

“Synthesis, Characterization, and evaluation of the bioefficacy of the Hg(II) complex with a mixed of hydrazinyl benzothiazole and phosphine (dppm) ligands ”

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Abstract :

The ligand was prepared in two steps and was a mixture of hydrazinayl, benzothiazole and methoxybenzaldehyde and the solvent was used in the first step ethanol and the second step methanol. Some complexes consisting of mercury(II), ligand and phosphine (dppm) were present, the complex $[Hg(L)_2(\kappa^1\text{-dppm})Cl]Cl$ where one mole of each mercuric chloride and phosphine (dppm) and a molle of ligand and the solvent was ethanol, and the complex was attended in a way, which is taking two moles of ligand and metal halide and a mole of phosphine where phosphine is a bridge ligand and is bound to mercury and the solvent was methanol , $[Hg_2(L)_2(\mu\text{-dppm})Cl_2]Cl_2$. The complexes were charactrizis with infrared spectroscopy, ultraviolet spectroscopy, nuclear magnetic resonance spectrometry, electrical conductivity, melting point measurement, scanning electron microscopy, X-ray diffraction spectra, and X-ray energy dispersion spectroscopy. The bacterial activity of the complexes on negative and positive bacteria, and molecular anchoring was measured .

Keywords: 2-Hydrazinobenzothiazole , FTIR , UV, NMR, Sem, XRD, EDX, Biological activity, docking.

“تحضير وتشخيص وتقييم الفعالية الحيوية لمعقد الزئبق (II) مع مزيج من ليكاندات الهيدرازينايل بنزو ثيازول والفوسفين” (dppm)

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مستخلص:

تم تحضير الليكاند في خطوتين وكان عبارة عن مزيج من الهيدرازينايل والبنزو ثيازول والميثوكسي بنزالدهيد وتم استخدام المذيب في الخطوة الاولى من الايثانول وفي الخطوة الثانية المذيب ميثانول . وحضر بعض المعقدات المكونة من الليكاند وفلز الزئبق (II) والفوسفين (dppm)، حيث تكون المعقد $[Hg(L)_2\eta^1(dppm)Cl_2]$ الذي تم تحضيره من تفاعل مول واحد من كل من كلوريد الزئبق (II) والفوسفين (dppm) ومولين من الليكاند وكان المذيب الايثانول وتكونت بلورات لونها اخضر. حيث تكون المعقد $[Hg_2(L)_2(\mu\text{-dppm})Cl_2]Cl_2$ الذي تم تحضيره من تفاعل مولين من كل من كلوريد الزئبق (II) والفوسفين (dppm) و الليكاند وكان المذيب الميثانول وتكونت بلورات لونها بني. تم تشخيص المعقدات باستخدام التحليل الطيفي للأشعة تحت الحمراء ، التحليل الطيفي للأشعة فوق البنفسجية ، قياس الرنين المغناطيسي النووي ، التوصيل الكهربائي، قياس درجة الانصهار، المجهر الالكتروني الماسح أطياف حيود الأشعة السينية ، مطيافية تشتت الطاقة بالأشعة السينية ، وتم قياس النشاط البكتيري والارساء الجزيئي للمعقدات على البكتيريا السالبة والموجبة.

الكلمات المفتاحية: 2 -هيدرازينو بنزو ثيازول ، طيف الأشعة تحت الحمراء ، طيف الأشعة فوق البنفسجية، أطياف الرنين النووي المغناطيسي ، المجهر الالكتروني الماسح ، أطياف حيود الأشعة السينية ، مطيافية تشتت الطاقة بالأشعة السينية ، بس (ثنائي فنييل فوسفينو) ميثان ، الفعالية الحيوية ، الارساء الجزيئي.

1- Introduction

Benzothiazole is one of the heterocyclic organic compounds that have importance in biological activity and plays an important role in the medical field, especially in pharmacy and the drugs used in it, as the compensated benzothiazole rings are of great importance in the chemical formula of drugs used in the treatment of many diseases, as they showed their vital effectiveness against fungi^[1], against microbes^[2], against cancerous tumors^[3] and against malaria^[4], in addition to its vital effectiveness against viruses and worms^[5] and anti-inflammatory^[6] and antibacterial^[7]. Benzothiazole derivatives are also used in solvent extraction^[8] and are used as an organic reagent in chemical analysis^[9]. The compound 2-hydrazino benzothiazole, which belongs to the class of heterocyclic compounds (benzothiazole) and compensated at the site (2) hydrazine group and the compound 2-hydrazino benzothiazole with methoxybenzaldehyde proved its effectiveness against bacteria^[10]. Benzothiazole and hydrazino benzothiazole are among the Schiff bases due to the presence of the formula (HC=N)

^[11] In general, Schiff bases are solid and crystalline^[12] and have many uses, including as pigments^[13], catalysts^[14] and polymeric stabilizers.^[15] And also in optical applications such as light-emitting organic diodes^[10]. The mercury ion (II.) ^[16] is a toxic ion, so caution must be exercised when it is handled and is present in human blood at a concentration of 0.007 mg/L. The researchers were able to estimate mercury ion spectrally in biological models. For both urea and blood in humans^[17]. Research objective A number of Hg(II) ligand [2-(2-(4-methoxy benzyldiene) hydrazineyl)benzo[d]thiazole] complexes and tertiary phosphates were prepared, diagnosed and studied their biological efficacy.

2- Experimental

All chemicals and solvents necessary for the preparation of complexes were provided and used without purification. The melting point was measured on the automatic melting point device (SMP30). The conductivity of a solution of concentration ³⁻¹⁰ of DMSO was measured using the digital conductivity meter (Starter 3100c) Spectra were recorded. Infrared ra-

diation for compounds as disk KBR tablets using Shimadzu FTIR 8400S spectrophotometer (4000-400 cm) and nuclear magnetic resonance spectra was obtained on the Bruer 400 MHz spectrometer in DMSO as a solvent measuring electron spectroscopy using a device (200-900nm), was measured scanning electron microscope was measured at degree of magnification up to half a million times, and X-ray diffraction spectra were measured to know the crystal size of nanomaterials, X-ray energy dispersion spectroscopy for analyze elements to determine their chemical properties.

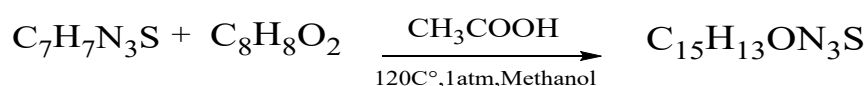
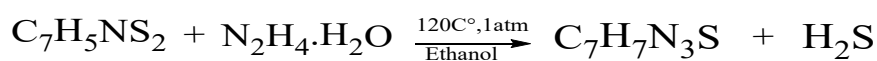
2-1-Methods

2-1-1-Preparation of the Ligand(2-(2-(4-methoxybenzylidene (hydrazineyl) benzo[d]thiazole)

Of aqueous (1.494ml 0.029mol) hydrazine was added in a glass conical flask and (5.00g,0.029mol) of 2-Mer-

capto benzothiazole The mixture refluxion at a temperature of (120°C) after (20) minutes, the color turned from yellow to dark brown and the appearance of the smell of (H₂S) and a brown foam was formed, then (8 ml) of ethanol was added, then the refluxion was completed for (5) hours, then the result was filtered and a light yellow precipitate was formed, washed with cold ethanol and dried at room temperature(g3.13, 63%,163-166°C M.P).

A warm solution of 2-hydrazino-benzothiazole (3.00g,0.018mol) in (20ml) of methanol was added to a solution of 4-methoxybenzaldehyde (2.47ml,0.018mol) in (5ml) of methanol with some drops of ice Acetic acid, the mixture was refluxion for 3 hours at (100°C), then the yellow precipitate was filtered, washed with cold methanol and then dried at laboratory temperature. (170-173°C M.P,80.1%, 3.9g).



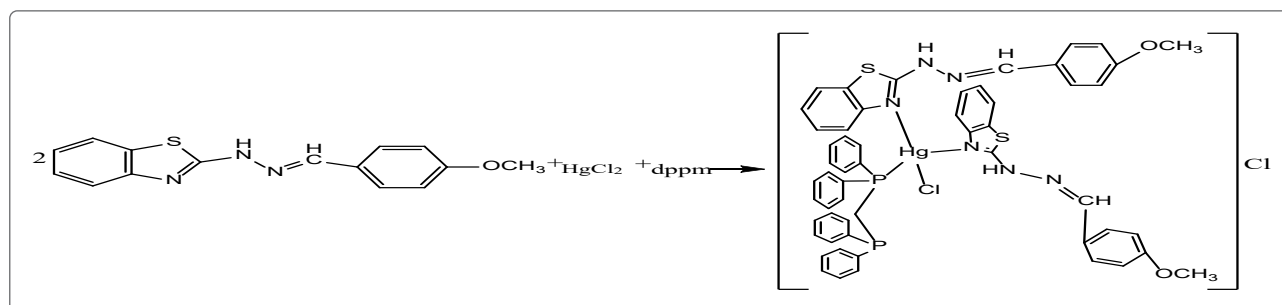
2-1-2-Synthesis of the complex [Hg(L)₂(κ¹-dppm)Cl]Cl

A solution of ligand (L) (0.158g,

0.56mmol) was added in (5ml) of absolute ethanol to a solution of HgCl₂ (0.071 g, 0.28mmol) in (5ml) of ab-

solute ethanol The mixture refluxion for an hour at a temperature of (100°C) and added to it (0.107g, 0.28mmol) from dppm and refluxion for three hours at a temperature of (120°C), the solution of the final mixture was left to

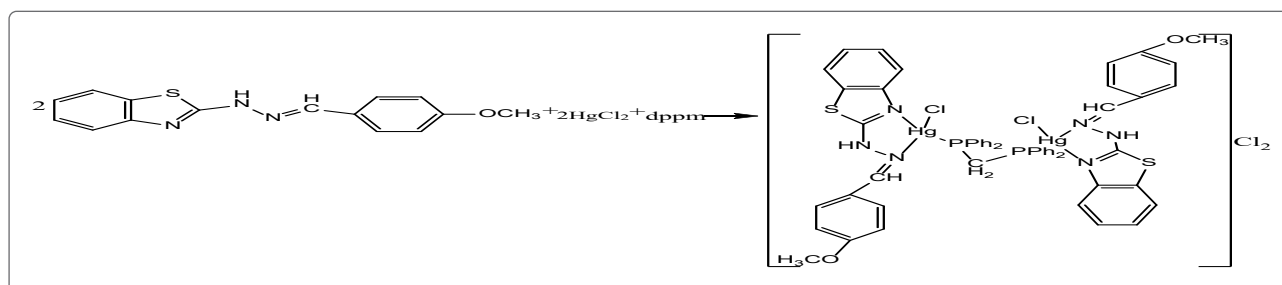
evaporate at room temperature in half, then filtered, washed with cold ethanol and dried at room temperature to evaporate and yellowish-green crystals were formed. (g0.4, 95.82%, M.P 190-193°C).



2-1-3-Synthesis of the complex $[Hg_2(L)_2(\mu-dppm)Cl_2]Cl$

A solution of ligand (L) (0.158g, 0.56mmol) was added in (7ml) of absolute methanol to a solution of $HgCl_2$ (0.152g, 0.56mmol) in (7ml) of absolute methanol The mixture refluxion for an hour at a temperature of (80°C) and added (0.107g, 0.28mmol) from

dppm and refluxion for three hours at a temperature of (100°C), the final mixture solution was left to evaporate at room temperature in half, then filtered, washed with cold methanol and dried at room temperature to evaporate and formed light brown crystals. (0.37g, 90.1%, M.P180-183°C).



3- Results and discussion

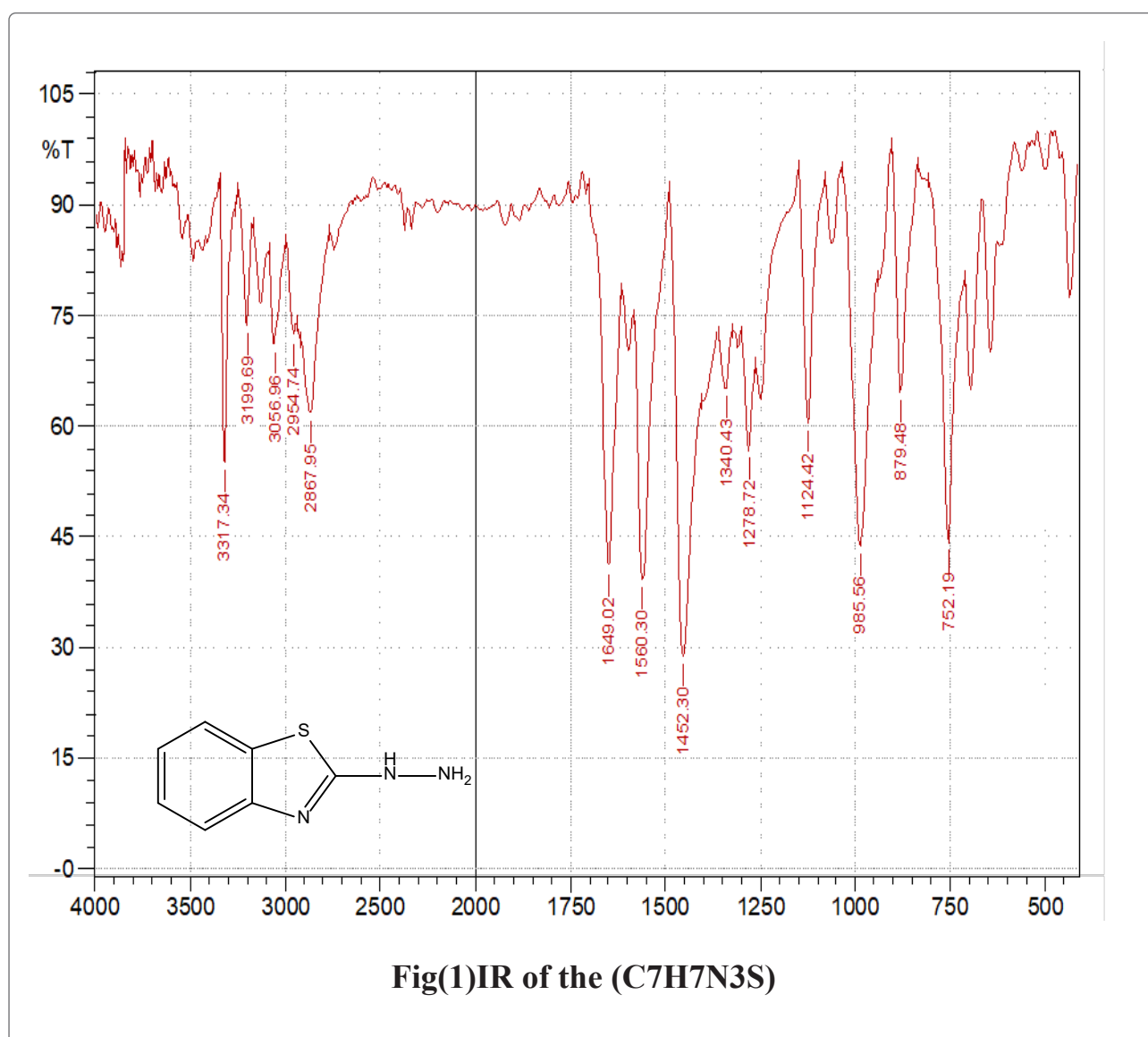
3-1- FTIR

The infrared spectrum of 2-hydrazino benzothiazole showed a beam at

frequency ($3317cm^{-1}$) belonging to the stretching of the $\nu(NH_2)$ group^[18], the appearance of a beam at ($3199cm^{-1}$) which is due to the stretching of the

$\nu(\text{NH})$ group^[19], the appearance of a beam at (3056cm^{-1}) belonging to the extension of the $\nu(\text{C-H})$ aromatic group^[19], the appearance of a beam at (1649cm^{-1}) belonging to the stretching of the $\nu(\text{C}=\text{N})$ group^[19], the appearance of a beam at (1560cm^{-1}) returning to the stretching of the $\nu(\text{C}=\text{C})$ group^[20], the appearance of a beam at (1452cm^{-1}) re-

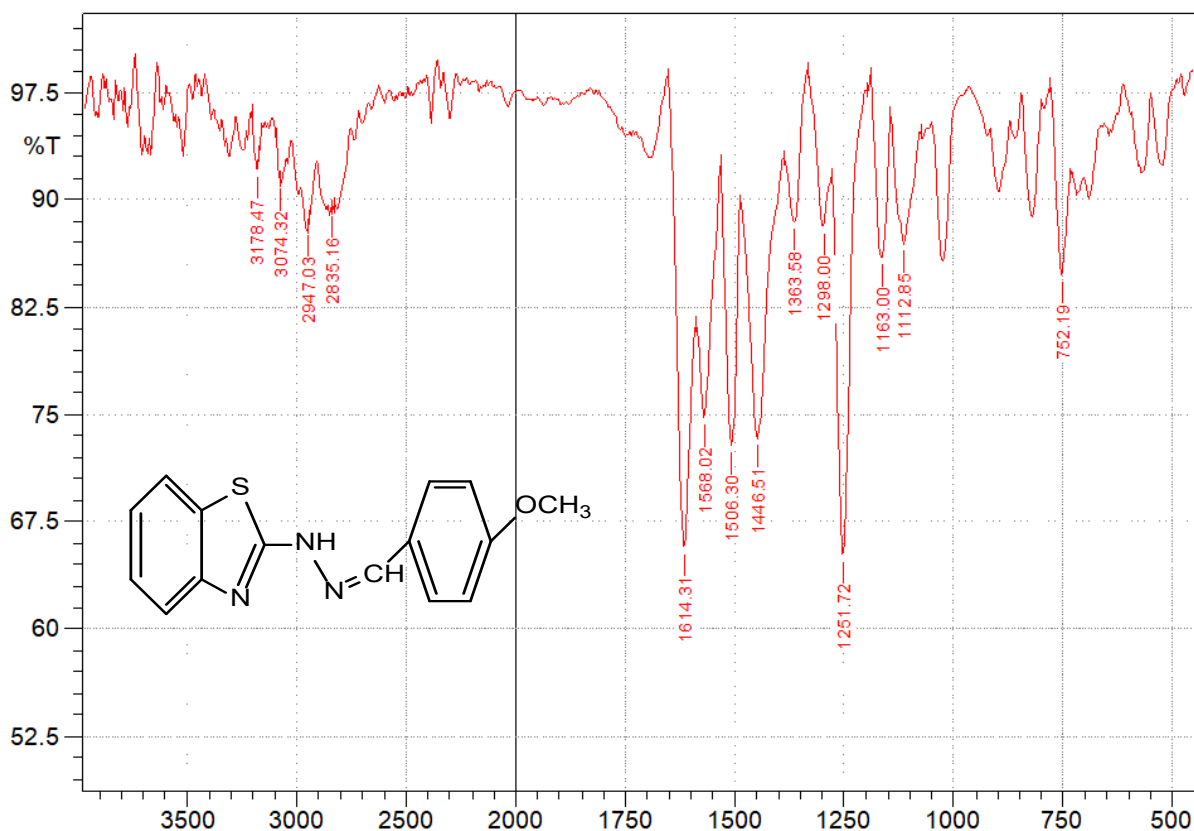
turning to the stretching of the $\nu(\text{C}=\text{N})$ group^[19] of the thiazole ring and the appearance of a beam At (1340cm^{-1}) it returns to the stretch of the $\nu(\text{N-N})$ group^[19], the appearance of a beam at (1278cm^{-1}) returns to the stretch of the $\nu(\text{C-N})$ group^[19], and the appearance of a beam at (752cm^{-1}) returns to the stretch of the $\nu(\text{C-S})$ group^[21].



Fig(1)IR of the (C₇H₇N₃S)

The infrared spectrum of the lican showed a beam at (3178cm^{-1}) which is due to the stretch of the $\nu(\text{NH})$ group^[22], the appearance of a beam at (3074cm^{-1}) belonging to the stretch of the $\nu(\text{C-H})$ aromatic group^[23], the appearance of two beams at (2947cm^{-1} , 2835cm^{-1}) belonging to the stretch of the $\nu(\text{C-H})$ group^[25] and the appearance of a beam at (1614cm^{-1}) due to the stretching of the $\nu(\text{C=N})$ group^[22], the appearance of a beam at (1568cm^{-1}) due to the stretching of the $\nu(\text{C=C})$ group^[22] and

the emergence of A beam at (1506cm^{-1}) returns to the stretching of the $\nu(\text{C=N})$ group^[22] of the thiazole ring, the appearance of a beam at (1363cm^{-1}) returns to the stretching of the $\nu(\text{N-N})$ group^[20], the appearance of a beam at (1251cm^{-1}) returns to the stretching of the methoxy group $\nu(\text{C-O})$ ^[25], the appearance of a beam at (1163cm^{-1}) returns to the stretch of the $\nu(\text{C-N})$ group^[22] and the appearance of a bundle at (752cm^{-1}) returns to the stretch of the $\nu(\text{C-S})$ group^[21].

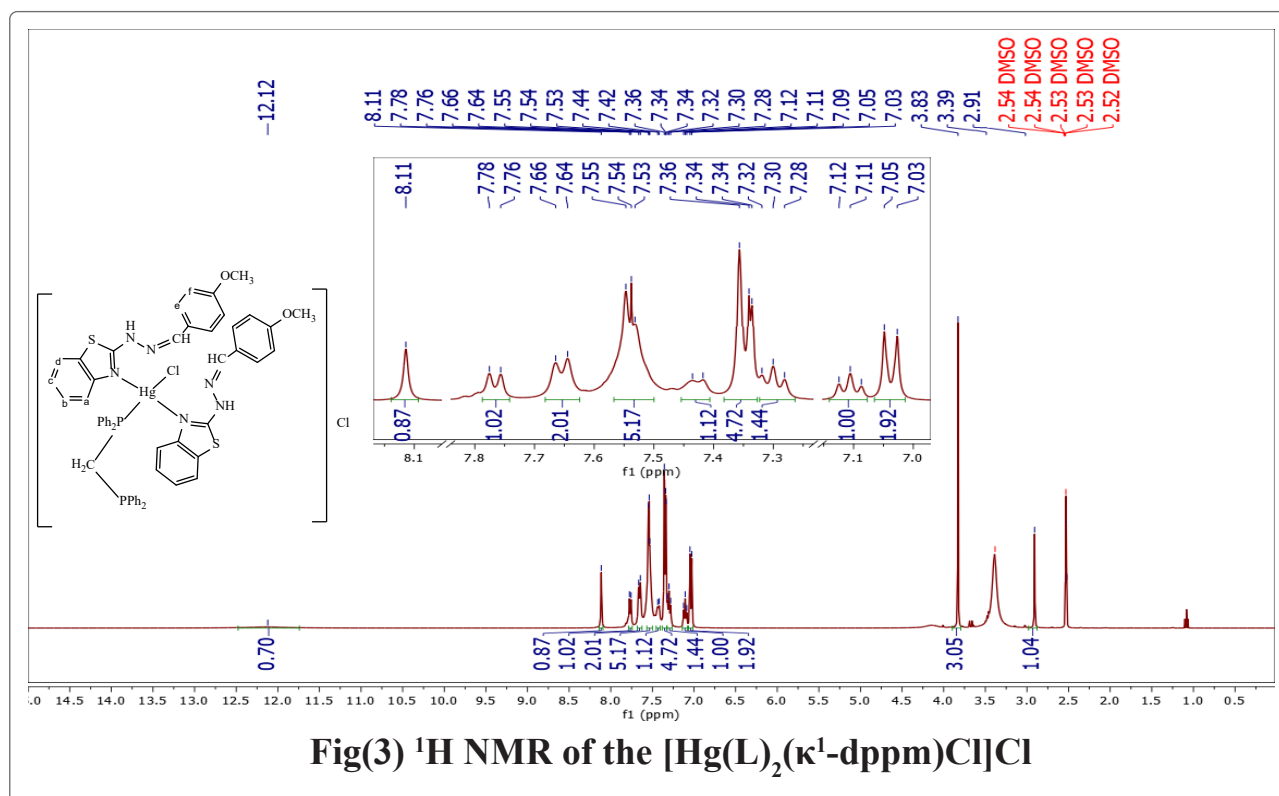


Fig(2) IR of the (C₁₅H₁₃ON₃S)

3-2- Nuclear magnetic resonance spectra(NMR)

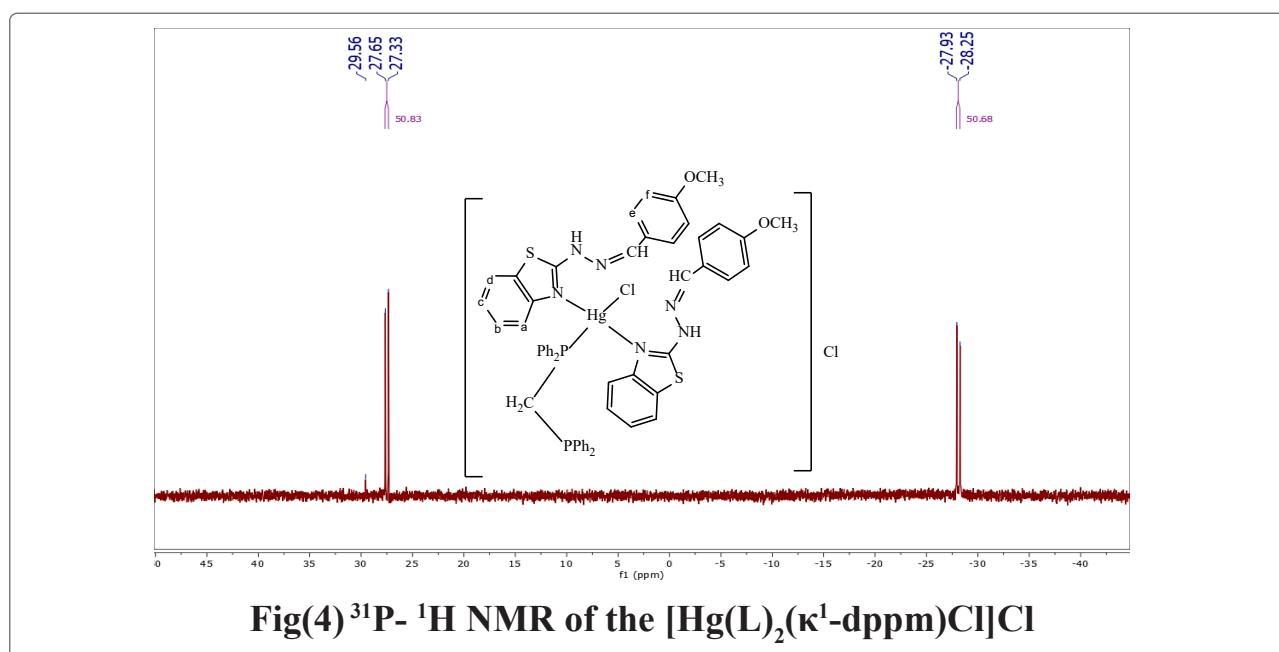
The spectrum of ^1H NMR of the complex $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$ showed a single signal at ($\delta\text{H}=12.16\text{ppm}$) belonging to the group (NH) and with the integration of one proton and also the appearance of a single signal at ($\delta\text{H}=8.12\text{ppm}$) belonging to the proton group (CH) and with the integration of a proton and a binary signal appeared at ($\delta\text{H}=7.78\text{ppm}$) belonging to (H_a) and with a constant of ($^3J_{\text{H-H}}=7.73\text{Hz}$) and with a single proton integration and also a binary signal at ($\delta\text{H}=7.68\text{ppm}$) belonging to (H_c) and with a constant of ($^3J_{\text{H-H}}=8.70\text{Hz}$) and with the integration of two protons, as well as the appearance of a binary signal at ($\delta\text{H}=7.45\text{ppm}$) and the conjugate constant ($^3J_{\text{H-H}}=8.15\text{Hz}$) and the integration of a proton return to (H_d) and the appearance of a triple signal at ($\delta\text{H}=7.31\text{ppm}$) and the constant of comparison ($^3J_{\text{H-H}}=7.67\text{Hz}$) and the integration of a proton return to (H_c) and also the appearance of a triple signal at ($\delta\text{H}=7.12\text{ppm}$) back to (H_b) and the constant of coupling ($^3J_{\text{H-H}}=7.75\text{Hz}$) and the integration of one proton and the appearance of a bi-

nary signal at ($\delta\text{H}=7.04\text{ppm}$) back to (H_f) and the constant of ($^3J_{\text{H-H}}=8.73\text{Hz}$) and the integration of two protons as it showed that there are multiple signals at ($\delta\text{H}=7.49\text{ppm}$) and ($\delta\text{H}=7.35\text{ppm}$) belonging to the protons of the phenyl group (Ph) With the integration of 10 protons and the appearance of a single-signal beam at ($\delta\text{H}=3.8\text{ppm}$) returns to the protons of the methoxy group (CH_3) and the integration of three protons, Also, a single signal at ($\delta\text{H}=3.0\text{ppm}$) belongs to the group (CH_2) associated with the two phosphorus atoms in phosphine (dppm) and the integration of one proton, where the integration ratios indicate the presence of 2 moles of ligand versus one mole dppm.



Fig(3) ^1H NMR of the $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$

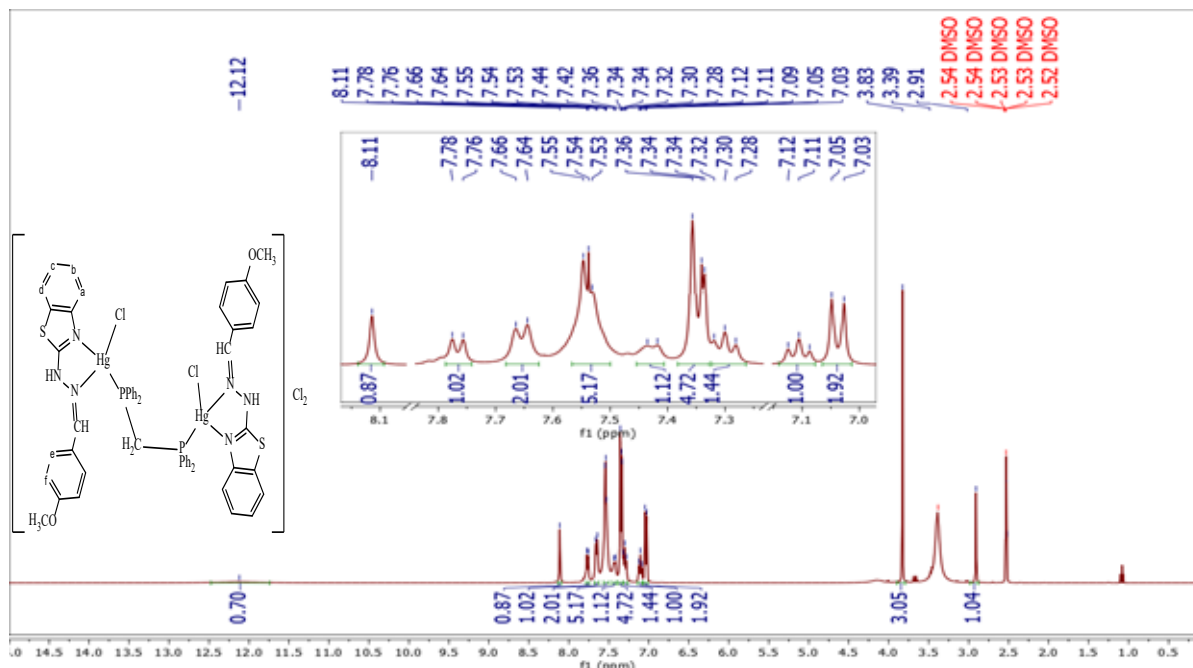
The spectrum of $^{31}\text{P}\{^1\text{H}\}$ NMR of the complex $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$ showed two binary signals at chemical displacement ($\delta^{31}\text{P}=27.49\text{ppm}$) with a conjugate constant ($^2J_{\text{P-P}}=50.83\text{ Hz}$) and at ($\delta^{31}\text{P}=-28.09\text{ppm}$) with a conjugate constant ($^2J_{\text{P-P}}=50.68\text{Hz}$), where the two signals indicate that one phosphorus atom is bonded with the metal and the other is free respectively.



Fig(4) $^{31}\text{P}\text{-}^1\text{H}$ NMR of the $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$

The ^1H NMR spectrum of the complex $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$ showed a single signal at ($\delta\text{H}=12.12\text{ppm}$) belonging to the (NH) group and with one proton integration, and also a single signal appeared at ($\delta\text{H}=8.11\text{ppm}$) belonging to the group (CH) and with the integration of a proton and the appearance of a binary signal at ($\delta\text{H}=7.77\text{ppm}$) belonging to (H_a) and with the integration of a proton and a constant coupling ($^3J_{\text{H-H}}=7.58\text{Hz}$), as well as a binary signal appeared at ($\delta\text{H}=7.65\text{ppm}$) belonging to (H_e) and with the integration of two protons and a constant coupling ($^3J_{\text{H-H}}=8.02\text{Hz}$), as well as multiple signals appeared at ($\delta\text{H}=7.34\text{ppm}$) returning For the phenyl group (Ph) and the integration of 5 protons and a binary signal appeared at ($\delta\text{H}=7.43\text{ppm}$) back to (H_d) and with a coupling constant ($^3J_{\text{H-H}}=7.04\text{Hz}$) and with the integration of one proton two protons and also multiple signals appeared at ($\delta\text{H}=7.54\text{ppm}$) and with the integration of 5 protons belonging to the phenyl group (Ph) and the emergence of a binary signal at ($\delta\text{H}=7.30\text{ppm}$) returns to (H_c) and with the integration of one proton the appearance of a binary signal at ($\delta\text{H}=7.11\text{ppm}$) and a constant coupling

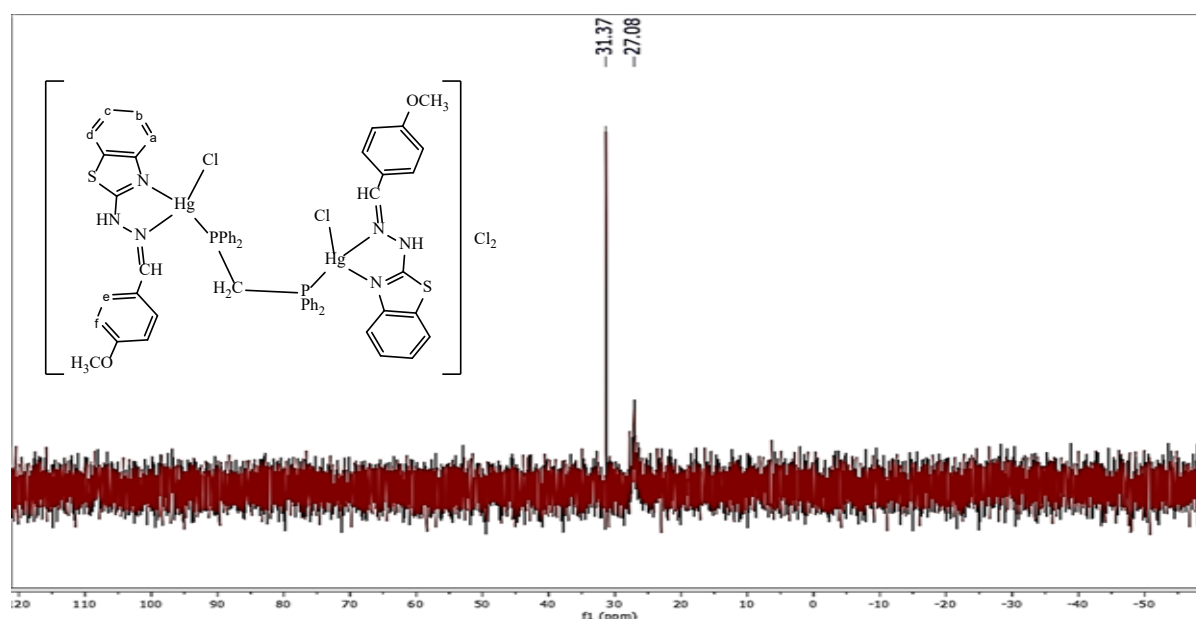
($^3J_{\text{H-H}}=7.50\text{Hz}$) returns to (H_b) and the integration of one proton and there is a binary signal at ($\delta\text{H}=7.04\text{ppm}$) returns to (H_f) and a constant coupling ($^3J_{\text{H-H}}=8.68\text{Hz}$) and the integration of two protons and a single signal appeared at ($\delta\text{H}=3.83\text{ppm}$) belonging to the group (CH_3) and the integration of three protons as well as a single signal appeared at ($\delta\text{H}=2.91\text{ppm}$) back to (CH_2) with the integration of one proton where the integration ratios indicated the presence of 2 moles From the ligand opposite one mall from dppm.



Fig(5) 1H NMR of the $[Hg_2(L)_2(\mu-dppm)Cl_2]Cl_2$

The $^{31}P\{^1H\}$ NMR spectrum of the complex $[Hg_2(L)_2(\mu-dppm)Cl_2]Cl_2$ showed two signals at chemical displacement ($\delta^{31}P=31.37$ ppm) while the

other signal at chemical displacement ($\delta^{31}P=27.08$) is expected to disappear if the sample is cooled.

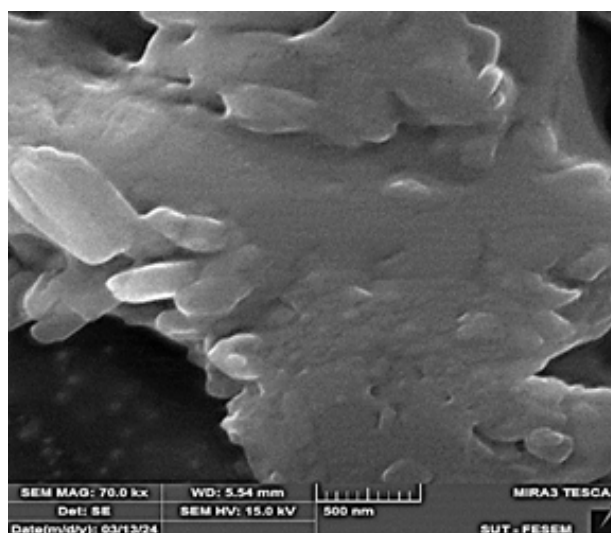
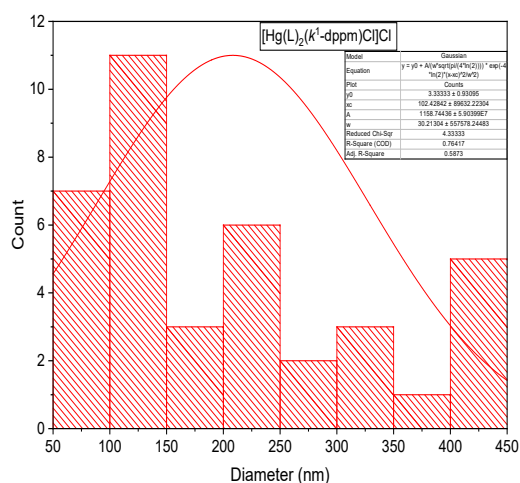


Fig(6) ^{31}P - 1H NMR of the $[Hg_2(L)_2(\mu-dppm)Cl_2]Cl_2$

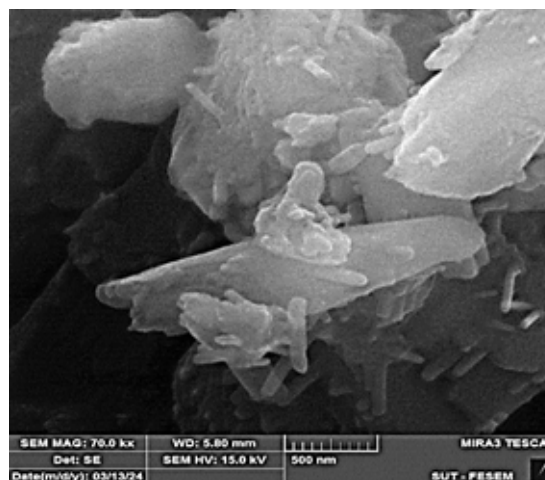
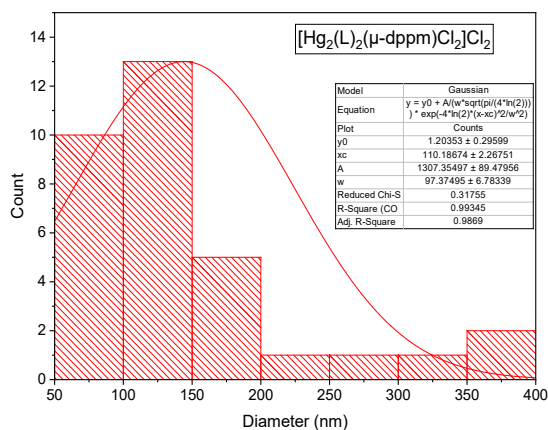
3-3- Results of SEM and EDX

SEM analysis of complex $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$, $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$, where it was used for an area of (500nm), (500nm), for complexes respectively, and the magnification power of the complexes was

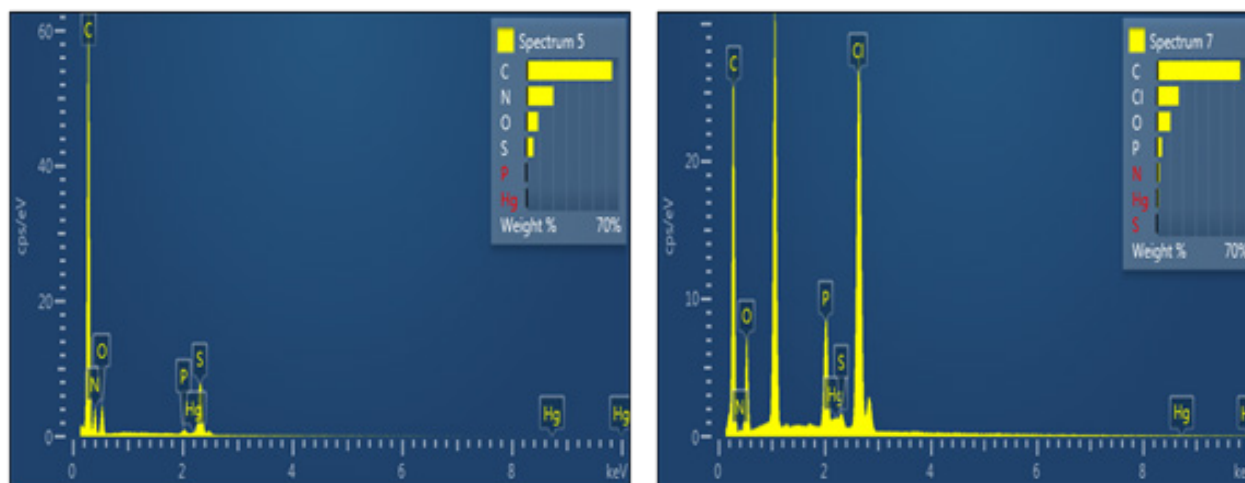
(HV:15.0KV), where the peak of the particle radii of the complexes according to Gaussian curves (102.48nm) and (110.18nm) respectively was among the nanocrystals^[26]. The results of the (EDX) showed the presence of peaks indicating the presence of the following elements (C, S,N,P,O,Hg,Cl).



Fig(7) SEM $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$



Fig(8) SEM $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$



Fig(9)EDX $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$ and $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$

3-4-Results XRD, Electrical Conductivity

The results of the (XRD) of the powder complexes showed that it has a degree of crystallization ranging between (49.63% - 49.59%) by calculating the percentage of the total areas under the crystal top (A_c) and dividing it by the total area ($A_c + A_a$), where (A_a) represents the area below the baseline and

this was measured through the Origin program and this result matches the surface images of the complexes using the ^[27]SEM technique. The electrical conductivity of the prepared complexes was measured at a concentration of (10^{-3}) molar in a solution (DMSO) at a temperature of (20 °C). The melting point of the complexes was also measured as shown in the following table.

Table 1 :XRD for Complex $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$, $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$

Complexes	Conductivity	XRD		
		A_c	$A_c + A_a$	$[A_c / A_c + A_a]\%$
$[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$	12	9747.535	19637.28	49.63%
$[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$	4.5	8890.14	8890.14	49.59%

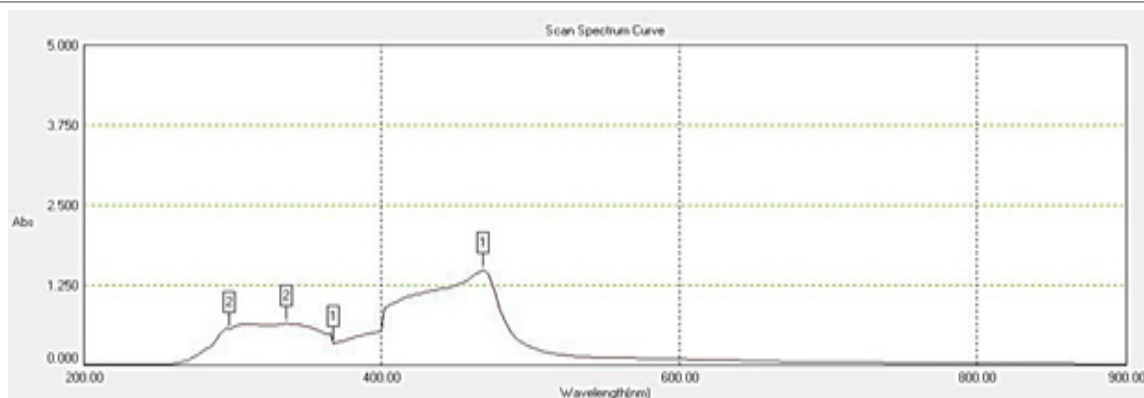
3-5- (UV) Results

The prepared complexes show absorptions of wavelengths within the visible region of the electromagnetic

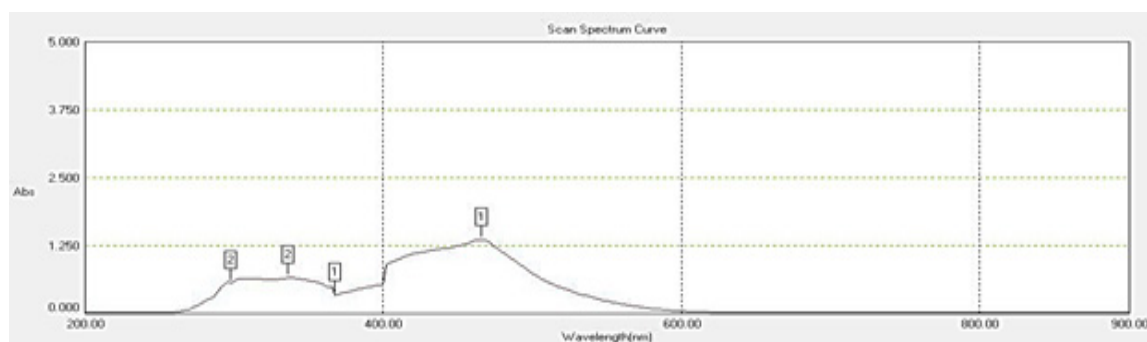
radiation spectrum, and there are additional absorptions in the far ultraviolet region adjacent to it^[28] As shown in the following table:

Table 2 (UV) for Complex $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$, $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$

Complexes	Wave Length(nm)	Wave Number(cm^{-1})	Transfer Type
$[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$	298	34482	$n \rightarrow \sigma^*$
	336	29940	$n \rightarrow \pi^*$
	368	27777	$\pi \rightarrow \pi^*$
	466	21929	C.T
$[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$	296	33783	$n \rightarrow \sigma^*$
	324	3864	$n \rightarrow \pi^*$
	356	28089	$\pi \rightarrow \pi^*$
	440	22727	C.T



Fig(10)(UV) $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$



Fig(11) (UV) $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$

3-6- Bacterial Acctivity

Mercury complex solutions prepared in advance using DMSO solvent were prepared and each complex has three concentrations (10^{-1} , 10^{-2} , 10^{-3} mg/mol),

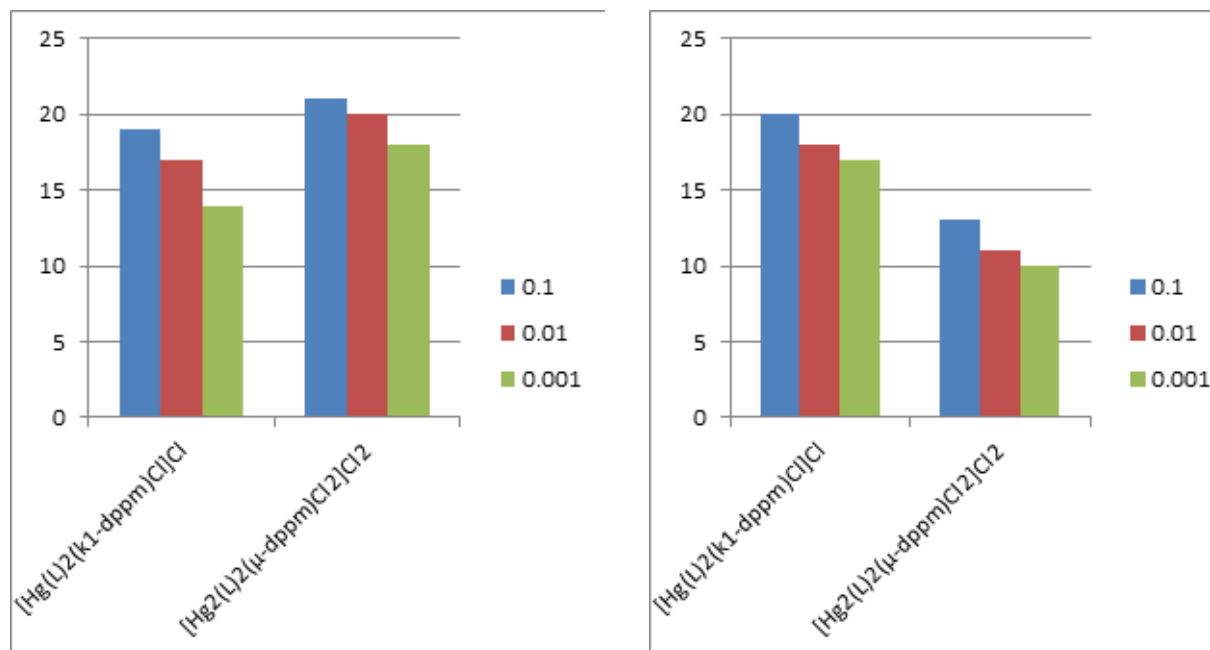
and the bacterial activity was measured by drilling method and for two types of positive bacteria (Staphylococcus aureus) and negative (Escherichia coli). The complexes showed high biological efficacy against bacteria.

Table 3 : Bacterial for Complex $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$, $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$

Complexes	Conc	Staphylococcus aureus(+)	Escherichia coli(-)
$[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$	10^{-1}	20	19
	10^{-2}	18	17
	10^{-3}	17	14
$[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$	10^{-1}	13	21
	10^{-2}	11	20
	10^{-3}	10	18

Escherichia coli (-)

Staphylococcus aureus (+)



fig(12) Bacterial Acctivity of Staphylococcus aureus and Escherichia coli

3-7- Results of the molecular docking study of some prepared compounds

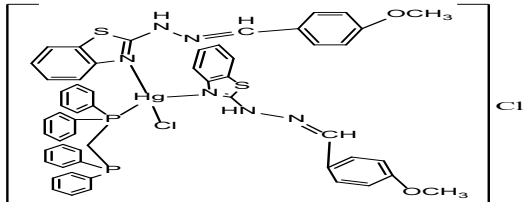
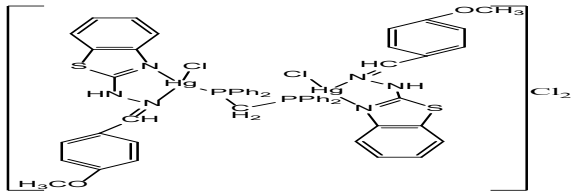
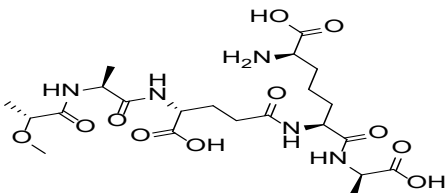
Positive and negative bacteria were used as a model organism to study the molecular fusion of prepared compounds ($[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$, $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$). MOE (2014) was used to calculate the binding energy. The proteins were downloaded from the (pdb) and prepared and

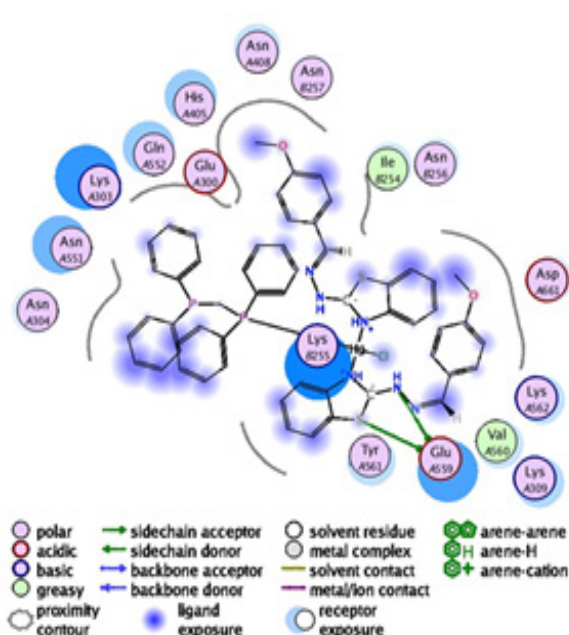
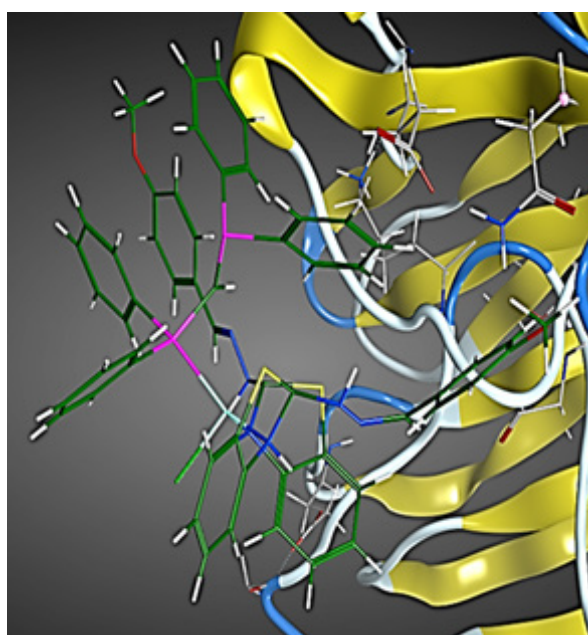
the missing elements and bonds were added. The chemical compounds were drawn in the chemoffice program and then converted into the (moe) program in a three-dimensional format, and molecular fusion was performed and the results showed that in the negative bacteria protein the binding energy of the complex $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$ is higher and in the protein of positive bacteria the binding energy of the complex $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$ is higher.

Table 4: Docking Compounds prepared in bacteria *Staphylococcus aureus*(+)

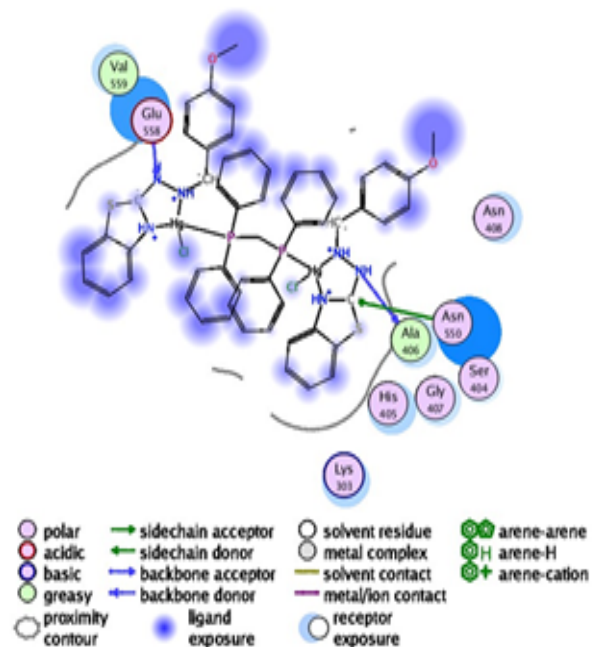
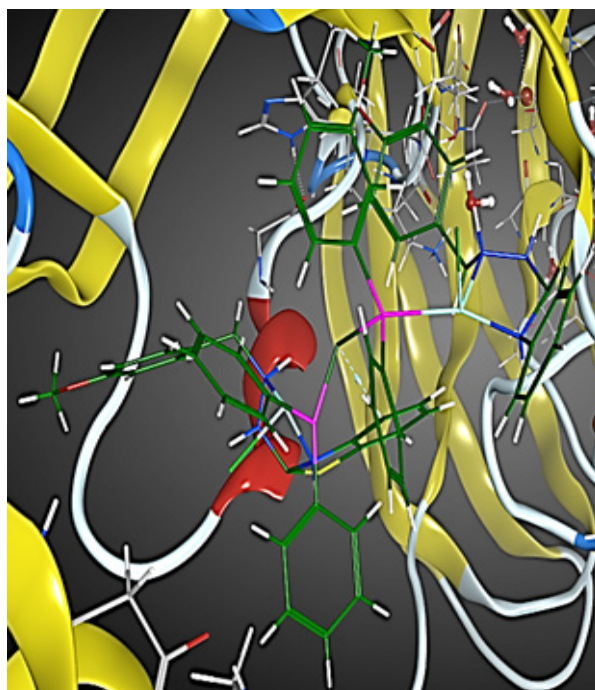
Compound	Structure	Docking Score (kcal/mol)
$[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$		-7.6118
$[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$		-6.798
native_ligand_6H5O		-10.738

Table 5 : Docking Compounds prepared in bacteria Escherichia coli (-)

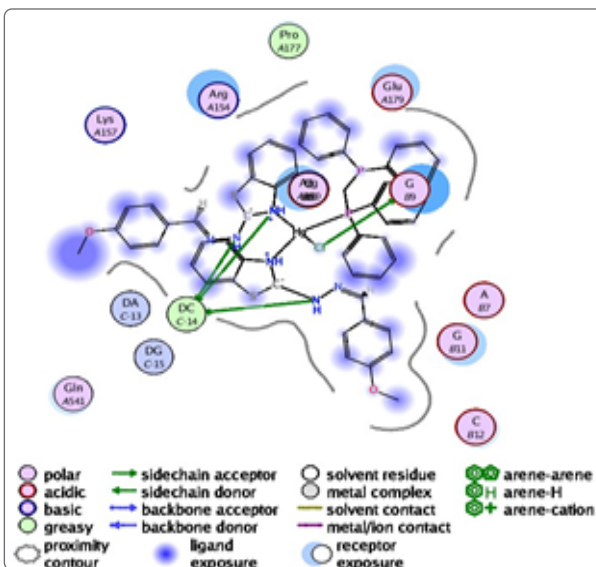
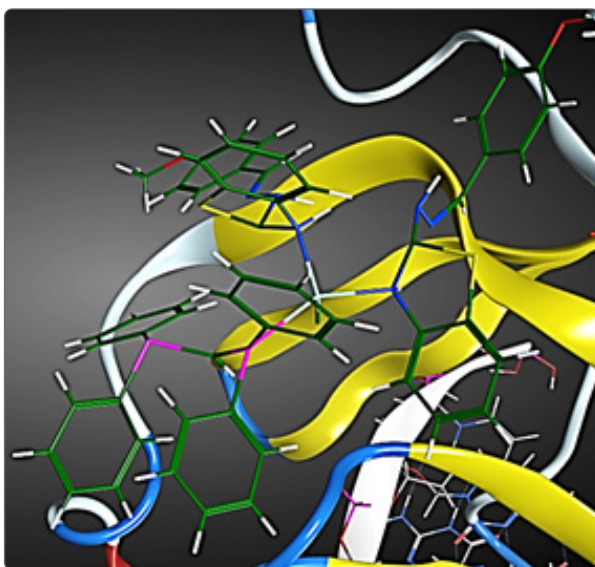
Compound	Structure	Docking Score (kcal/mol)
$[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$		-7.0648
$[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$		-8.3
native_ligand_6Top		-11.241



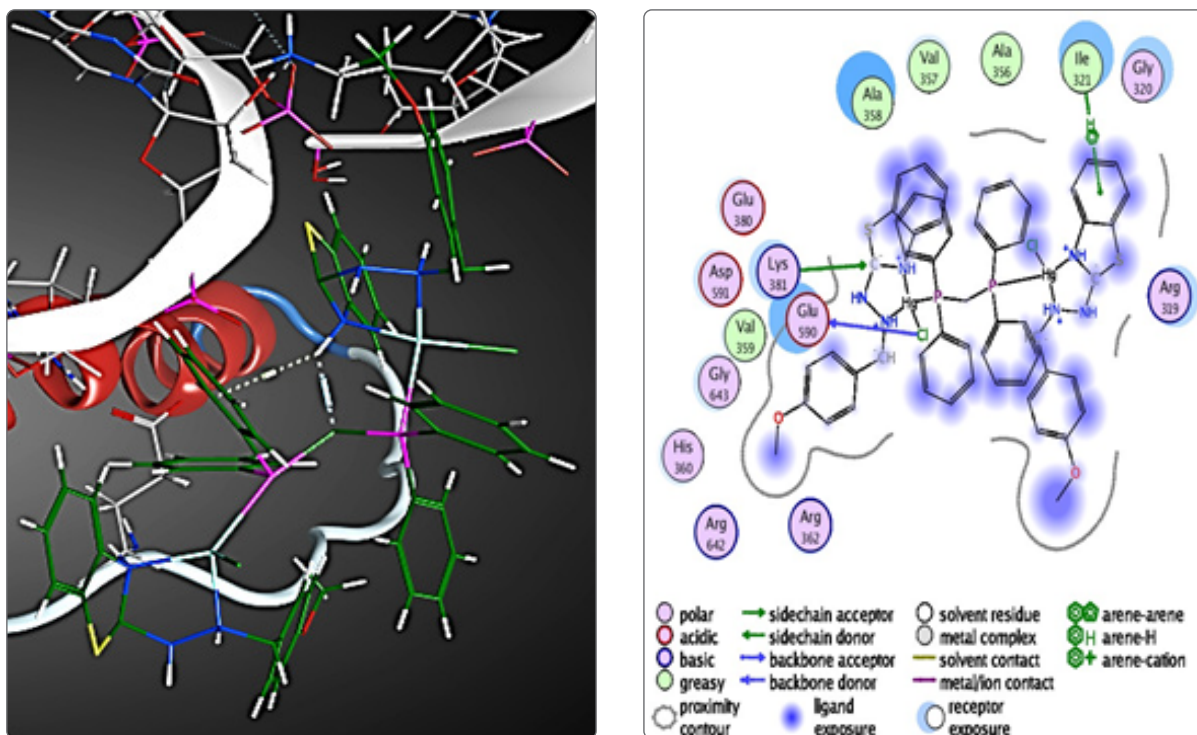
Fig(13) Staphylococcus aureus(+) $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$



Fig(14) *Staphylococcus aureus*(+)[Hg₂(L)₂(μ-dppm)Cl₂]Cl₂



Fig(15) *Escherichia coli* (-)[Hg(L)₂(κ¹-dppm)Cl]Cl



Fig(16) Escherichia coli (-) $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$

4- Conclusion

In this research, we found that ligand methoxybenzaldehyde hydrazino benzothiazole can bind with mercury ion in monodent or bi-toothed form. Where the chemical compound $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$ ligand is bind bidental-ly binds to mercury and phosphine is bidental bridge and the product is in the form of brown crystals, while the chemical compound $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$ is mono-tooth ligand bound to mercury and phosphine is bonded to

a phosphorus atom with mercury and the other phosphorus atom is free unbonded and the product is in the form of green crystals. The results of bacterial activity and molecular anchoring of positive and negative bacteria where The $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$ positive bacteria results higher than the complex $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$, but in negative bacteria it is the opposite where the complex $[\text{Hg}_2(\text{L})_2(\mu\text{-dppm})\text{Cl}_2]\text{Cl}_2$ has higher values than the complex $[\text{Hg}(\text{L})_2(\kappa^1\text{-dppm})\text{Cl}]\text{Cl}$.

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