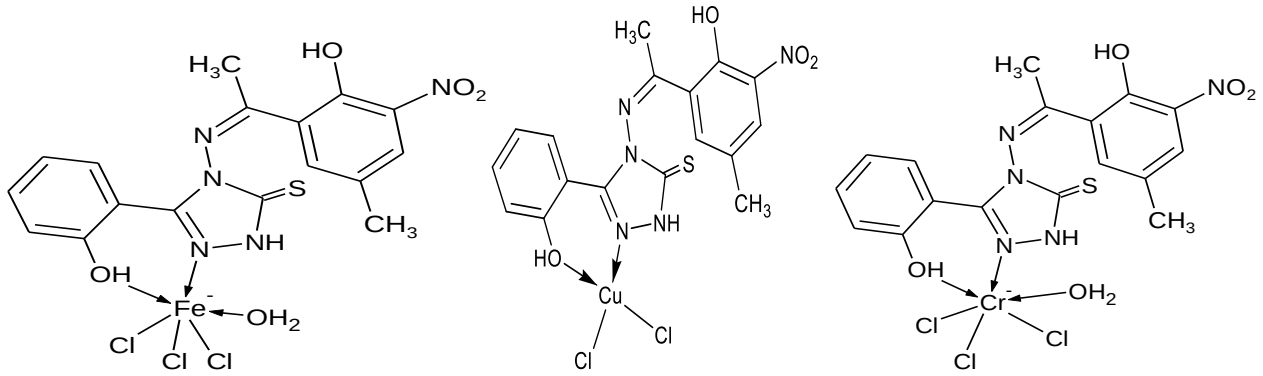


Fig (3)

3. Results and Discussion

3.1. Physical Properties, Magnetic Susceptibility and Molars Conductivity

Table 1. The physical, molar conductivity, and magnetic properties

No.	Compound	Colour	M(g/mol)	ʌ s cm² mol⁻¹	M.p ⁰C	μeff. B.M
1	$C_{17}H_{15}N_4O_4S$	yellow	385	……	248	……
2	[Fe(L_1) Cl_3. H_2O]	brown	565	10.64	193	2.3
3	[Cr(L_1) Cl_3.H_2O]	yellow	560	11.12	210	3.73
4	[Cu(L_1) Cl_2] . H_2O	green	537	14	245	1.9

3.2. Infrared Spectrum (FT-IR)

There were nine main bands visible on the free ligand (L) at (3298), (3193), (3091-3027), (2914),(1619),(1541), and (1496). These bands are attributed to the free molecule and the number of bands is considered as an indication of the number of conformations that the molecule may have adopted. These are in agreement with (υOH), Table (2) and Figure (5) list (υN-H), (υC-H aro), (υC-H Elaph), (υC=N)oxo, and (υC=N) end. New bands that matched the bonded (M-N), the area (682-686 cm-1, and the (M-Cl) displayed at the region were formed (304-327) cm^{-1}. As illustrated in figure (11-14) and table (2).

Table 2. Ligand and its complexes infrared spectra (υ cm^{-1})

Assignment	Wave number (cm^{-1})			
	L1	Fe	Cu	Cr
OH	3298	3298	3271	3298
NH	3193	3194	3116	3194
Ar(C-H)	3091-3027	3109	3055	3055
Elf(C-H)	2914	2943	2966	2943

Azo(C=N)	1619	1631	1639	1631
Het(C=N)	1541	1531	1531	1531
(C=C)	1496	1481	1458	1450
Asy(C-O-O)	1241	1229	1230	1319
Sym(C-O-C)	1067	1072	1010	1072
M-N	-------	686	682	686
M-Cl	--------	324	304	327

3.3. Nuclear Magnetic Resonance

Data from the 1HNMR spectra of the ligand (L) was demonstrated in figure (15). The spectrum exhibited two signals at (2.52 and 3.55 ppm) attributed to (DMSO), water, respectively. The spectrum also exhibited a third signal at (3.71 ppm, 3 H) attributed to the methyl group. Also, signals were observed at the (7.54-7.86 ppm,m,6H) return to protons at the Azomethine and aromatic regions. The spectrum is characterized by the presence of signals at (10.13 ppm and 10.84 ppm, 2 H) due to protons of two different groups of hydroxyl, a signal at (14.31 ppm, s,1H) due to N-H [34, 35] as depicted in figure (15).

3.4. Mass Spectra

The ligand's mass mass spectrum is 385 m/z, this is the molecular peak that is associated with the molecular formula $C_{16}H_{15}N_5O_4S$(L) and the base spectrum in 10 m/z that returns to [C15H7N4OS].+. The spectra demonstrated another prominent peak at 368 m/z, 275 m/z, 192 m/z, 177 m/z, 152 m/z, 121 m/z, 93 m/z and 76 m/z. Assigned to the subsequent fragments $[C_{17}H_{14}N_5O_3S]^{\cdot+}$,$[C_{15}H_7N_4S]^{\cdot+}$, $[C_9H_9N_2O_3]^{\cdot+}$, $[C_8H_6N_2O_3]^{\cdot+}$ and $[C_7H_6NO_3]^{\cdot+}$ respectively.

The mass spectrum of the complex's Fe(III) content exhibits peaks at 565 m/z that are associated with the molecular ions $[Fe(L)Cl_3.H_2O]^{\cdot+}$. The spectrum of the complex exhibits a series of peaks at 546 m/z that are attributed to the loss of one water molecule, 512 m/z, 476 m/z and 441 m/z that are attributed to the loss of the tree's chloride atoms, respectively. The mass spectrum of the Cr(lII) complex showed a fragment peak at 561 m/z corresponding to $[Cr(L)Cl_3.\ H_2O].H_2O^{\cdot+}$, showing the corresponding molecular ion peak. The complex exhibited One water molecule is lost, causing fragmentation to peak at 543 m/z. and at 507 m/z, 473 m/z, and 437 m/z as a result of the two chlorine atoms being lost, respectively, Peaks due to the desorption of water molecules and chlorine atoms were observed at 411 m/z and 385 m/z in the spectrum, respectively, while the mass spectrum of the Cu(II) complex showed a molecular ion peak corresponding to $[Cu(L)Cl_2].H_2O^{\cdot+}$ at 520 m/z. The spectra showed fragmentation peaks at 484 m/z and 447 m/z due to the loss of chlorine atoms, respectively, as shown in Figures (16-19).

3.5. Magnetic Susceptibility

The magnetic susceptibilities (μeff B.M) of the metal ions listed in Table 1 give details regarding the complexes' central ions' electrical structure. the Fe(III) complex's (μeff B.M) value is 2.3 BM, which indicates the presence of an octahedral shape orbital contribution.

the (μeff B.M) value for Cr(III) is 3.73 BM and this value refers to the octahedral shape. 1.9 BM of Cu(II) is attributed to the tetrahedral structure [20].

3.6. Antimicrobial Activity

The antimicrobial activity test was performed using the Andrews-based disk diffusion method: 10 mg of Sterile paper disks with a diameter of 6 mm were coated with the ligand and its complexes that had been dissolved in DMSO. After that, the discs were vacuum-dried at 40°C to remove the solvent. The discs were set on top of a Mueller-Hinton agar-infected petri dish. For twenty-four hours, the infected plates were incubated at 37°C. By measuring the zone of inhibition, which includes the discs, against the test microorganisms, antimicrobial activity was assessed. The ligands and their complexes were screened for antibacterial activity against Staphylococcus aureus and Pseudomonas aeruginosa compared to ampicillin, and all test compounds showed moderate to good antibacterial activity at concentrations of 15 mg/mL, as shown in Figures (4), (5) and Table (3).

Figure 4. Antimicrobial of ligand and its complex against Staphylococcus

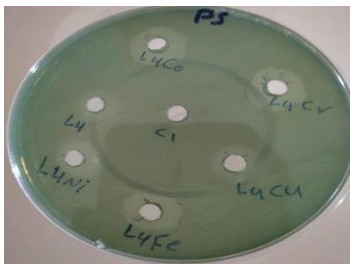


Figure 5. Antimicrobial of ligand and its complex against pseudomonas

Table 3. Antibacterial data

Compound	Inhibition zone (mm) Staphylococcus aureus	Inhibition zone (mm) pseudomonas aeruginosa
Ligand (L)	6	8
(L)Cr	12	18
(L)Fe	8	17
(L)Cu	17	11
Ampicillin	8	0
DMSO	0	0

3.7. Electrostatic Potential (MEP). Molecular.

Using the Hyperchem 8.02 program, we drew the optimized structures of the ligands and produced the electrostatic potentials, which are thought to be crucial for determining the free ligands' active sites. As seen in Figure (6-10), we found tetrahedral for Cu(II) complexes and octahedral for Cr(III) and Fe(III) complexes.

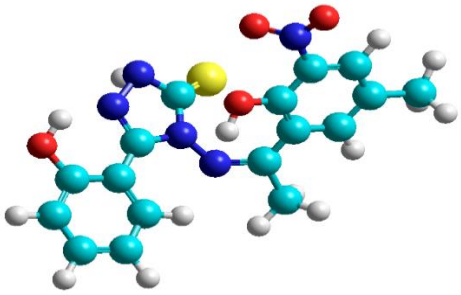


Figure 6. Ligand

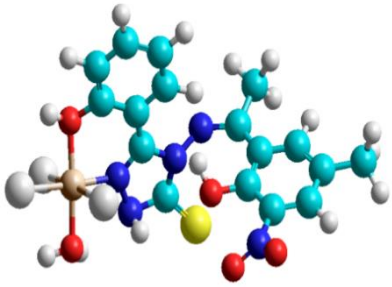


Figure 7. [$LFeCl_3H_2O$]

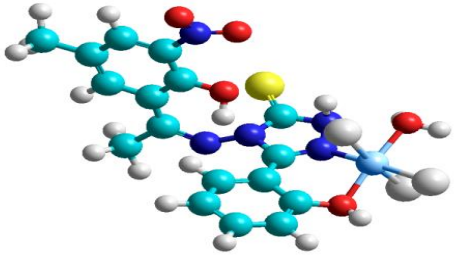


Figure 8. [$LCrCl_3H_2O$]H_2O

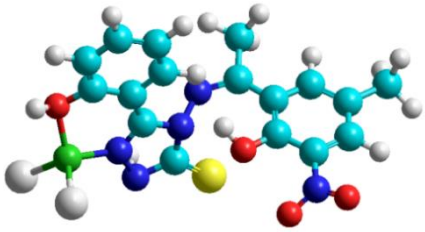


Figure 9. [$LCuCl_2$]

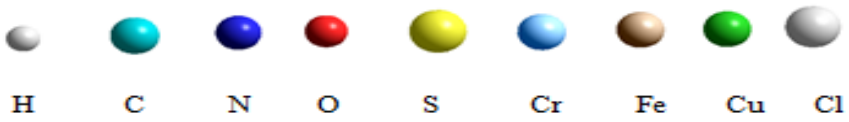


Figure 10

4. Conclusion

In the paper, a new triazole derivative ligand was synthesized and characterized. mass spectrum, it was confirmed that the prepared ligand is bidentate. From the theoretical study and determination of the electronic density distribution, the binding sites were determined, which were identical to the shift of the bands resulting from the complexation, in addition to determining the geometric shape of each of the chromium and iron complexes as octahedral, while for copper, it is tetrahedral. As for the electrical properties, through measuring the electrical conductivity, it was proven that all complexes are non-electrolytic. As for the biological activity against bacteria, the chromium and copper complexes showed clear inhibition against bacteria, about twice the inhibition of ampicillin used as a control against *Staphylococcus aureu* bacteria, and the ligand showed inhibition close to the inhibition of the control against *Staphylococcus aureu*. The ligand and complexes also showed very large inhibition compared to the effect of ampicillin on *pseudomonas aeruginosa* bacteria.

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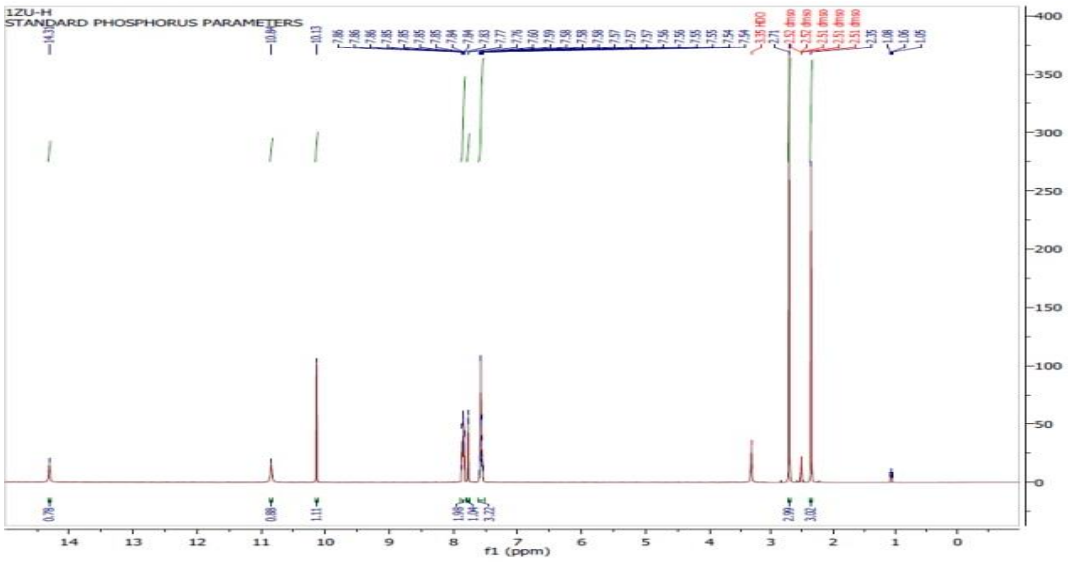
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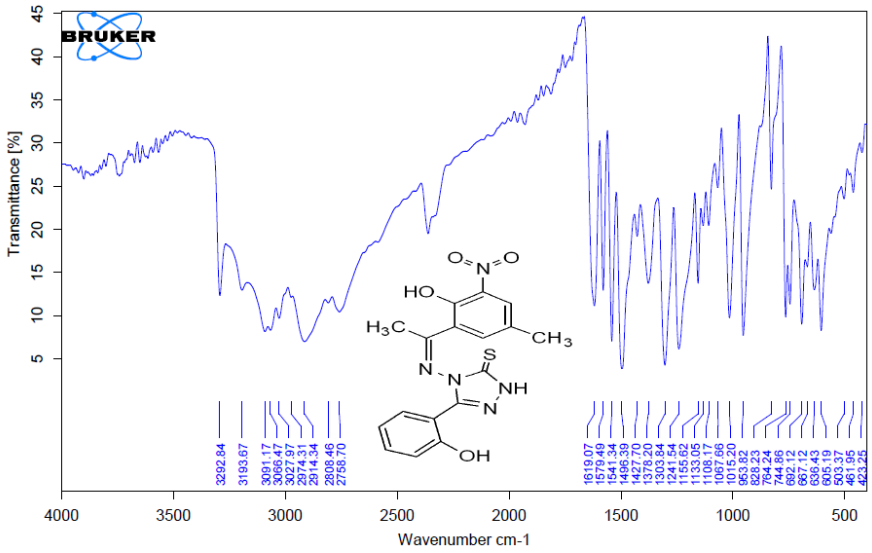
f1 (ppm)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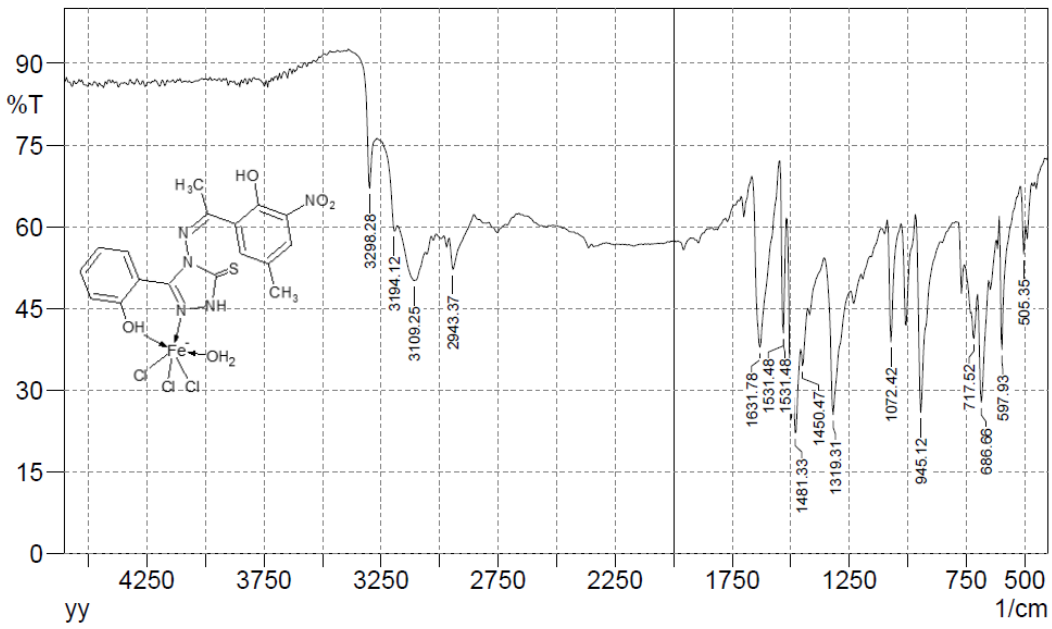
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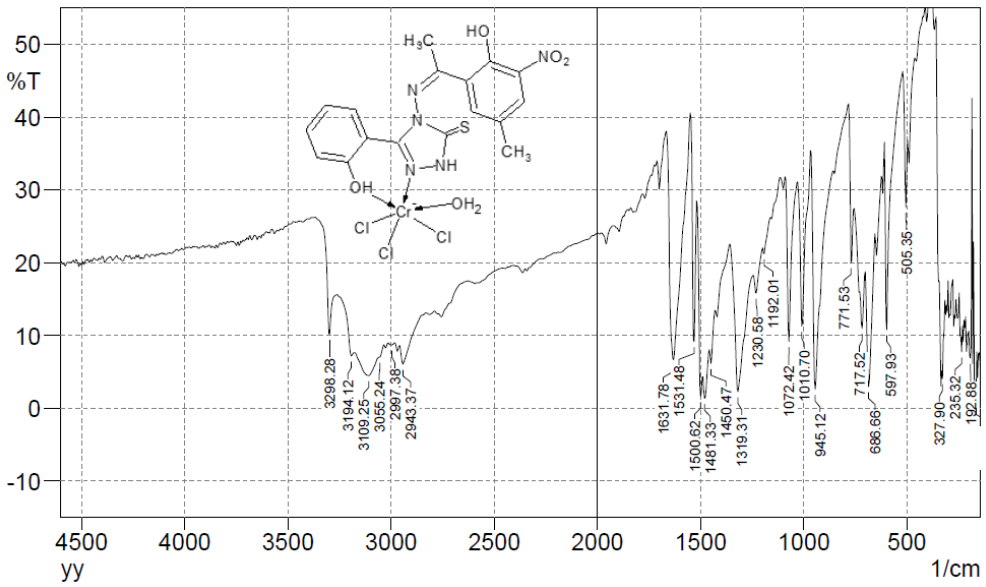
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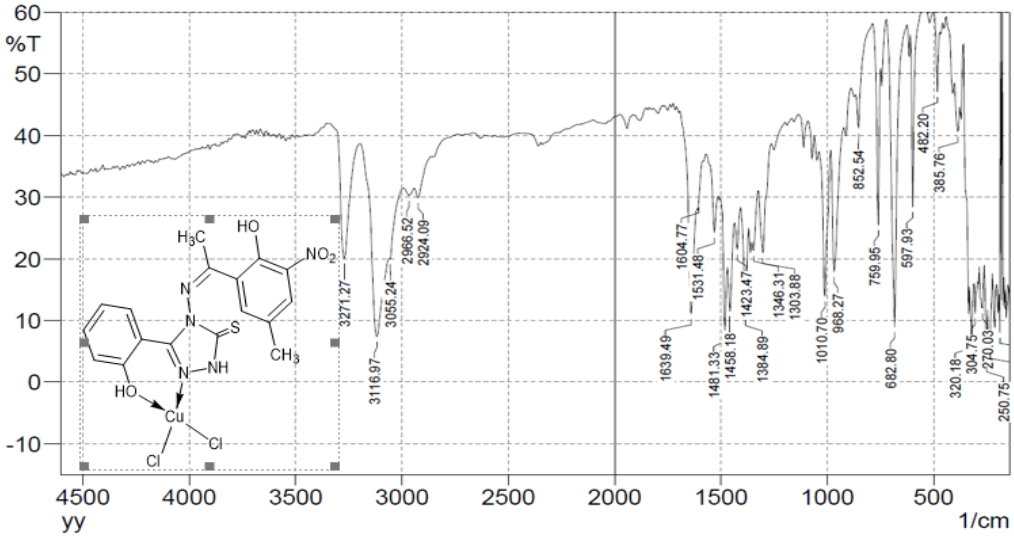
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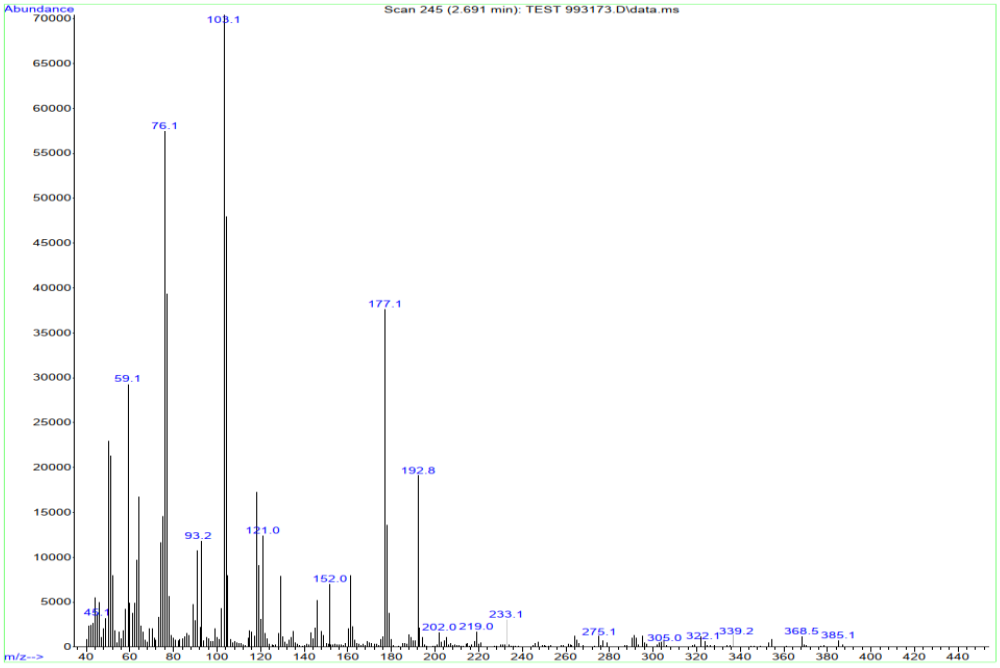

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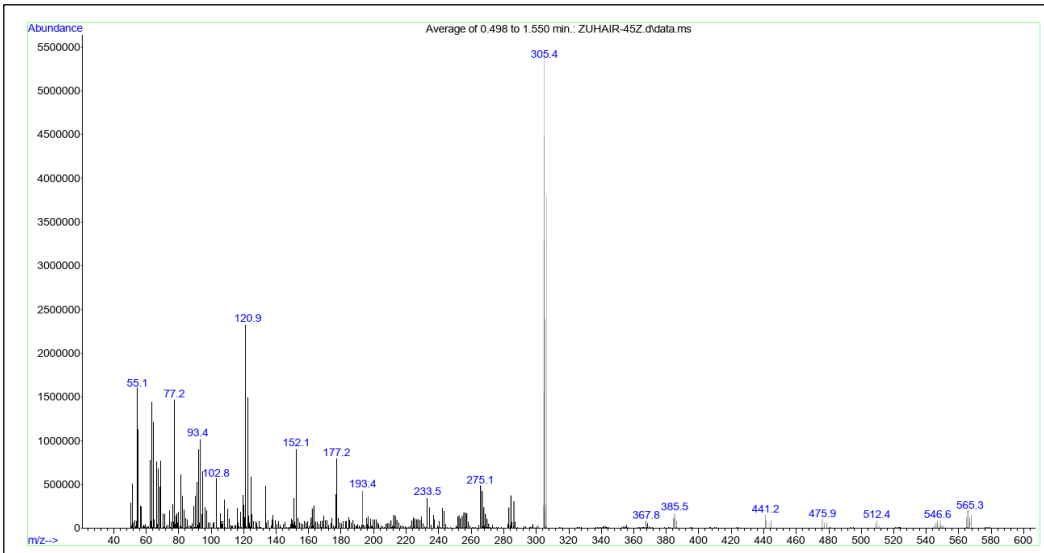

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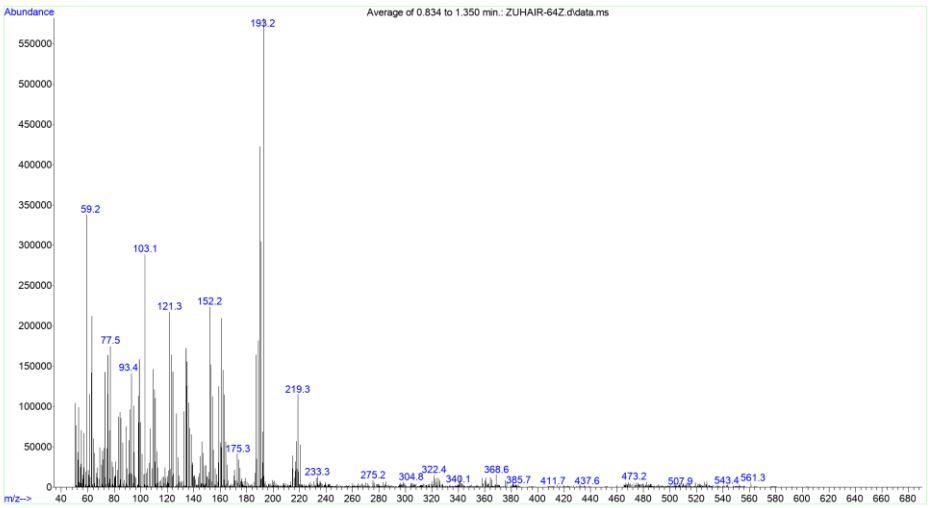

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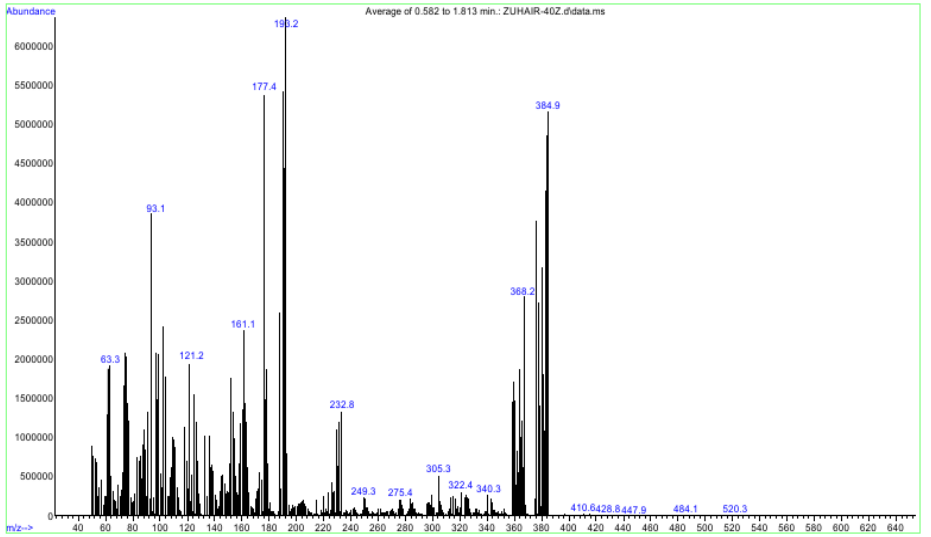

[LCuCl$_2$]