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## Synthesizing, Structuring, and Characterizing Bioactivities of Cr(III), La(III), and Ce(III) Complexes with Nitrogen, Oxygen and Sulphur donor bidentate Schiff base ligands

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### Abstract:

Two Schiff bases, namely, 3-(benzylidene amino) -2-thioxo-6-methyl 2,5-dihydropyrimidine-4(3*H*)-one (LS)] and 3-(benzylidene amino)-6-methyl pyrimidine 4(3*H*, 5*H*)-dione(LA) as chelating ligands, were used to prepare some complexes of Cr(III), La(III), and Ce(III) ions. Standard physico-chemical procedures including metal analysis M%, element microanalysis (C.H.N.S) , magnetic susceptibility, conductometric measurements, FT-IR and UV-visible Spectra were used to identify Metal (III) complexes and Schiff bases (LS) and (LA). According to findings, a [Cr(III) complex] showed six coordinated octahedral geometry, while [La(III), and Ce(III) complexes] were structured with coordination number seven. Schiff's bases and mineral complexes were examined in vitro to investigate potential inhibition against Gram-positive bacteria such as *Pseudomonas aeruginosa* and Gram-negative bacteria such as *Staphylococcus aureus*. The low concentration for inhibition has been also determined by studying the minimal inhibitory concentrations MIC. Antibiotics (Ampicillin, Amoxicillin) have been chosen to contrast their activity. Furthermore, Anti-fungal activity against two types of fungi "*Aspergillus flavus*" and "*Penicillium Spp.*" was studied for these compounds. The results of the antibacterial activity were better compared to the standard drugs.

**Keywords:** Antimicrobial activity, Complexes of Pyrimidine Derivatives, lanthanide Metal Complexes, Spectroscopic analysis, Transition Metal Complexes.

### Introduction:

Pyrimidine derivatives have attracted a lot of attention by the chemists because they play a vital role due to their wide range of applications, such as industrial application, biological activities and therapeutic. The synthesis of chiral pyrimidine Schiff bases was prepared via the condensation of thiosemicarbazide or semicarbazide alcohols with benzaldehyde in the presence of ethyl acetoacetate and used as ligands. The pyrimidine ring has sulfur atom or oxygen atoms with the substituent having a donating group in the structure which enables these compounds to possess a good coordination behavior with, various transition and inner-transition metals. Spectrum chemotherapeutic properties were exhibited by chiral complexes schiff bases such as antibacterial<sup>1</sup>, antifungal<sup>2</sup>, anti HIV<sup>2,3</sup>, antiviral<sup>2,4</sup>, anti-tubercular and anticancer<sup>5</sup>.

In continuation of our work in synthesis pyrimidine derivatives<sup>6</sup>, we have synthesized new Schiff's bases metals ions complexes such as Cr(III), La(III), and Ce(III). The antibacterial study of the ligands and their complexes was determined against selected types of bacteria and fungi.

### Materials and Methods:

Gallenkamp MFB600-010f m.p was used to measure melting points (uncorrected). A Thin-layer chromatography technique TLC was used to check the purity of the new compounds utilized a mixture of acetone and dichloromethane (2: 2 v / v) with different proportions of (acetone: methyl acetate) mixture of solvents as eluents, iodine chamber to indicate spot location. A Shimadzu, (FT-IR)-8400s spectrophotometer was used to identify the functional groups in the synthesized ligands and their complexes between the range on

[4000–300]  $\text{cm}^{-1}$  using Cesium iodide as a disc. Atomic absorption type Shimadzu model 6809 was used to determine the elements for complexes and for ligands by using (C.H.N.S) analyzer. UV-visible spectrophotometer was used to measure the electronic spectrum between range 900-200 nm. Conductivity meter (CON 510 bench) containing 2-ring stainless Conductivity Electrode using DMSO as a solvent and (0.001M) solution to record the molar conductivity for the prepared complexes. Magnetic susceptibility balance "Sherwood scientific" was used to measure the magnetic susceptibility at 25°C as a solid state using Gouy method.

#### A- Preparation of (LS and LA Ligands):

Depending on the previous procedure, the Schiff base LS and LA was prepared <sup>6</sup>.

#### B- Preparation of Complexes:

##### 1- Cr(III) Complex

With stirring, the salt of  $[\text{CrCl}_3 \cdot 6\text{H}_2\text{O}]$  (0.266g, 1mmole) was dissolved in EtOH and added to EtOH solution of ligands LS (0.245g, 1mmole) or LA(0.229g, 1mmole) respectively. The mixture was warmed up for 3 hours under reflux. The precipitation was completed form, filtered, and washed with EtOH. The precipitation was dried

under vacuum for four hours; the physical properties are shown in (Table 1).

#### 2-La (III) and Ce (III) Complexes

$\text{LnCl}_3 \cdot 7\text{H}_2\text{O}$  (Ln = La, Ce) (0.5 mmol) was dissolved in EtOH and gradually added with stirring to the EtOH solution of LS (0.245g, 1mmole) or LA(0.229g, 1mmole) ligands respectively. It was stirred magnetically for 6 hours at room temperature. After reducing the solution to half the volume, the precipitation was separated, filtered, and washed with EtOH and dried under drain on anhydrous calcium chloride for four hours.

#### Results and Discussion:

##### 1- Physical measurements data:

Complexes Cr(III), La(III), and Ce(III) were synthesized with Schiff bases LS and LA in powder form. All complexes are stable in air, without hygroscopicity and also decomposed above 200°C, in addition, some complexes are soluble in DMF and DMSO and insoluble in other organic solvents. Elemental analysis suggests that the molar ratios Cr(III) complex has 1:1 (metal; ligand), while La(III), and Ce (III) complexes have 1:2 (metal; ligand), as shown in Table 1.

**Table 1. The Physical properties of new LS and LA Ligands and its metal complexes**

Comp . No.	Color	Melting Point °C Deco.	M.Wt g.mol <sup>-1</sup>	Elemental Analysis Found (calc.)				M% Metal Found (calc.)	M:L	Suggested Formula for Compounds
				C	H	N	S			
CrLS	Dark green	205	457.4	31.33 (31.48)	3.90 (3.72)	10.05 (9.18)	7.15 (6.99)	11.68 (11.35)	1:1	$[\text{CrLS}(\text{H}_2\text{O})_2\text{Cl}_2] \text{Cl}(\text{H}_2\text{O})_5$
CrLA	Dark green	215	441.4	32.68 (32.62)	4.03 (3.85)	9.88 (9.51)	-	12.02 (11.76)	1:1	$[\text{CoLA}(\text{H}_2\text{O})_2\text{Cl}_2] \text{Cl}(\text{H}_2\text{O})$
LaLS	Light yellow w	260	789.4	36.91 (36.48)	3.79 (3.55)	10.82 (10.64)	9.03 (8.11)	17.89 (17.59)	1:2	$[\text{La}(\text{LS})_2(\text{H}_2\text{O})_2\text{Cl}] \text{Cl}_2 \cdot \text{H}_2\text{O}$
LaLA	Light brown	255	757.4	38.18 (38.02)	3.97 (3.69)	11.14 (11.09)	-	18.62 (18.34)	1:2	$[\text{La}(\text{LA})_2(\text{H}_2\text{O})_2\text{Cl}] \text{Cl}_2 \cdot \text{H}_2\text{O}$
CeLS	Light yellow w	265	790.5	36.76 (36.43)	3.73 (3.54)	10.89 (10.63)	8.33 (8.09)	17.97 (17.71)	1:2	$[\text{Ce}(\text{LS})_2(\text{H}_2\text{O})_3\text{Cl}] \text{Cl}_2 \cdot \text{H}_2\text{O}$
CeLA	Off white	245	740.5	39.04 (38.89)	3.81 (3.51)	11.64 (11.34)	-	19.12 (18.91)	1:2	$[\text{Ce}(\text{LA})_2(\text{H}_2\text{O})_2\text{Cl}] \text{Cl}_2$

\*Where Dec =decomposition degree.

#### 2- Infrared spectra:

In Table 2, the main characteristic infrared absorption bands of LS and LA and its Cr(III), La(III), and Ce (III) complexes are provided along with their assignments.

#### A- The free ligand LS and its Cr(III), La(III) and Ce(III) complexes:

The LS infrared spectrum exhibited two absorption bands at (1699 and 1645)  $\text{cm}^{-1}$ , assignable to  $\nu\text{C}=\text{O}$  and  $\nu\text{C}=\text{N}$  of the carbonyl and azomethine groups respectively and an intense band was observed at (1095)  $\text{cm}^{-1}$  attributed to the C=S stretching of thio carbonyl group [7-9]. When

comparing the positions of these bands and those observed in the infrared spectra of their complexes Cr(III), La(III), and Ce(III)] indicated that the band did not show a marked shift at 1698 cm<sup>-1</sup>, it was discussed that the complexation toward Cr(III), La(III), and Ce(III) ions did not share carbonyl group, while those bands at 1645 and 1095 cm<sup>-1</sup> were assigned to stretching vibration motions C=N and C=S of azomethine and thio carbonyl moiety is mild decreasing in an intensity. The results suggested the coordination of LS through the nitrogen (C=N) of azomethine and sulfur (C=S) of thio carbonyl. Proof of coordination to the N and S atoms are submitted by the appearance of the new absorption bands with in (511-506) cm<sup>-1</sup>, (483-480) cm<sup>-1</sup>, (445-440) cm<sup>-1</sup> and (380-366) cm<sup>-1</sup> attributed to stretching frequency of  $\nu$ M-N,  $\nu$ M-O, M-S and M-Cl respectively, in IR spectra of all complexes<sup>10,11</sup>, Table 2.

### B- The free ligand LA and its Cr(III), La(III) and Ce(III) complexes:

The infrared spectrum of the LA exhibited two bands at approximately (1674), and (1595) cm<sup>-1</sup>, and assigned to stretching mode of C=O, and C=N respectively<sup>8</sup>. The ligand behave as bidentate

coordinating with metal ions through two-donor atoms (oxygen of carbonyl & nitrogen of the azomethine groups); in all Cr(III), La(III), and Ce(III) complexes. Thus, the two bands shifted to lower values in the three LA complexes due to the involvement of the oxygen & nitrogen atoms in the bonding with the metal's ions, Table 2. Also, new band was observed indicating the  $\nu$  (M-O, and M-N) respectively, Table 2. A broad band was observed around (3433-3386) cm<sup>-1</sup> in all spectra of LS and LA complexes corresponding to (O-H) stretching. The findings suggest that the appearance peak around 822-840 cm<sup>-1</sup> was attributed to the rocking mode of the water molecule<sup>9</sup>. This confirmed by the presence of H<sub>2</sub>O molecules in the crystal lattice of the complexes<sup>7,9</sup>.

**Table 2. Frequencies of FT-IR bands (cm<sup>-1</sup>) to new metal complexes (LS and LA Ligands)**

Comp.	$\nu_{C=N}$	$\nu_{C=O}$	$\nu_{C=S}$	$\nu_{OH}$	M-N	M-O	M-Cl	M-S
CrLS	1631	1697	1031	3433	510	482	366	440
CrLA	1512	1635	-	3402	512	485	363	-
LaLS	1608	1697	1083	3386	506	480	370	445
LaLA	1572	1640	-	3434	498	486	388	-
CeLS	1600	1695	1028	3438	511	483	380	443
CeLA	1624	1642	-	3390	509	481	376	-

### 3- Electronic spectra, Magnetic susceptibility and Molar conductance

#### A- Cr complexes of LS and LA

The Cr(III) complexes exhibited three absorption bands at (12345, 16501 and 29850) cm<sup>-1</sup> for LS and (12376, 16528 and 29940) cm<sup>-1</sup> for LA. These bands were typical of octahedral Cr(III) complexes<sup>12</sup>. The ( $\nu_2/\nu_1$ ) ratio is (1.33) which is similar to the results obtained for pure octahedral Cr(III) complexes<sup>12,13</sup>. The solid complex gave a

magnetic moment value to be (3.89 B.M) and the molar conductivity in (DMF) demonstrated that the complex was electrolyte, (table 3). Magnetic moment of Cr complexes of [LS, LA] are (3.79, 3.81) B.M respectively. More over conductivity measurements of Cr complexes of [LS, LA] are conductance. All measurements indicate the octahedral geometry around Cr(III) ions<sup>13-15</sup>, Table 3.

**Table 3. Electronic Spectral data, Electrical conductivities and Magnetic sensitivities of its mineral ligands and complexes**

Comp. No.	Absorption band(nm)	Assignment of the band	Molar conductivity $\text{Ohm}^{-1}.\text{cm}^2.\text{mol}^{-1}$	Magnetic sensitivities B.M
[LS]	(273) (300)	$\pi \rightarrow \pi^*$ $n \rightarrow \pi^*$	-	-
[LA]	(277) (310)	$\pi \rightarrow \pi^*$ $n \rightarrow \pi^*$	-	-
[CrLS]	(810) (606) (335)	$^4a_{2g} \rightarrow ^4t_{2g}(F)$ $^4a_{2g} \rightarrow ^4t_{1g}(F)$ $^4a_{2g} \rightarrow ^4t_{1g}(P)$	35	3.79
[CrLA]	(808) (605) (334)	$^4a_{2g} \rightarrow ^4t_{2g}(F)$ $^4a_{2g} \rightarrow ^4t_{1g}(F)$ $^4a_{2g} \rightarrow ^4t_{1g}(P)$	40	3.81
[LaLS]	(280) (323) (342)	$\pi \rightarrow \pi^*$ $n \rightarrow \pi^*$ La $\rightarrow$ LS (CT)	76	0.21
[LaLA]	(291) (337) (348)	$\pi \rightarrow \pi^*$ $n \rightarrow \pi^*$ La $\rightarrow$ LA (CT)	73	0.23
[CeLS]	(282) (325) (343) (384)	$\pi \rightarrow \pi^*$ $n \rightarrow \pi^*$ La $\rightarrow$ LA (CT) F $\rightarrow$ F	78	2.46
[CeLA]	(295) (339) (350) (388)	$\pi \rightarrow \pi^*$ $n \rightarrow \pi^*$ La $\rightarrow$ LA (CT) F $\rightarrow$ F	70	2.53

### B-La and Ce complexes of LS and LA

The f-f transitions of the lanthanide complexes were hypersensitive to stereochemistry, therefore, it appeared very weak as well as the strong charge transfer(CT) transition bands of the ligands obscured the bands corresponding to this transition<sup>11,16,17</sup>.

The maximum absorbance bands ( $\lambda_{max}$ ) of the LS and LA are (300,310) and (273,277) nm respectively, these bands can be attributed to n -  $\pi^*$  and  $\pi$ - $\pi^*$  transition respectively<sup>11</sup>. The absorption peaks of the [La complexes of LS and LA] solutions in DMSO showed well resolved bands at [342,323 and 280 nm] for LaLS and [348,337 and 291 nm] for LaLA transitions, respectively. The isolated CeLS complex showed all expected bands at [384,343,325 and 282 nm], which are assigned to F $\rightarrow$ F, LS $\rightarrow$ Ce, n- $\pi^*$  and  $\pi$ - $\pi^*$  transitions, respectively<sup>18,19</sup>. The CeLA complex spectrum displayed bands at [388,350,339 and 295 nm], due to F $\rightarrow$ F, LS $\rightarrow$ Ce, n- $\pi^*$  and  $\pi$ - $\pi^*$  transitions, respectively (10,17,20). This fact shows that there is coordination between LS and LA ligands with

lanthanide ions (La<sup>3+</sup>, Ce<sup>3+</sup>) forming a  $\pi$ -conjugated system, the data are listed in Table 3. The magnetic moment of [La complexes of LS and LA] is (0.21 and 0.23 B.M) of the present La(III) complex (4f<sup>0</sup>) configuration with <sup>1</sup>S<sub>0</sub> state. While magnetic moment of solid [Ce complexes of LS and LA], table 3, found to be (2.46 and 2.53 B.M) which agreed well with one unpaired electron, (4f<sup>1</sup>) configuration and <sup>2</sup>F<sub>5/2</sub> state<sup>16,18-21</sup>. The data is described in Table 3. Conductivity in (DMSO) solution showed that the La and Ce complexes bearing LS and LA were ionic.

### 4-Biological Studies:

The LS and LA ligands and new complexes were examined in vitro to investigate the potential growth inhibition of "*Pseudomonas aeruginosa*" and a representative "*Bacillus subtilis*". This study was also conducted using DMSO as blank solvent against "*Penicillium Spp.*" And "*Aspergillus flavus*" fungi, as shown in Table (4).

**Table 4. Antibacterial and Antifungal Activities for the Schiff bases [LS , LA ligands] and [La complexes of LS and LA] and [Ce complexes of LS and LA]**

Compound	<i>(Pseudomonas aeruginosa)</i>	<i>(Bacillus subtilis)</i>	<i>(Penicillium Spp.)</i>	<i>(Aspergillus flavus)</i>
DMSO as blank	-	-	-	-
[LS]	3.5	5.5	34.5	47.5
[LA]	-	-	39.5	43.5
[CrLS]	12	8	25	30
[CrLA]	10	8	28	36
[LaLS]	8	10	33	32
[LaLA]	6	8	38	42
[CeLS]	10	8	35	30
[CeLA]	8	6	30	39

**Where:**  
**6-8 (+)**  
**8-10 (++)**  
**>10 (+++)**

**Where:**  
**30-40 (+++)**  
**20-30 (++++)**  
**10-20 (++++)**

The following points were derived from the studies above contain:

1. (LS) has higher activity against the studied bacteria types comparing to [LA] activity.
2. Compared to the free ligands activity, the [LS] and [LA] metal complexes give higher activity against the studied bacteria types as shown in Table 4.
3. As shown in Table5, the findings of the minimum inhibitory concentration (MIC) compared with

those of the two antibiotics showed that at low concentrations, new complexes were more active.

4. Under the same experimental conditions, anti-activities of all metallic ion compounds including LS ligand were more toxic than metallic ion including LA ligand, and metal ion were LS chelating and LA ligands with free more toxic comparing with ligands towards microorganisms. table 5.

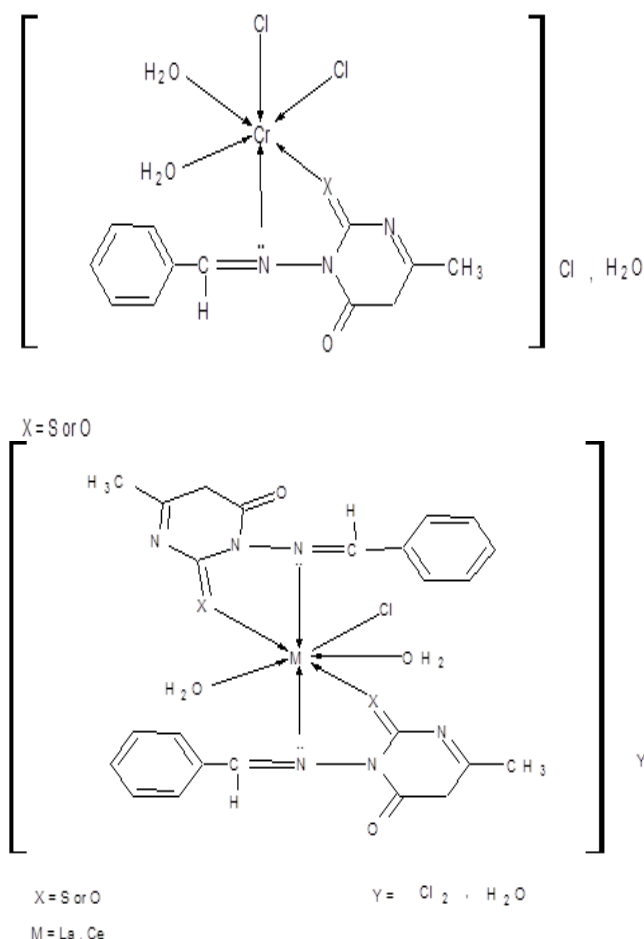
**Table 5. The lowest inhibitory concentration [MIC] of Schiff bases [LS, LA] ligands and complexes of [LS, LA]  $\mu\text{gm. } \mu\text{gm. ml}^{-1}$**

Symbol	<i>("Pseudomonas aeruginosa")</i>					<i>("Bacillus subtilis")</i>				
	0.025	0.05	0.075	0.1	0.5	0.025	0.05	0.075	0.1	0.5
[LS]	+	+	+	(*)	-	+	+	(*)	-	-
[LA]	+	+	+	+	(*)	+	+	+	+	(*)
[CrLS]	(*)	-	-	-	-	(*)	-	-	-	-
[CrLA]	(*)	-	-	-	-	+	+	(*)	-	-
[LaLS]	+	(*)	-	-	-	+	+	+	+	(*)
[LaLA]	+	+	+	+	(*)	+	+	+	+	+
[CeLS]	+	+	+	+	(*)	+	+	+	+	(*)
[CeLA]	+	+	+	+	+	+	+	+	+	(*)
Ampicillin	+	+	+	(*)	-	+	+	+	+	(*)
Amoxicillin	+	+	+	(*)	-	+	+	+	+	(*)

(\*) = [MIC]

### General Proposed Stereo Chemistry Structure of Complexes:

According to the results obtained from the elemental analysis, spectral studies, magnetic and conductivity measurements, the general structure of the above mentioned complexes can be illustrated as follows in **Figure (1)**



**Finger 1. Geometry Structure of the [LS, LA] Ligands with its metal complexes**

### Conclusions:

In this study, new novel complexes are synthesized and recognized by a variety of spectral and physicochemical analyses. The findings show that the synthesized ligand behave as bidentate coordinating with metal ions through two-donor atoms (O in C=O and N in C=N groups), therefore, the two bands shift to lower values for the three LA complexes, suggesting the involvement of the (O& N) nitrogen atoms in the bonding with metal's ions. Results of the anti-bacterial and antifungal activities for all compounds show that LS carries ligand more toxic metal ions compared to the effect of LA ligand metal ions, at the same time, metal ions chelate LS and LA are more ligands toxic compared to LS and LA by bonds towards the same microorganisms and give the same experimental conditions. Furthermore, the results of the Minimal

inhibitory concentration [MIC] comparing with those of the two antibiotics show more active at low concentration.

### Authors' declaration:

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are mine ours. Besides, the Figures and images, which are not mine ours, have been given the permission for republication attached with the manuscript.
- The author has signed an animal welfare statement.
- Ethical Clearance: The project was approved by the local ethical committee in University of Al-Mustansiriyah.

### Authors' contributions:

A.M. Rasheed, S.M.M. Al-Bayati, R.A.M. Al-Hasani and M.A. Shakir are contributed to the design and implementation of the research, to the analysis of the results and to the writing of the manuscript.

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## تخليق و دراسة تركيبية وتشخيص و فعالية بايولوجية لمعقدات Cr (III)

### و La (III) و Ce (III) مع النيتروجين والأكسجين والكبريت لقواعد شف ثنائية المنح

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#### الخلاصة:

تم استخدام قاعدتنا شف ، وهما: 3- (بنزيلدين أمينو)-6-مethyl-2-ثايوكسو-5,2-داي هايدرو بيريميدين-4-(3H)-أون (LS)، و 3- (بنزيلدين أمينو)-6-مethyl بيريميدين-4-(5 H,3H) داي أون (LA)، كالكاندات مخلبية لتحضير بعض المعقدات مع أيونات Cr(III) و La(III) و Ce(III). معقدات العناصر الثلاثية مع قواعد شف (LA) و (LS) تم تشخيصها عن طريق الطرائق الفيزيائية الكيميائية (تحليل المعادن، F. A. A. والتحليل الدقيق للعناصر C.H.N.S) وأطياف الأشعة تحت الحمراء FTIR والأشعة فوق البنفسجية-المرئية UV-vis وقياسات الحساسية المغناطيسية و التوصيلية). و وفقاً لهذه النتائج ، تم اقتراح شكل ثنائي السطوح مع معقد Cr(III) في حين أعطت المعقدات La(III) و Ce(III) أشكالاً متشابهة و ذات عدد تناسقي سبعة. تم فحص قواعد شف ومعقداتها المخلبية المعدنية في المختبر *in vitro* لتقييم قدرتها على التثبيط ضد (*Pseudomonas aeruginosa*) سالبة الصيغة و (*Staphylococcus aureus*) كيكثيريا موجبة الصيغة. كما تم دراسة أقل تركيز يحدث عنده التثبيط (MIC) لتحديد التركيز المنخفض للتثبيط. تم اختيار المضادات الحيوية (Ampicillin و Amoxicillin) لمقارنة فعاليتها مع المركبات الجديدة. كما تم دراسة الفعالية المضادة للفطريات ضد نوعين من الفطريات (*Penicillium Spp*) و (*Aspergillus flavus*) لجميع المركبات. أظهرت نتائج المركبات المحضرة نشاطاً مضاداً للبكتيريا أفضل من الأدوية.

الكلمات المفتاحية: الفعالية المايكروبية ، معقدات مشتقات البيريميدين ، معقدات العناصر اللانثانيد ، التحليل الطيفية ، معقدات العناصر الانتقالية.