

**Table (S1): Results of antibacterial bioassay of Salen ligand, metal salt and its mixed 8-hydroxy quinoline with Co, Ni, Cd, Al, La complexes against different strains of bacteria and fungi**

Compound	Mic of Bacteria mg mL <sup>-1</sup>			
	S. aureus (+ve)	B. subtilis (+ve)	E. coli (-ve)	P. vulgaris(-ve)
<b>S</b>	<b>14</b>	<b>13</b>	<b>12</b>	<b>15</b>
<b>Q</b>	<b>16</b>	<b>14</b>	<b>13</b>	<b>16</b>
<b>Gentamycin</b>	<b>24</b>	<b>26</b>	<b>30</b>	<b>25</b>
<b>CoSQ</b>	<b>18</b>	<b>15</b>	<b>13</b>	<b>13</b>
<b>NiSQ</b>	<b>20</b>	<b>16</b>	<b>14</b>	<b>15</b>
<b>CdSQ</b>	<b>26</b>	<b>30</b>	<b>28</b>	<b>30</b>
<b>AlSQ</b>	<b>31</b>	<b>25</b>	<b>23</b>	<b>24</b>
<b>LaSQ</b>	<b>29</b>	<b>30</b>	<b>20</b>	<b>27</b>
<b>CoCl<sub>2</sub>.6H<sub>2</sub>O</b>	<b>15</b>	<b>10</b>	<b>9</b>	<b>11</b>
<b>NiCl<sub>2</sub>.6H<sub>2</sub>O</b>	<b>16</b>	<b>9</b>	<b>12</b>	<b>13</b>
<b>CdCl<sub>2</sub>.H<sub>2</sub>O</b>	<b>19</b>	<b>23</b>	<b>24</b>	<b>24</b>
<b>AlCl<sub>3</sub>.6H<sub>2</sub>O</b>	<b>25</b>	<b>18</b>	<b>17</b>	<b>19</b>
<b>LaCl<sub>3</sub>.7H<sub>2</sub>O</b>	<b>22</b>	<b>26</b>	<b>14</b>	<b>23</b>
<b>Ref. 43</b>	<b>CoSI</b>	<b>11</b>	<b>13</b>	<b>11</b>
	<b>NiSI</b>	<b>12</b>	<b>15</b>	<b>12</b>
	<b>CdSI</b>	<b>20</b>	<b>33</b>	<b>25</b>
	<b>AlSI</b>	<b>NA</b>	<b>NA</b>	<b>NA</b>
	<b>LaSI</b>	<b>12</b>	<b>13</b>	<b>NA</b>

**Table (S2): Results of antifungal bioassay of Salen ligand, metal salt and its mixed 8-hydroxy quinoline with Co, Ni, Cd, Al, La complexes against different strains of bacteria and fungi**

Compound		Mic of Fungi mg ml <sup>-1</sup>	
		Candida albicans	Aspergillus flavus
<b>S</b>		<b>0</b>	<b>0</b>
<b>Q</b>		<b>13</b>	<b>16</b>
<b>Ketoconazole</b>		<b>16</b>	<b>20</b>
<b>CoSQ</b>		<b>0</b>	<b>0</b>
<b>NiSQ</b>		<b>0</b>	<b>0</b>
<b>CdSQ</b>		<b>23</b>	<b>28</b>
<b>AlSQ</b>		<b>37</b>	<b>28</b>
<b>LaSQ</b>		<b>38</b>	<b>25</b>
<b>CoCl<sub>2</sub>.6H<sub>2</sub>O</b>		<b>0</b>	<b>0</b>
<b>NiCl<sub>2</sub>.6H<sub>2</sub>O</b>		<b>0</b>	<b>0</b>
<b>CdCl<sub>2</sub>.H<sub>2</sub>O</b>		<b>14</b>	<b>20</b>
<b>AlCl<sub>3</sub>.6H<sub>2</sub>O</b>		<b>29</b>	<b>20</b>
<b>LaCl<sub>3</sub>.7H<sub>2</sub>O</b>		<b>27</b>	<b>19</b>
<b>Ref. 43</b>	<b>CoSI</b>	<b>0</b>	<b>0</b>
	<b>NiSI</b>	<b>0</b>	<b>0</b>
	<b>CdSI</b>	<b>20</b>	<b>30</b>
	<b>AlSI</b>	<b>0</b>	<b>0</b>
	<b>LaSI</b>	<b>0</b>	<b>0</b>

**Table S3:** Important optimized bond lengths (Å) and bond angles (°) of [Co(S)(Q)(H<sub>2</sub>O)]:

Type of bond	Bond length(Å)	Type of bond	Bond length(Å)	
	Complex		S	Complex
Co-N1	1.908	Co-O3	-	2.162
Co-N2	2.272			
Co-N3	1.993	N1...N2	3.788	2.709
Co-O4	2.113	N1...O2	4.261	2.720
Co-O2	2.007	N2...O2	7.003	3.045
Type of Angle	Angle (°)	Type of Angle	Angle (°)	
	Complex		Complex	
N1-Co-N2	80.28	O3-Co-N1	91.58	
N3-Co-O4	82.38	O3-Co-N2	93.53	
N1-Co-O4	91.04	O3-Co-N3	90.01	
N2-Co-N3	106.6	O3-Co-O4	79.26	
O2-Co-N1	88.00	N1-Co-N3	172.8	
O2-Co-N2	90.52	N2-Co-O4	168.6	
O2-Co-N3	89.90	O2-Co-O3	175.7	
O2-Co-O4	96.57	N1-N2-N3-O4	6.999*	

\*dihedral angle

**Table (S4): Results of Important optimized bond lengths (Å) and bond angles (°) of [Ni(S)(Q)(H<sub>2</sub>O)]**

Type of bond	Bond length(Å)	Type of bond	Bond length(Å)	
	Complex		S	Complex
Ni-N1	2.151	Ni-O3	-	1.997
Ni-N2	2.249			
Ni-N3	2.288	N1•••N2	3.788	2.777
Ni-O4	2.071	N1•••O2	4.261	2.717
Ni-O2	1.860	N2•••O2	7.003	2.950
Type of Angle	Angle (°)	Type of Angle	Angle (°)	
	Complex		Complex	
N1-Ni-N2	78.22	O3-Ni-N1	93.93	
N3-Ni-O4	78.98	O3-Ni-N2	92.55	
N1-Ni-O4	100.1	O3-Ni-N3	87.35	
N2-Ni-N3	102.8	O3-Ni-O4	83.65	
O2-Ni-N1	84.96	N1-Ni-N3	178.3	
O2-Ni-N2	91.27	N2-Ni-O4	175.7	
O2-Ni-N3	93.69	O2-Ni-O3	175.7	
O2-Ni-O4	92.46	N1-N2-N3-O4	-3.917*	

\*dihedral angle

**Table (S5): Results of Important optimized bond lengths (Å) and bond angles (°) of [Cd(S)(Q)(H<sub>2</sub>O)]:**

Type of bond	Bond length(Å)	Type of bond	Bond length(Å)	
	Complex		S	Complex
Cd-N1	2.227	Cd-O3	-	2.372
Cd-N2	2.409			
Cd-N3	2.312	N1...N2	3.788	2.886
Cd-O4	2.219	N1...O2	4.261	2.874
Cd-O2	2.231	N2...O2	7.003	3.349
Type of Angle	Angle (°)	Type of Angle	Angle (°)	
	Complex		Complex	
N1-Cd-N2	76.87	O3-Cd-N1	94.14	
N3-Cd-O4	77.40	O3-Cd-N2	90.38	
N1-Cd-O4	99.93	O3-Cd-N3	90.11	
N2-Cd-N3	106.2	O3-Cd-O4	84.06	
O2-Cd-N1	80.28	N1-Cd-N3	174.7	
O2-Cd-N2	92.34	N2-Cd-O4	173.4	
O2-Cd-N3	95.24	O2-Cd-O3	173.1	
O2-Cd-O4	92.80	N1-N2-N3-O4	-7.655*	

\*dihedral angle

**Table (S6): Results of Important optimized bond lengths (Å) and bond angles (°) of [Al(S)(Q)(H<sub>2</sub>O)]<sup>+</sup>**

Type of bond	Bond length(Å)	Type of bond	Bond length(Å)	
	Complex		S	Complex
Al- N1	1.974	Al- O3	-	2.052
Al- N2	2.122			
Al- N3	2.065	N1...N2	3.788	2.674
Al- O4	1.891	N1...O2	4.261	2.673
Al- O2	1.869	N2...O2	7.003	2.872
Type of Angle	Angle (°)	Type of Angle	Angle (°)	
	Complex		Complex	
N1-Al- N2	81.42	O3-Al- N1	90.01	
N3-Al- O4	83.86	O3-Al- N2	87.42	
N1-Al- O4	95.59	O3-Al- N3	88.39	
N2-Al- N3	-104.9	O3-Al- O4	82.89	
O2-Al- N1	88.13	N1-Al- N3	178.4	
O2-Al- N2	92.34	N2-Al- O4	169.9	
O2-Al- N3	91.84	O2-Al- O3	178.1	
O2-Al- O4	97.74	N1-N2-N3-O4	-5.790*	

\*dihedral angle

**Table S7:** Important optimized bond lengths (Å) and bond angles (°) of [La(S)(Q)Cl]

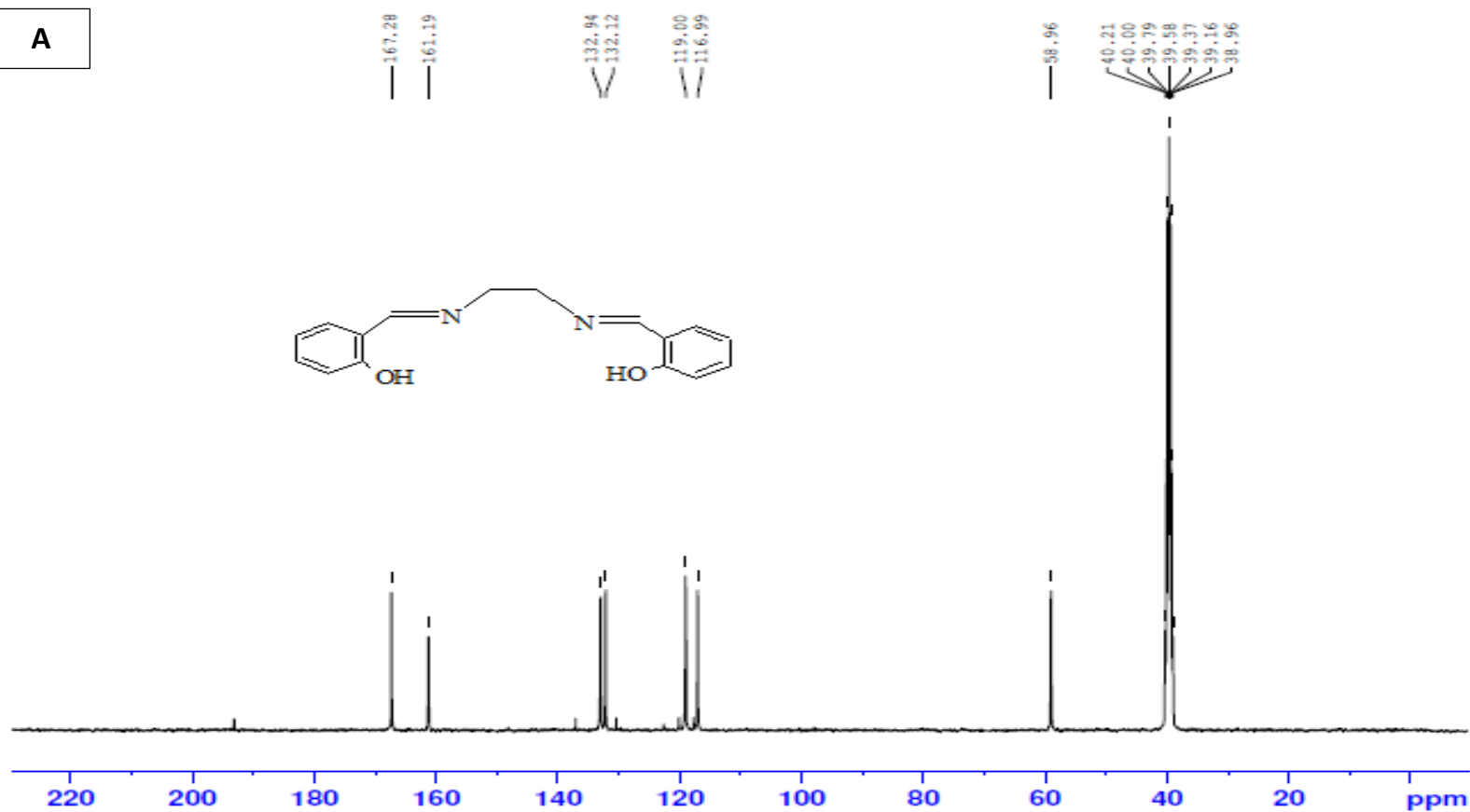
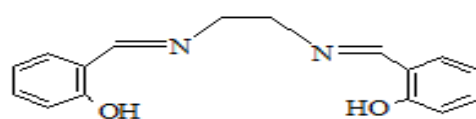
Type of bond	Bond length(Å) Complex	Type of bond	Bond length(Å) L                  Complex	
La-N1	2.534	La-O2	-	2.396
La-N2	2.704			
La-O3	2.402	N1- - - -N2	3.788	2.991
La-N3	2.621	N1- - - -O2	4.261	3.022
La-Cl	2.828	N2- - - -O2	7.003	3.674
Type of Angle	Angle (°) Complex	Type of Angle	Angle (°) Complex	
N1-La- N2	69.55	Cl-La-N1	94.01	
N3-La-O3	69.70	Cl-La-N2	88.38	
N1-La-O3	107.2	Cl-La-N3	93.10	
N2-La-N3	113.5	Cl-La-O3	91.66	
O2-La-N1	75.55	N1-La-N3	172.3	
O2-La-N2	91.96	N2-La-O3	176.8	
O2-La-N3	97.13	O2-La-Cl	168.7	
O2-La-O3	87.36	N1-N2-N3-O3	-5.859*	

\*dihedral angle

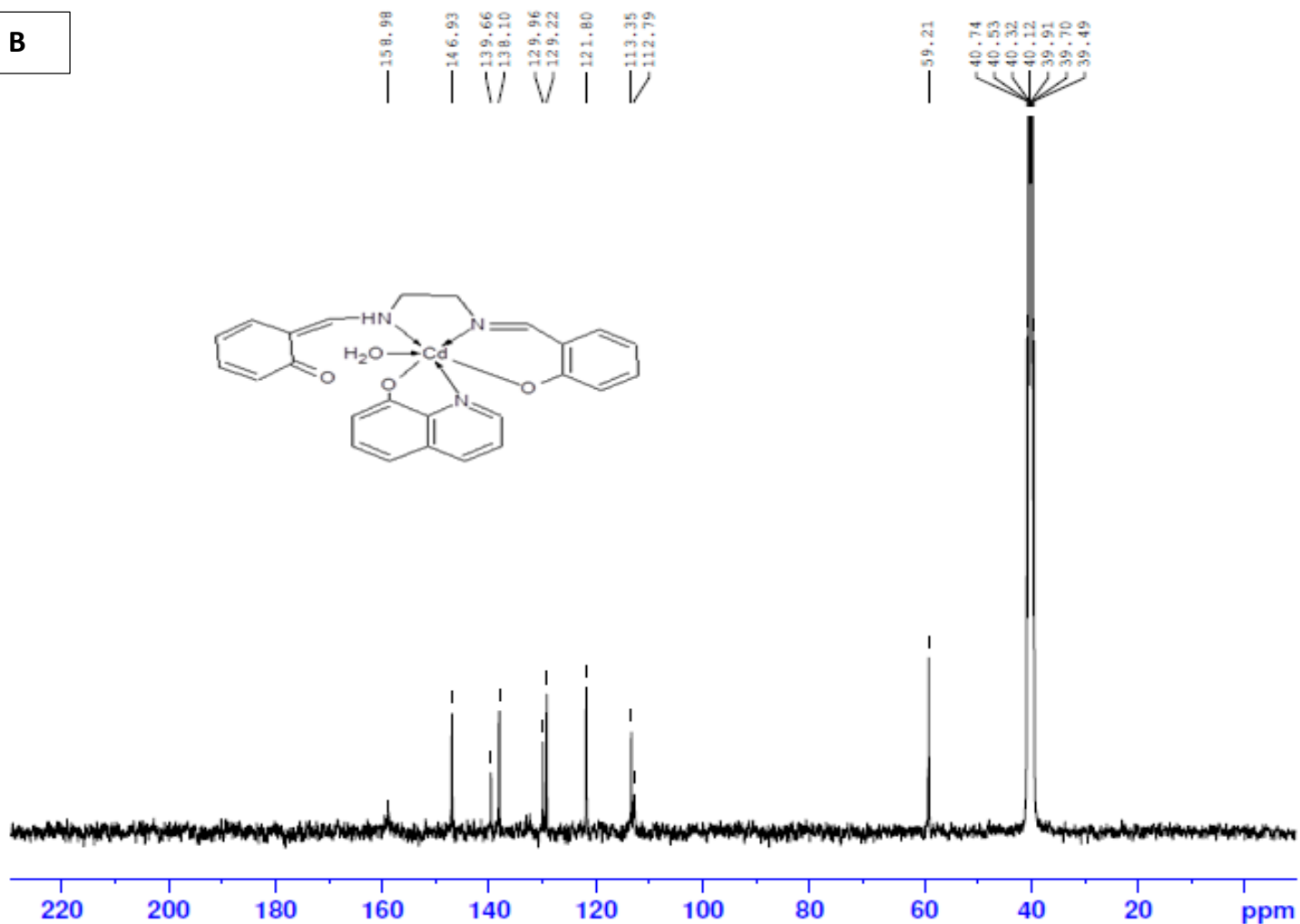
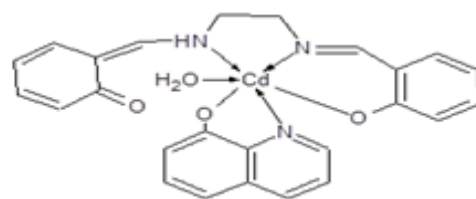




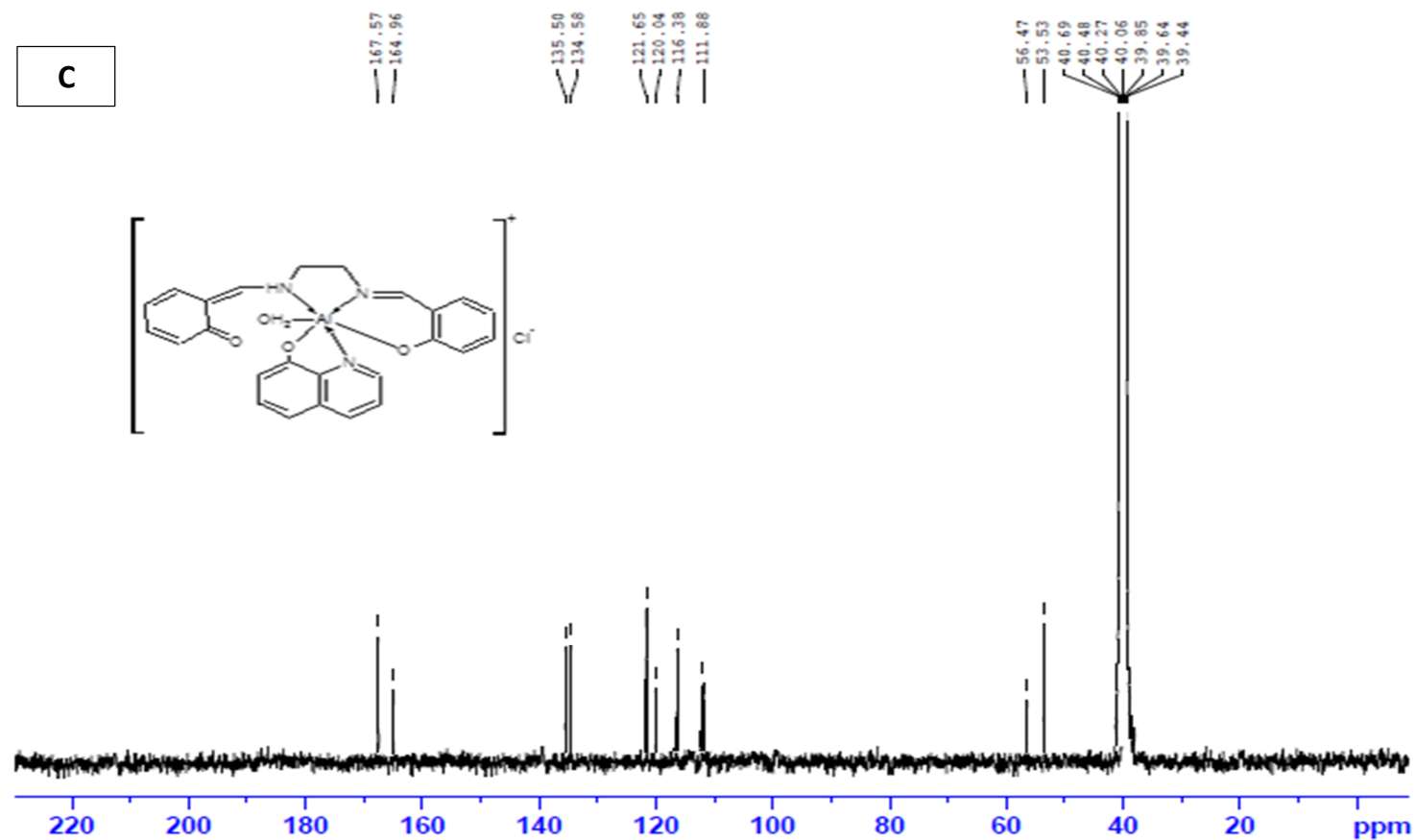
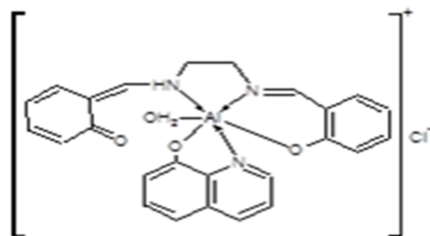
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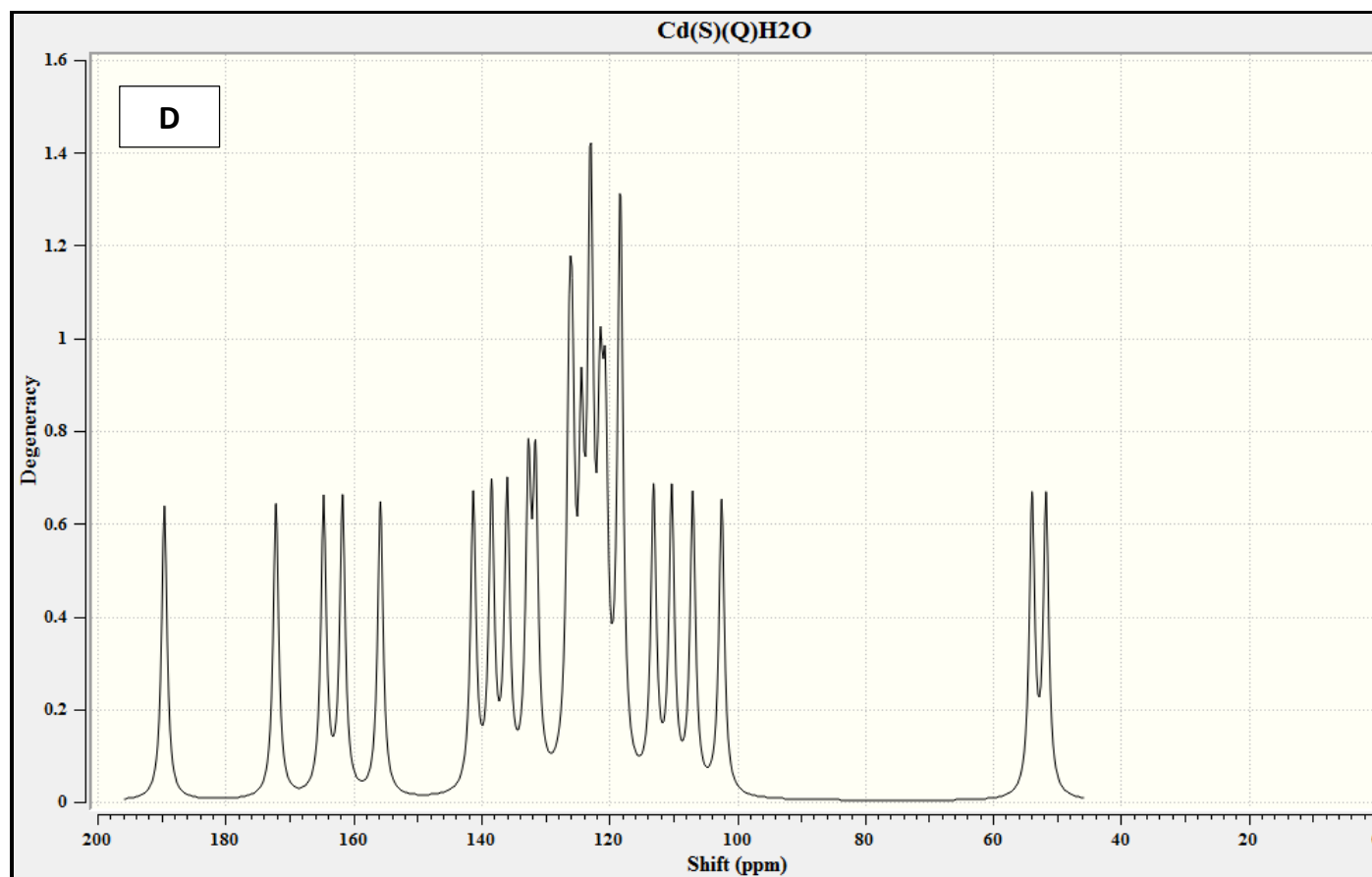


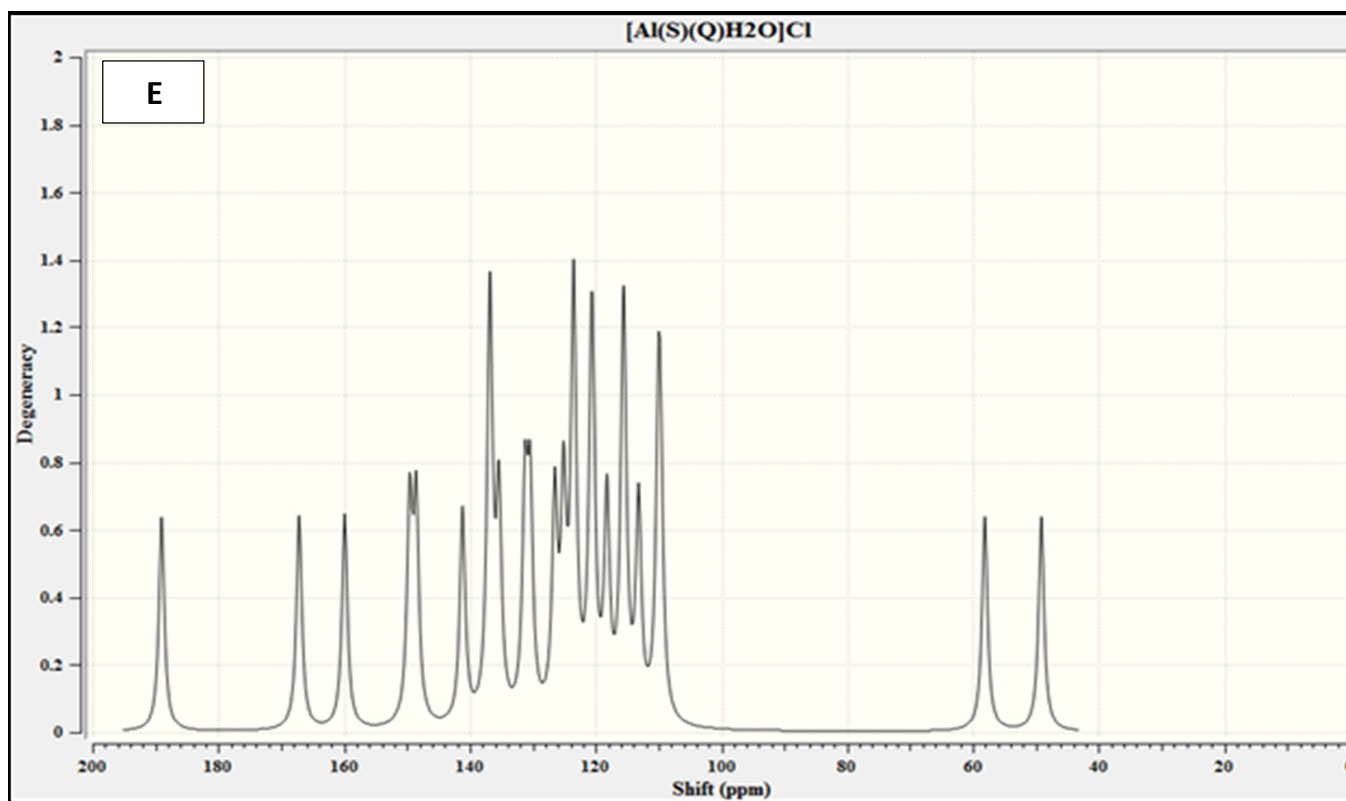
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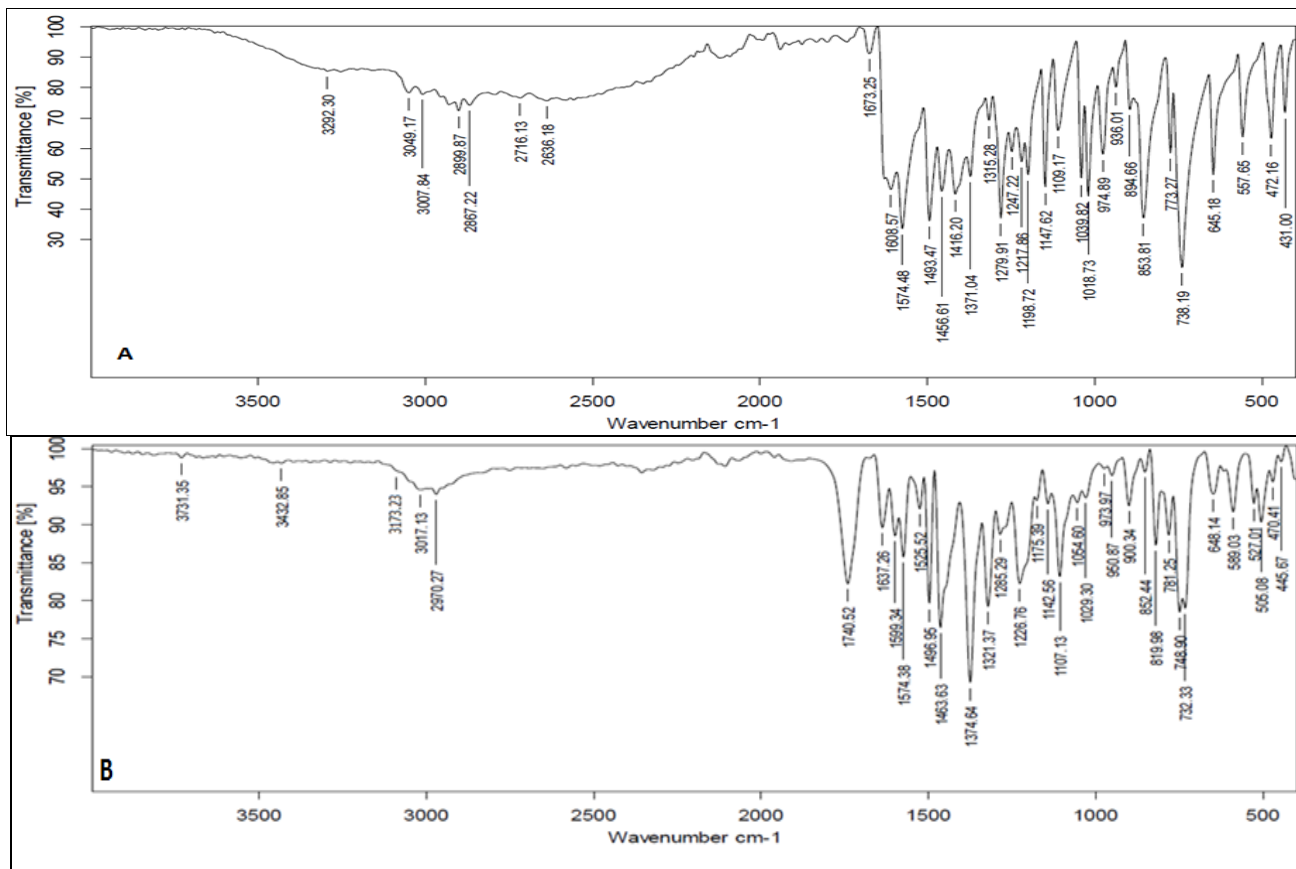
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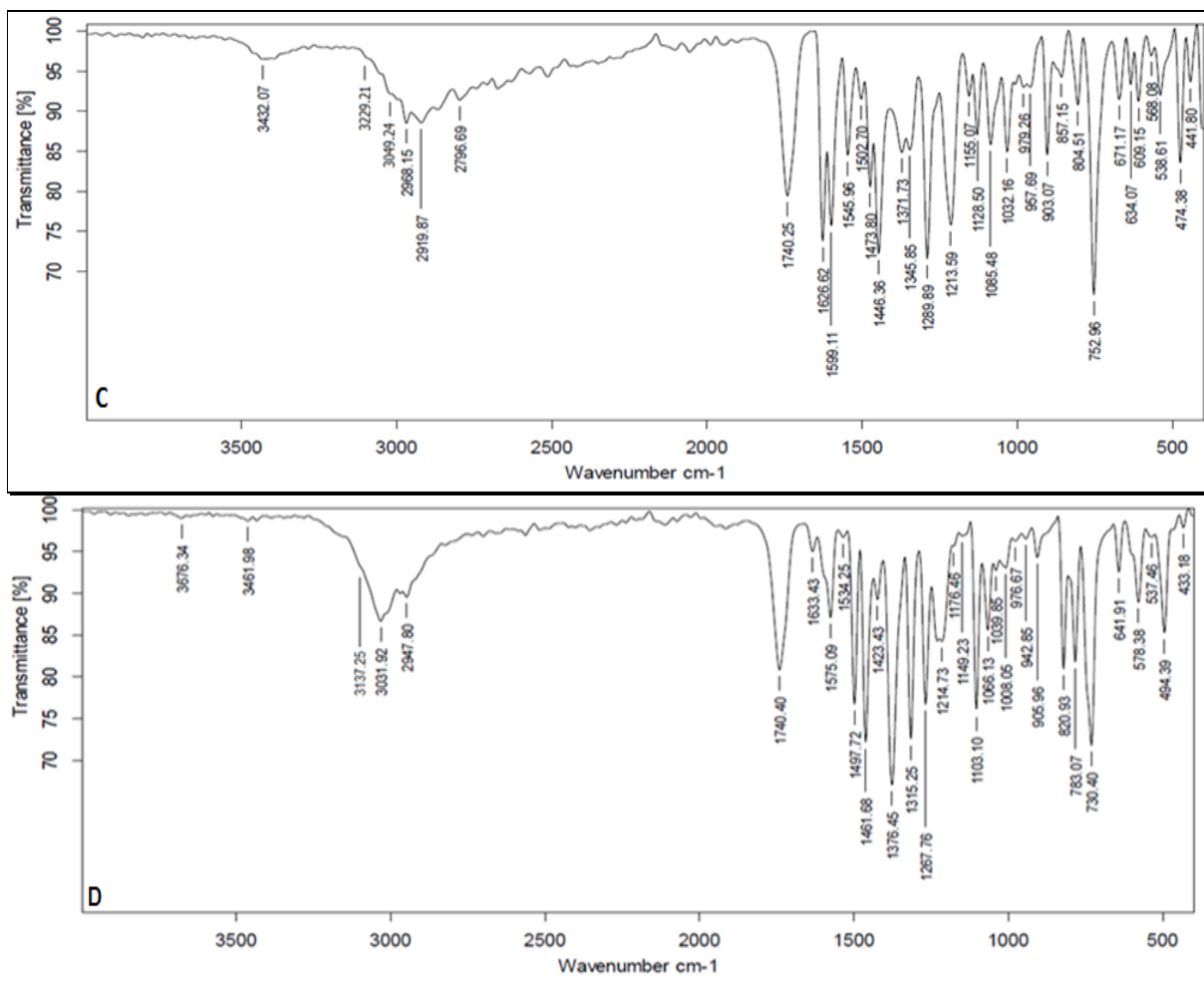


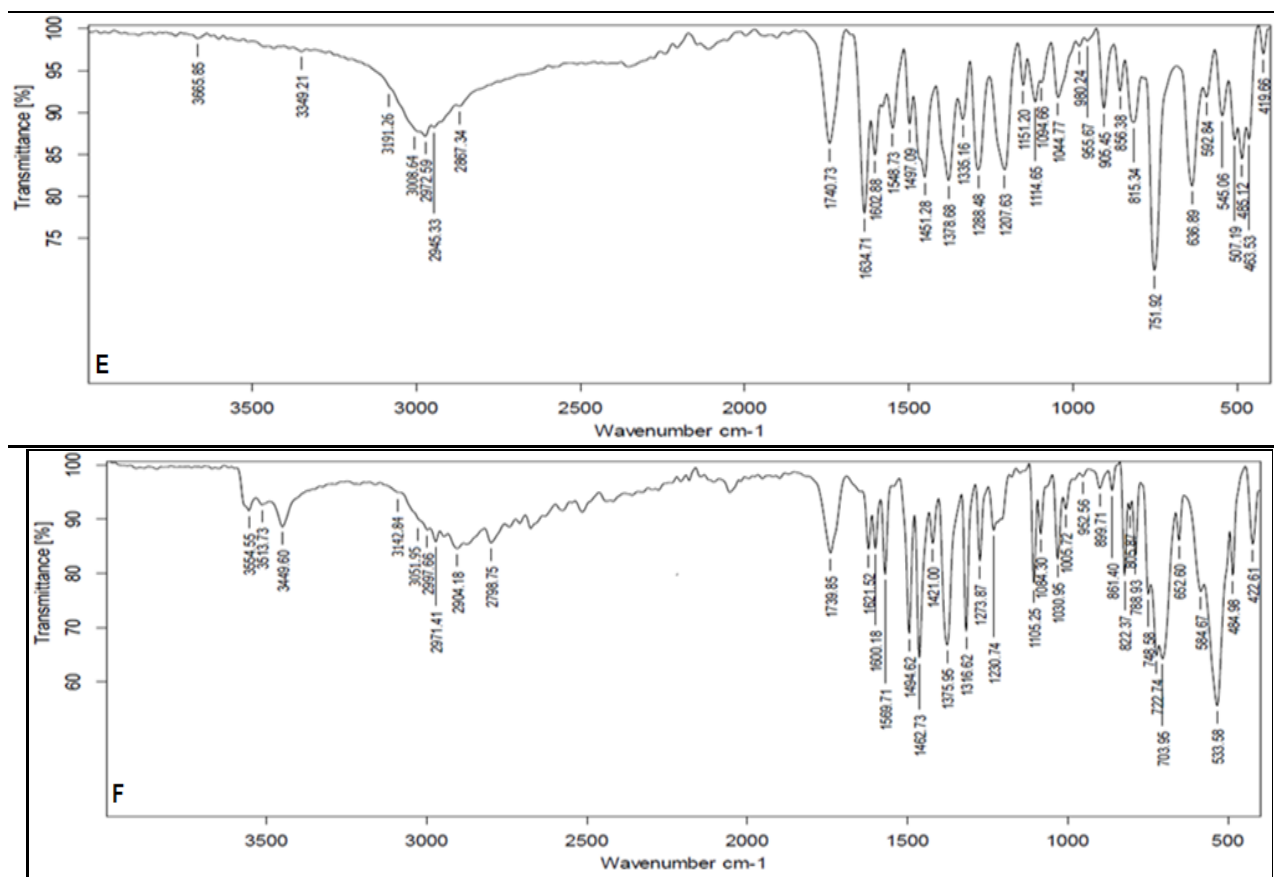




Figures (S1):  $^{13}\text{C}$  NMR spectra of Salen ligand (A) and Cd(B and D), Al(C and E) mixed 8-hydroxy quinoline complexes

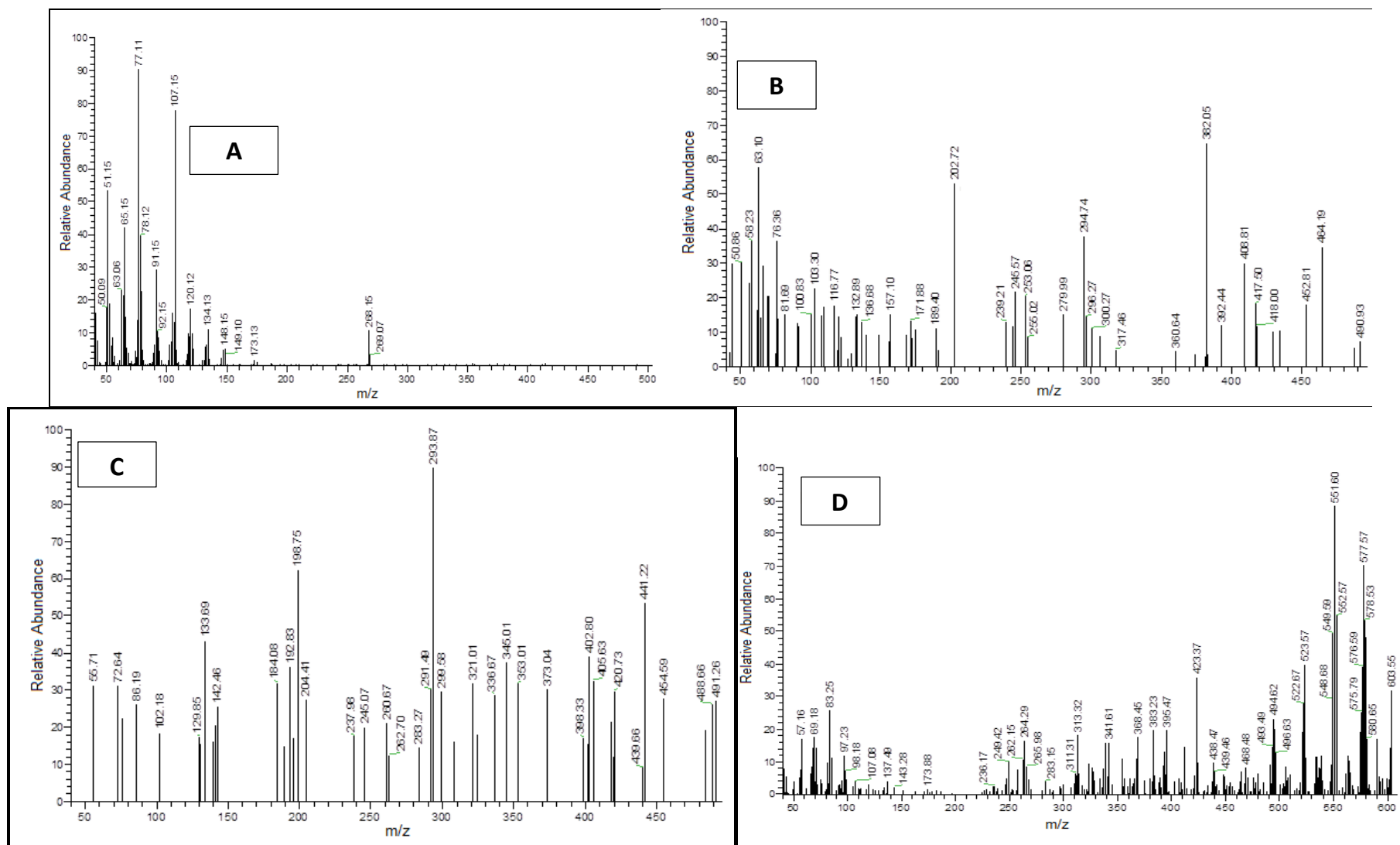




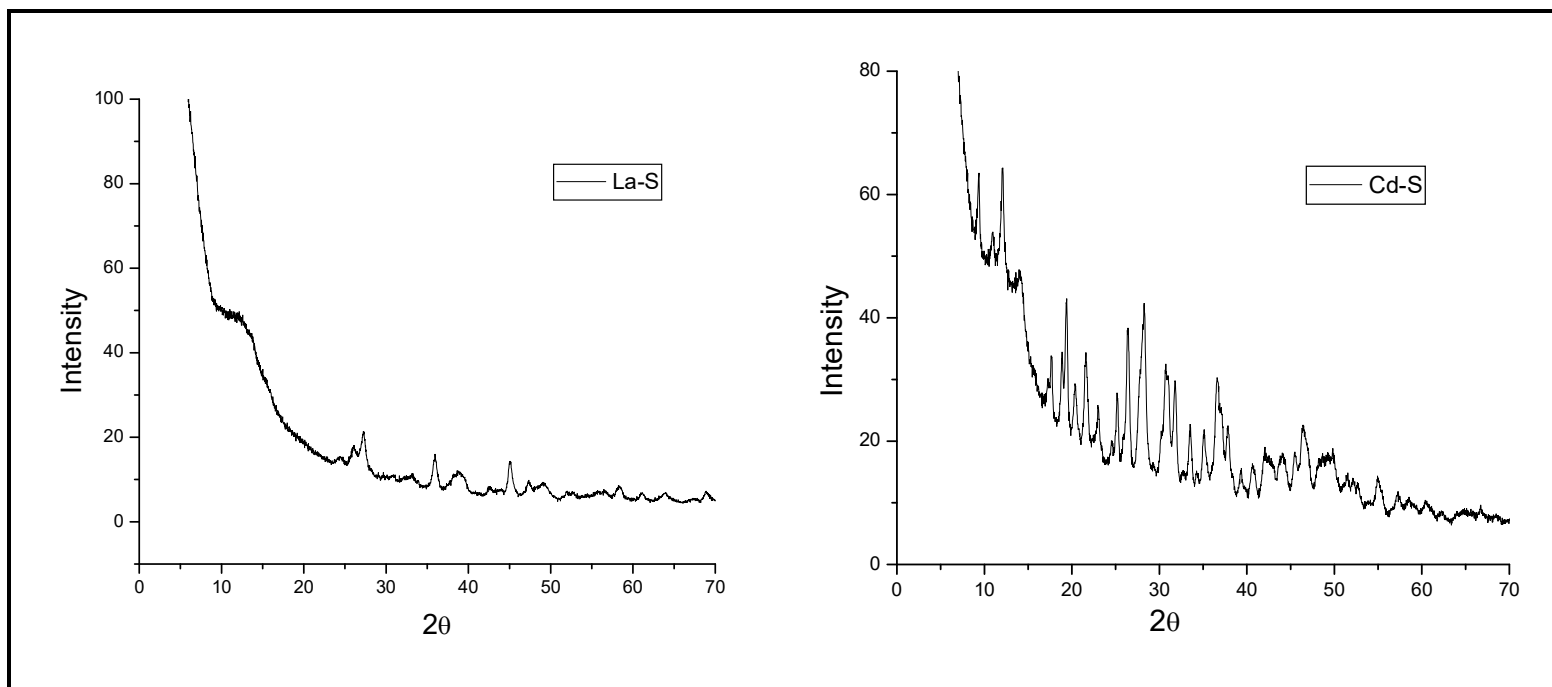


Figures (S2) : FT IR spectral of Salen Schiff base ligand (A) and its mixed 8-hydroxy quinoline (B)Co, (C)Ni, (D)Cd, (E)Al, (F)La complexes in 4000-400 cm<sup>-1</sup>

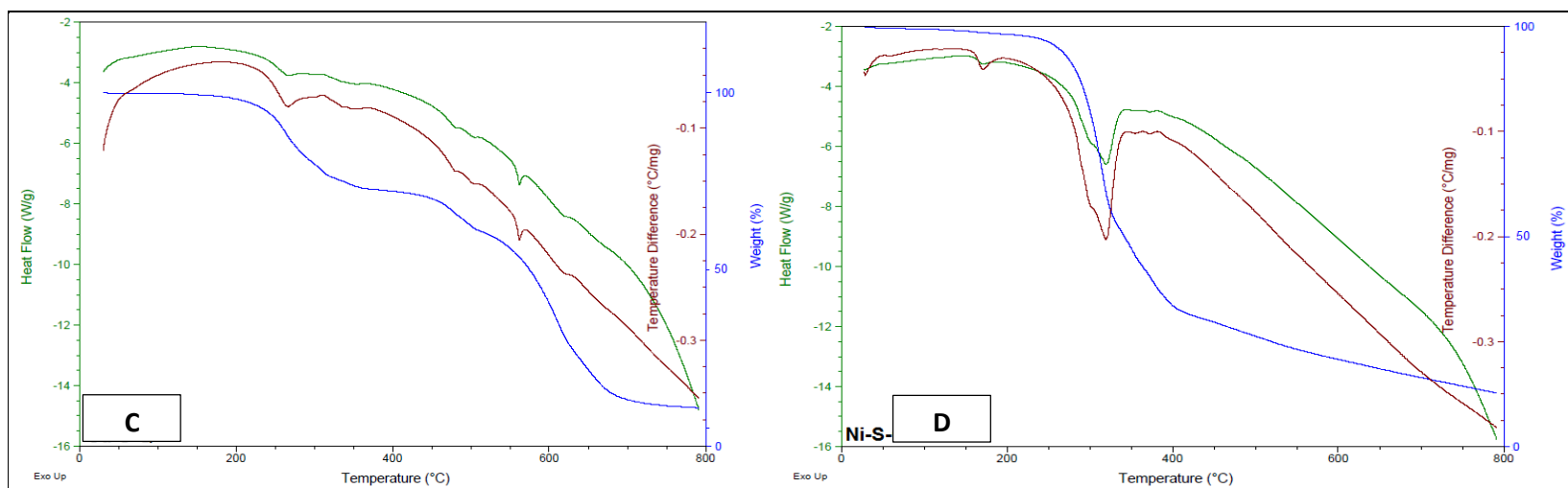
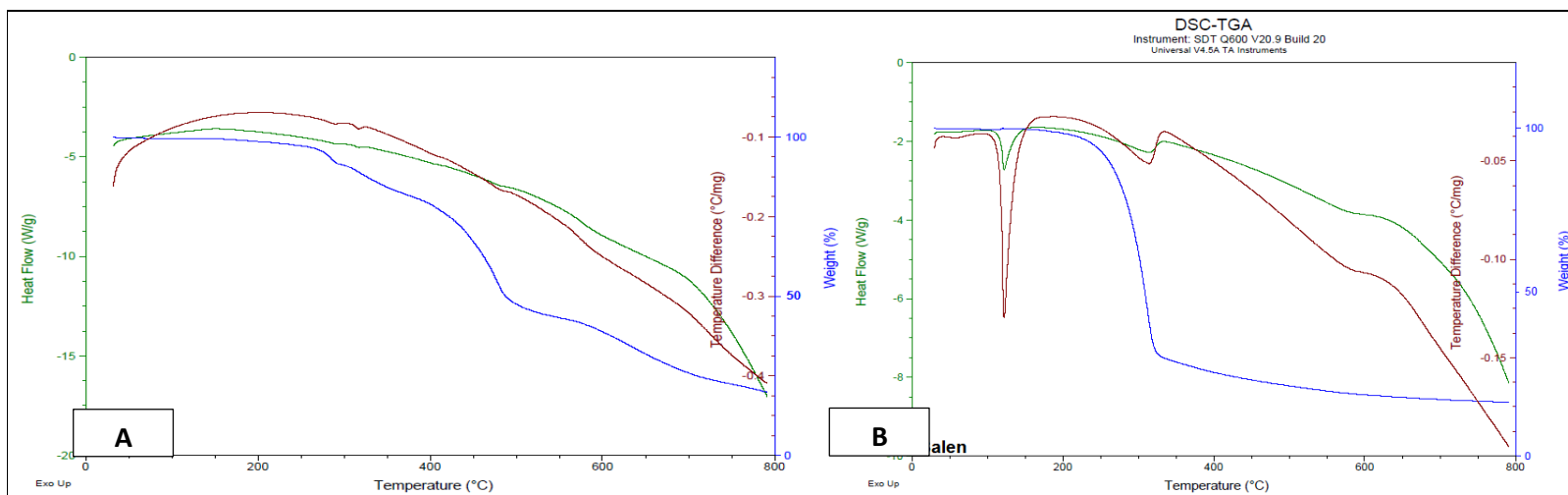


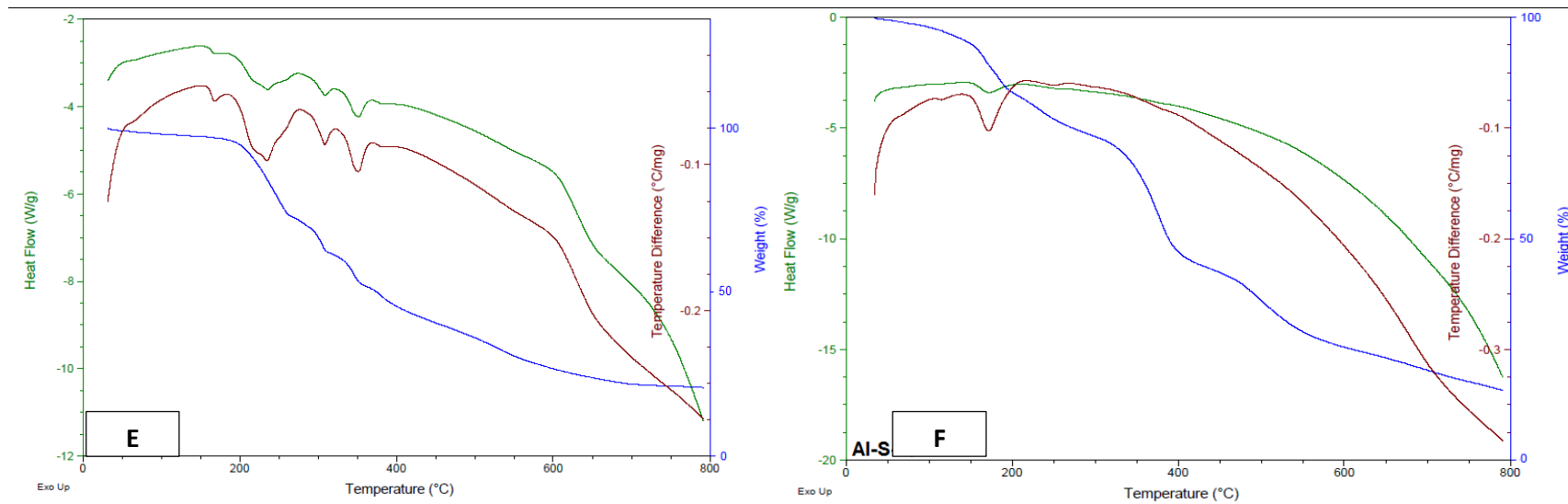


**Figures (S3):** The mass spectrum of Salen Schiff base ligand (A) and its mixed 8-hydroxy quinoline (B)CoSQ, (C)AlSQ, (D)LaSQ complexes

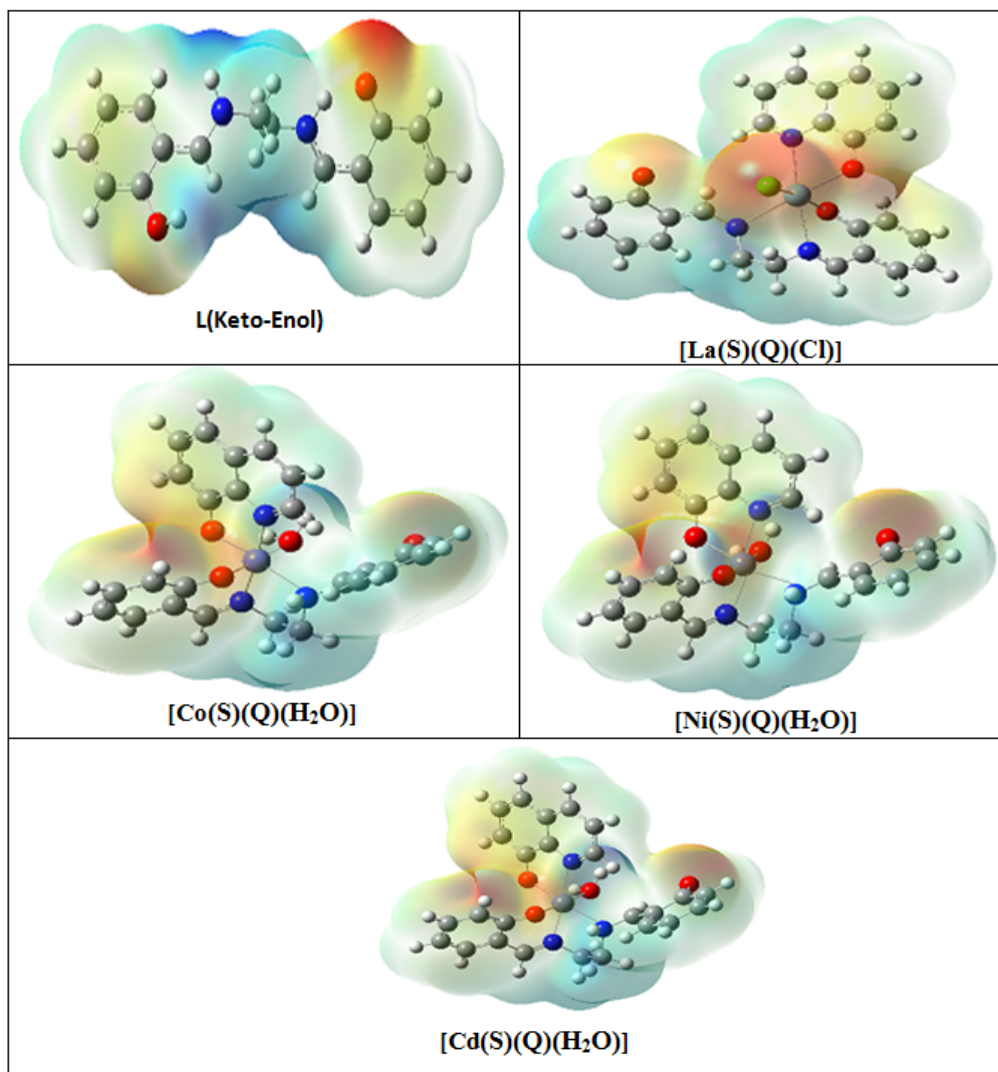


**Figures (S4):** PXRD powder pattern of Salen and its mixed CdSQ and LaSQ complexes. with 8-hydroxy quinolone

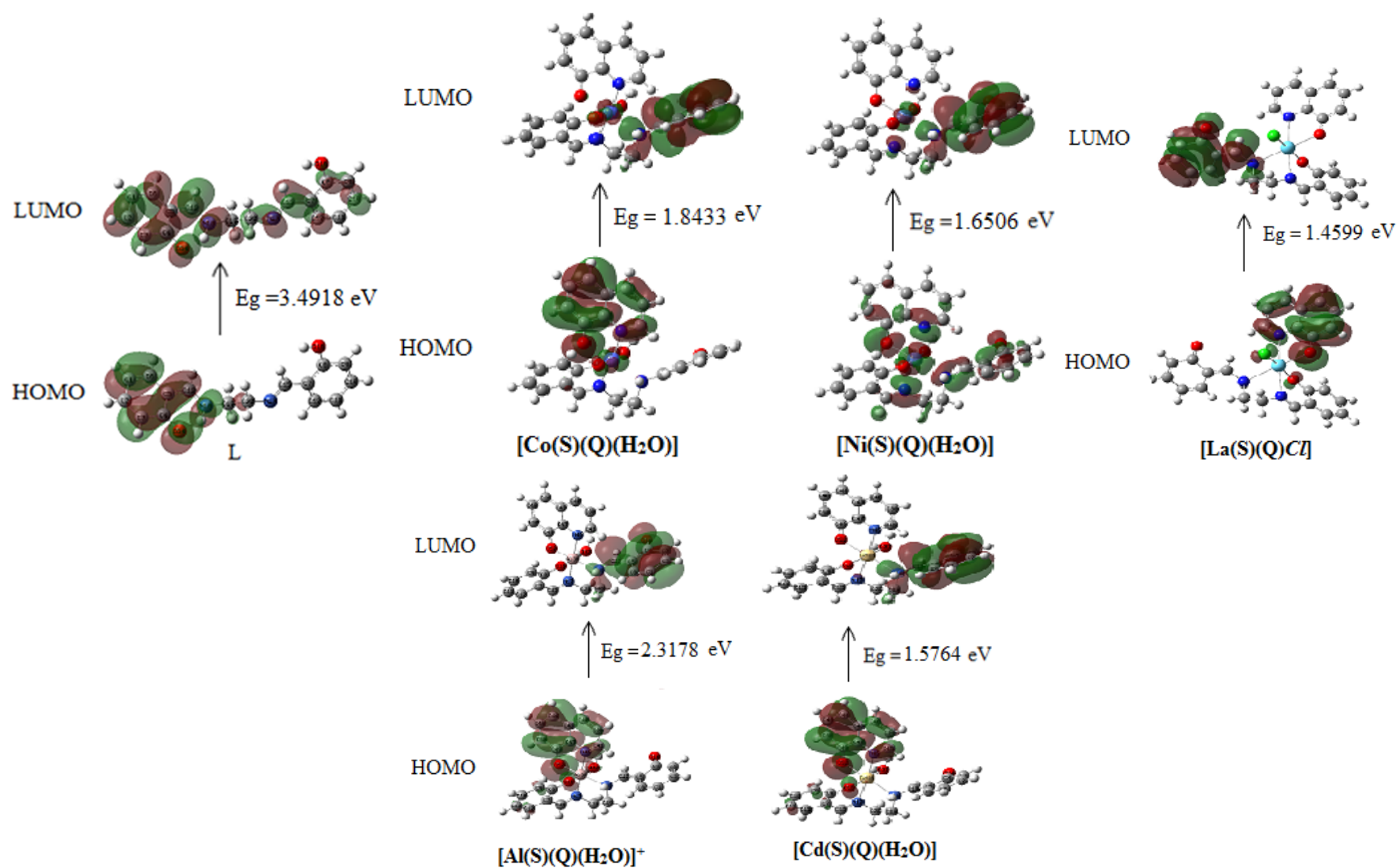




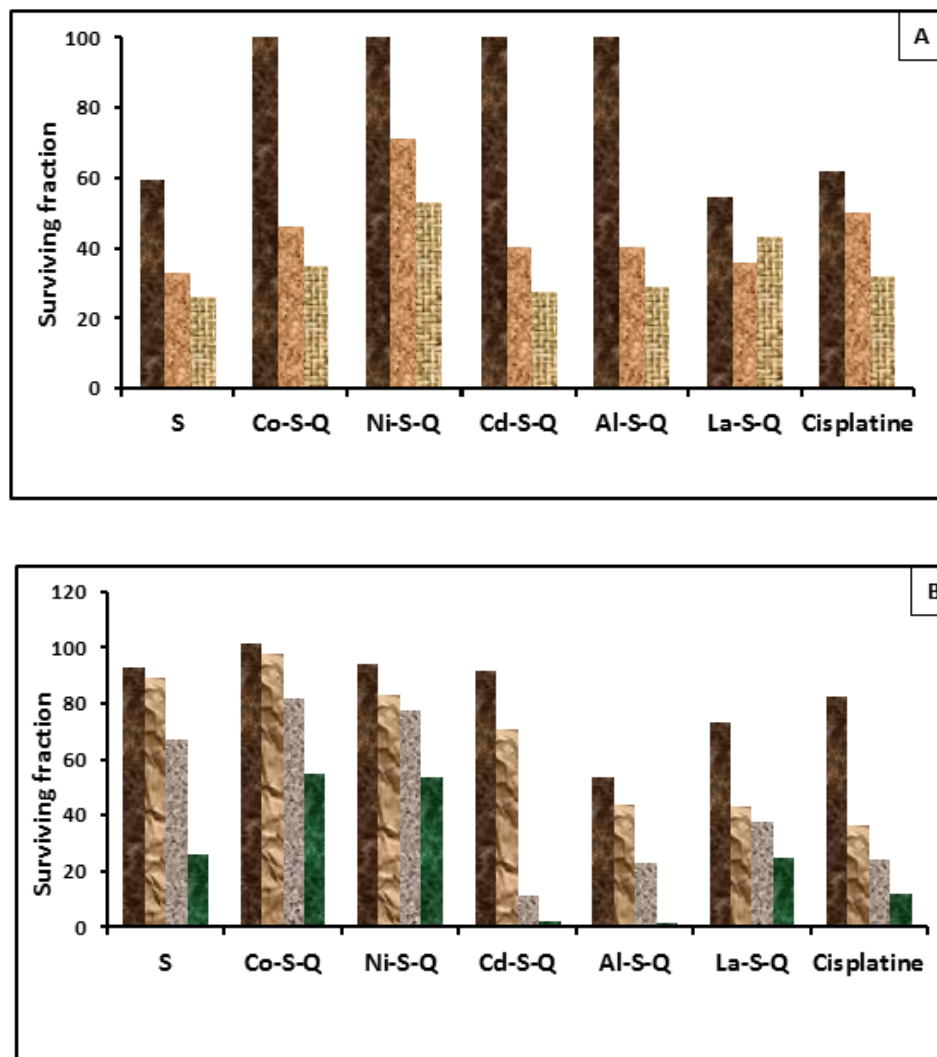
**Figures (S5):** Characteristic DSC-TGA curve of Salen ligand (A) and and its mixed 8-hydroxy quinoline (B)CoSQ, (C)NiSQ, (D)CdSQ, (E)AlSQ, (F)LaSQ complexes



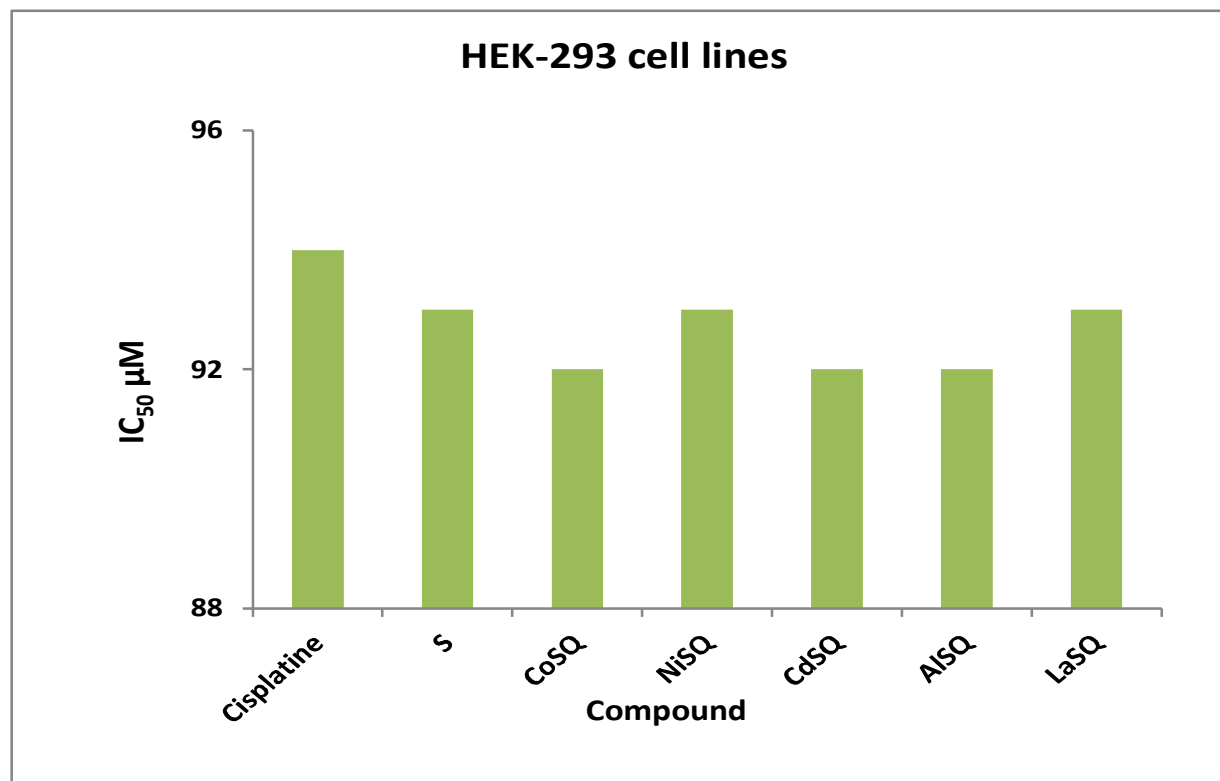
**Figure S6:** Molecular electrostatic potential (MEP) surface of ligand, L (Keto-Enol) and complexes [Co(S)(Q)(H<sub>2</sub>O)], [Ni(S)(Q)(H<sub>2</sub>O)], [Cd(S)(Q)(H<sub>2</sub>O)], and [La(S)(Q) Cl] using B3LYP/LANL2DZ.



**Figure S7:** HOMO and LUMO charge density maps of ligand and complexes [Co(S)(Q)(H<sub>2</sub>O)], [Ni(S)(Q)(H<sub>2</sub>O)], [Cd(S)(Q)(H<sub>2</sub>O)], [Al(S)(Q)(H<sub>2</sub>O)]<sup>+</sup> and [La(S)(Q)(Cl)] using B3LYP/LANL2DZ

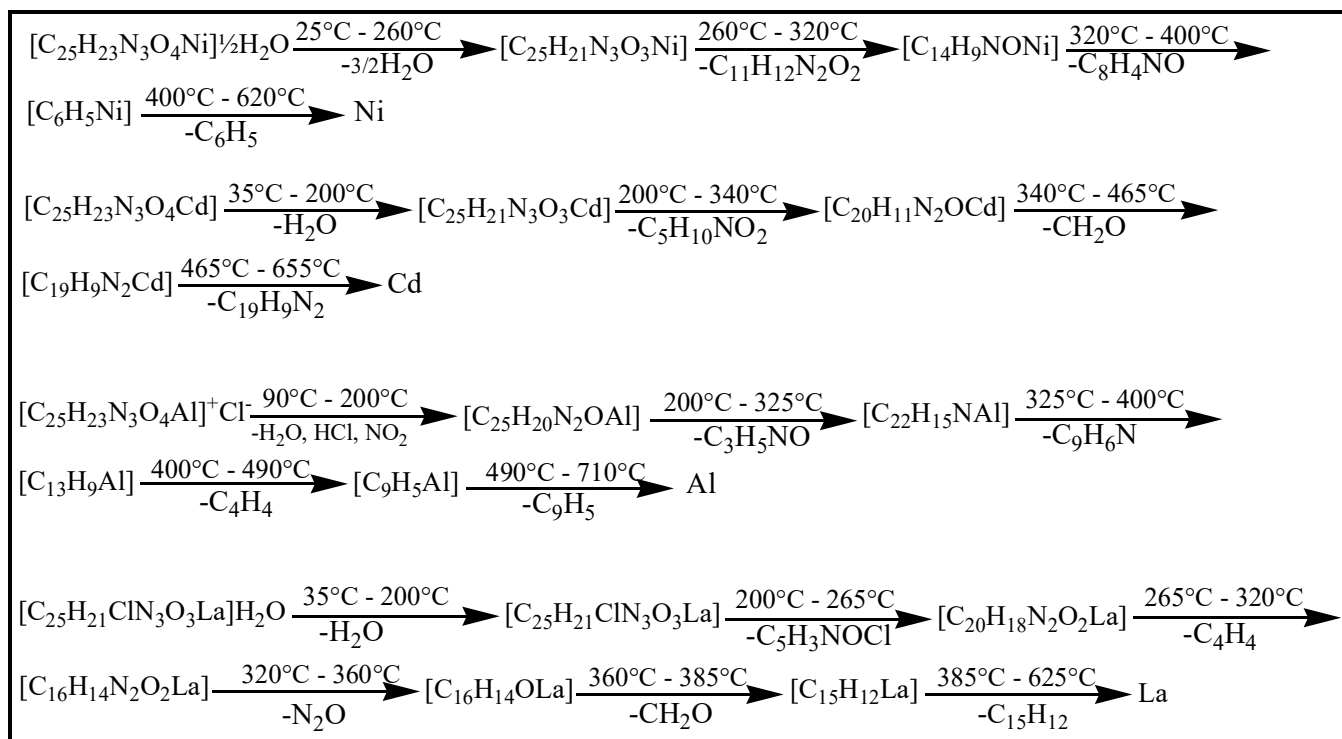


**Figure(S8): Graph showing values of % viability of (A) Hep-G2 and (B)MDA-MB231 breast cell lines in different concentration for Salen and its Co(II), Ni(II), Cd(II), Al(III), La(III) mixed 8-hydroxy quinoline -Salen Complexes**

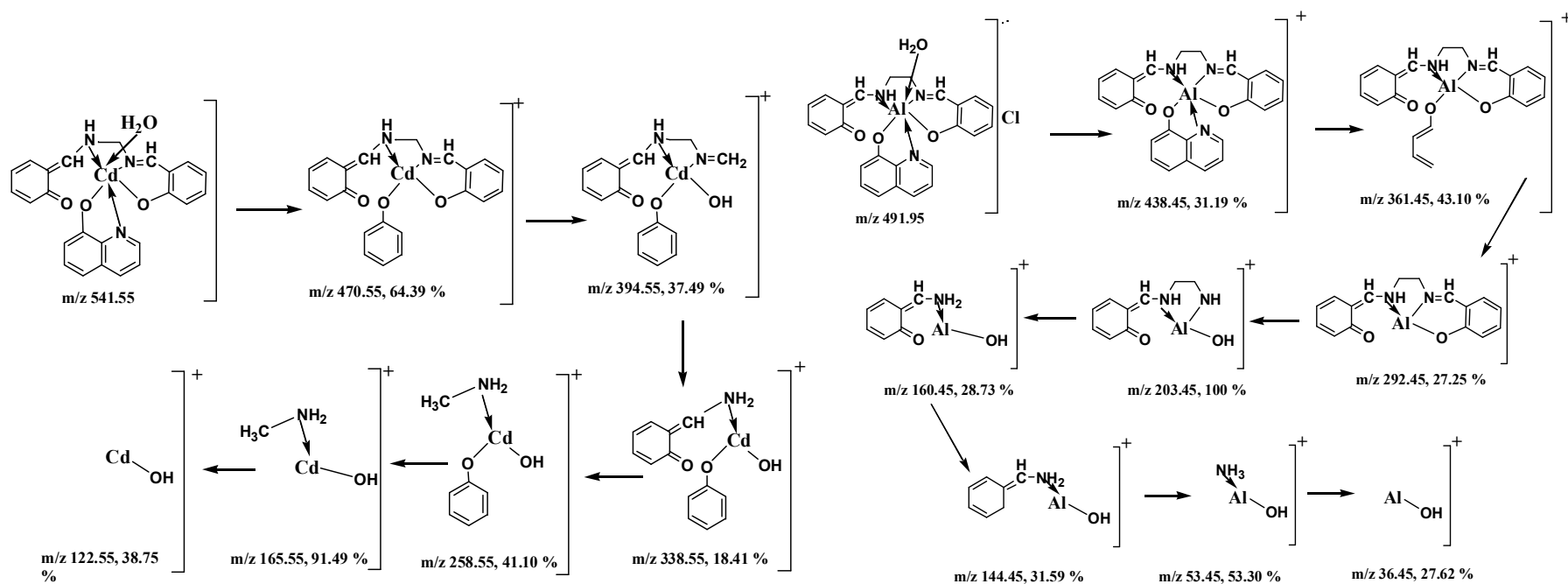


**Figure S9: IC<sub>50</sub> Values of Salen and its Cd(II), Al(III) and La(III) mixed 8-hydroxy quinoline complexes against HEK-293 cell lines compared to cisplatin.**





**Scheme S1:** Thermo gravimetric degradation steps for the prepared Mixed salen/8-hydroxy quinoline complexes with Ni(II), Cd(II), Al(III), La(III) from ambient temperature to 800 °C at heating rate of 10 °C / min



**Scheme S2:** Mass fragmentation of CdSQ and ALSQ complexes