

## SUPPLEMENTARY INFORMATION

### Cutting-Edge Green Synthesis and Characterization of Novel Ni(II) and Co(II) Fluoroimine Complexes: A Multifaceted Evaluation of Anticancer, Antioxidant, and Antimicrobial Activities

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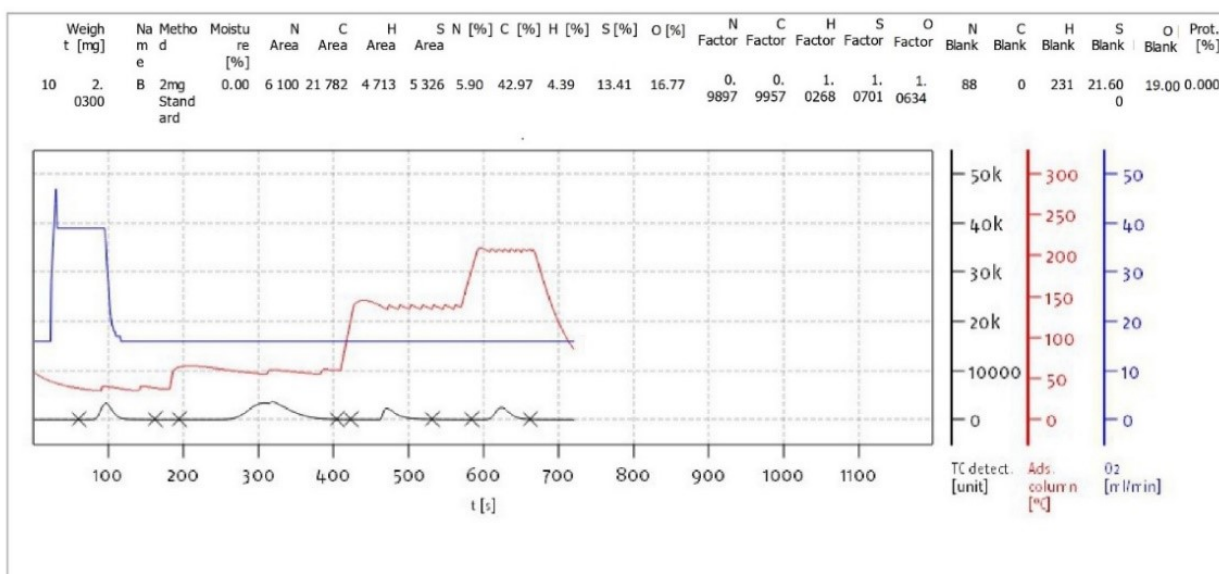
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#### analytic functional testing

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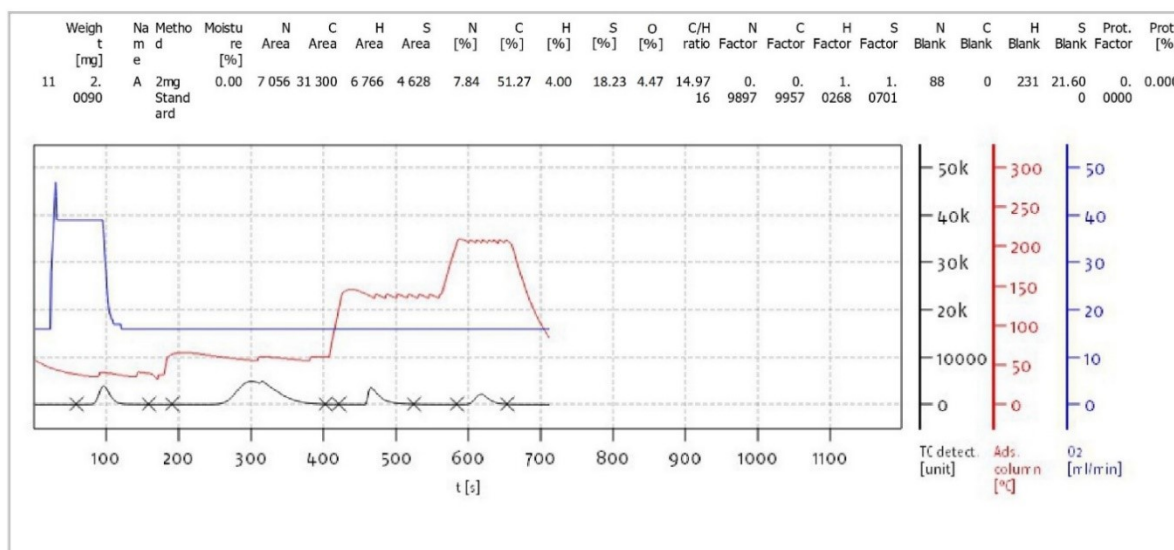
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Page 1 (from 6)

Fig. S1- Elemental analysis data of  $[\text{Ni}(\text{L}_1)(\text{OAc})(\text{H}_2\text{O})_3]$

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 Serial No: 0400.191001  
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Page 2 (from 6)

Fig. S2- Elemental analysis data of  $[\text{Ni}(\text{L}_1)_2 (\text{H}_2\text{O})_2]$

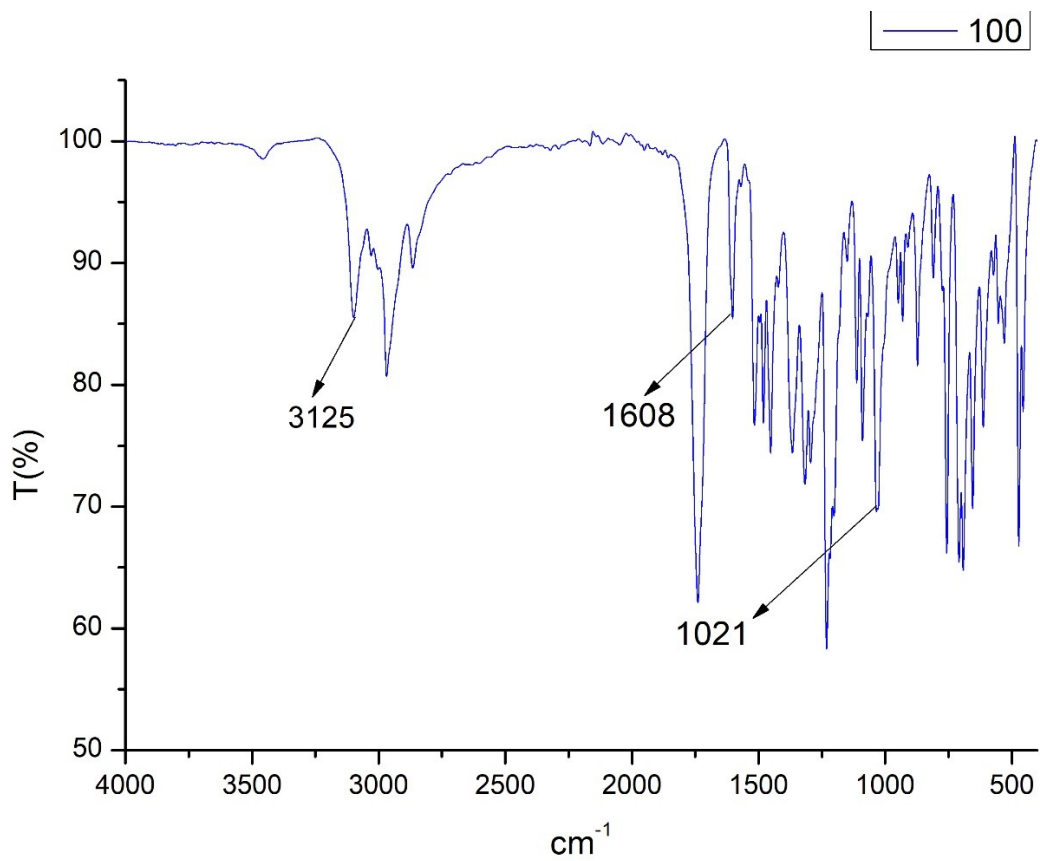


Fig. S3- FT-IR spectrum of ligand L<sub>1</sub>H

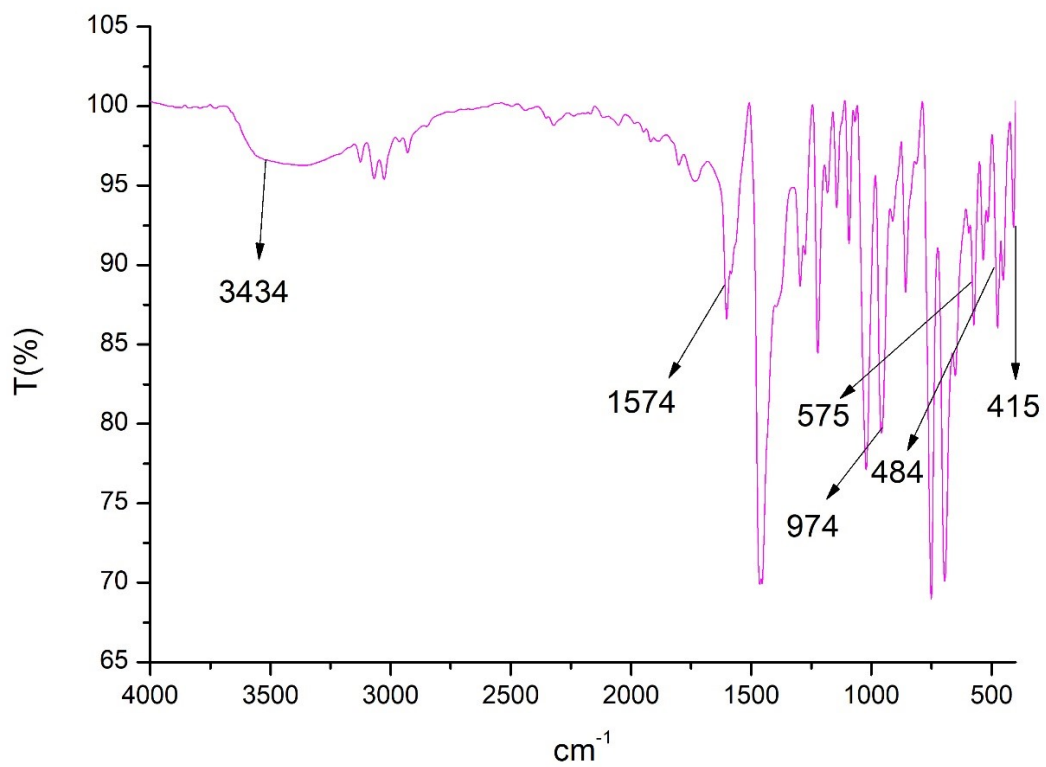


Fig. S4- FT-IR spectrum of complex [Ni(L<sub>1</sub>)(OAc)(H<sub>2</sub>O)<sub>3</sub>]

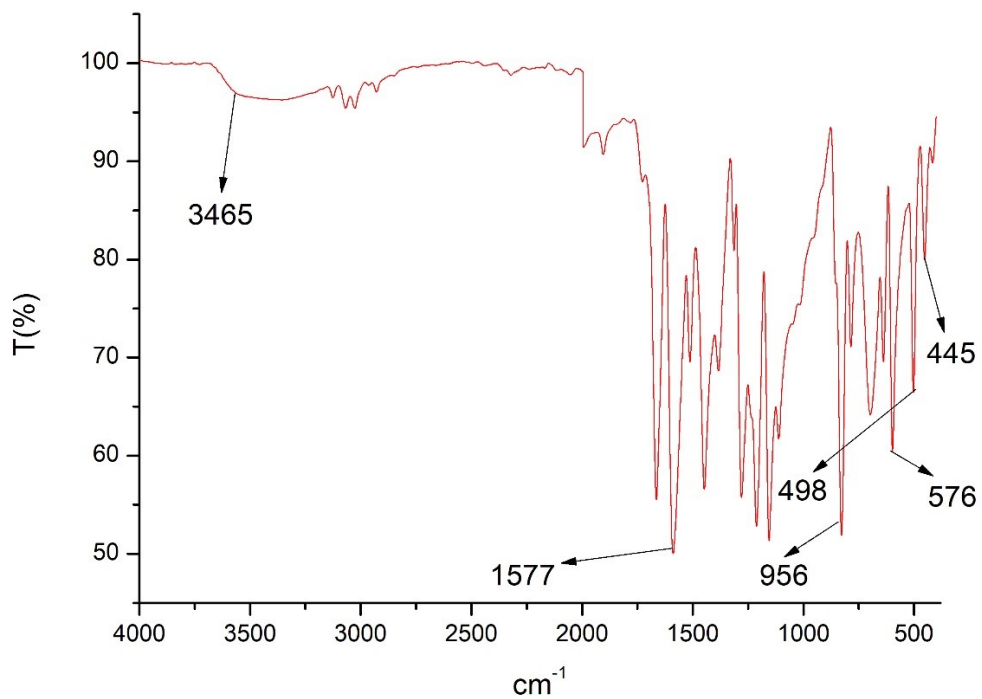


Fig. S5- FT-IR spectrum of complex  $[\text{Ni}(\text{L}_1)_2(\text{H}_2\text{O})_2]$

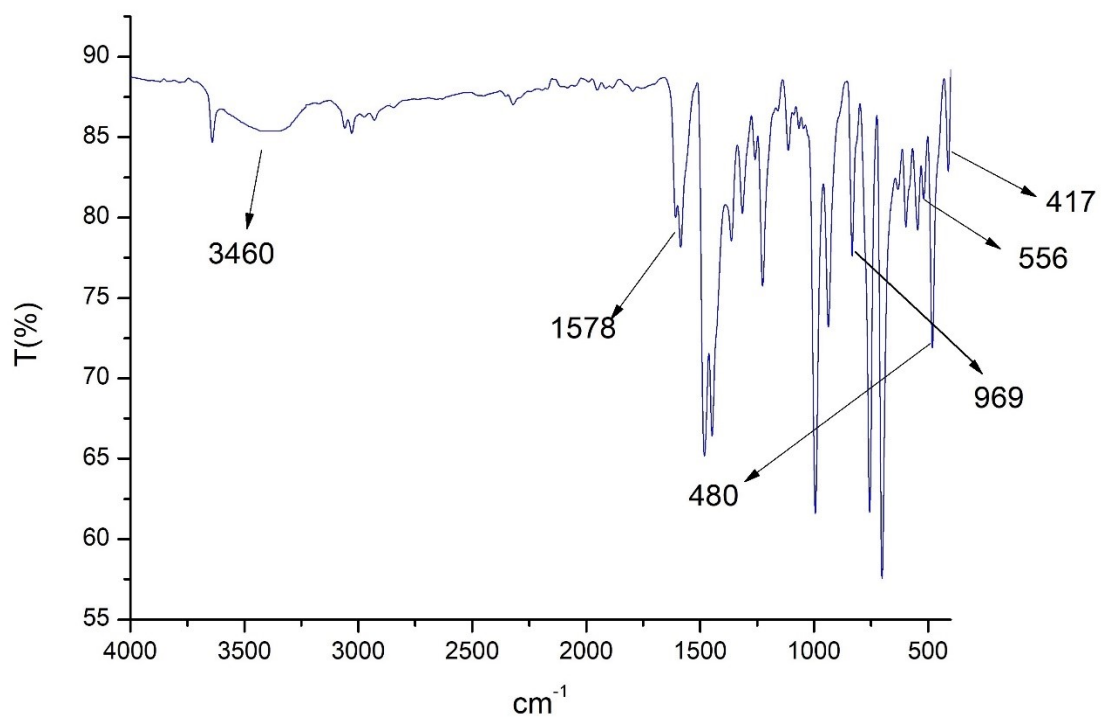


Fig. S6- FT-IR spectrum of complex  $[\text{Co}(\text{L}_1)(\text{OAc})(\text{H}_2\text{O})_3]$

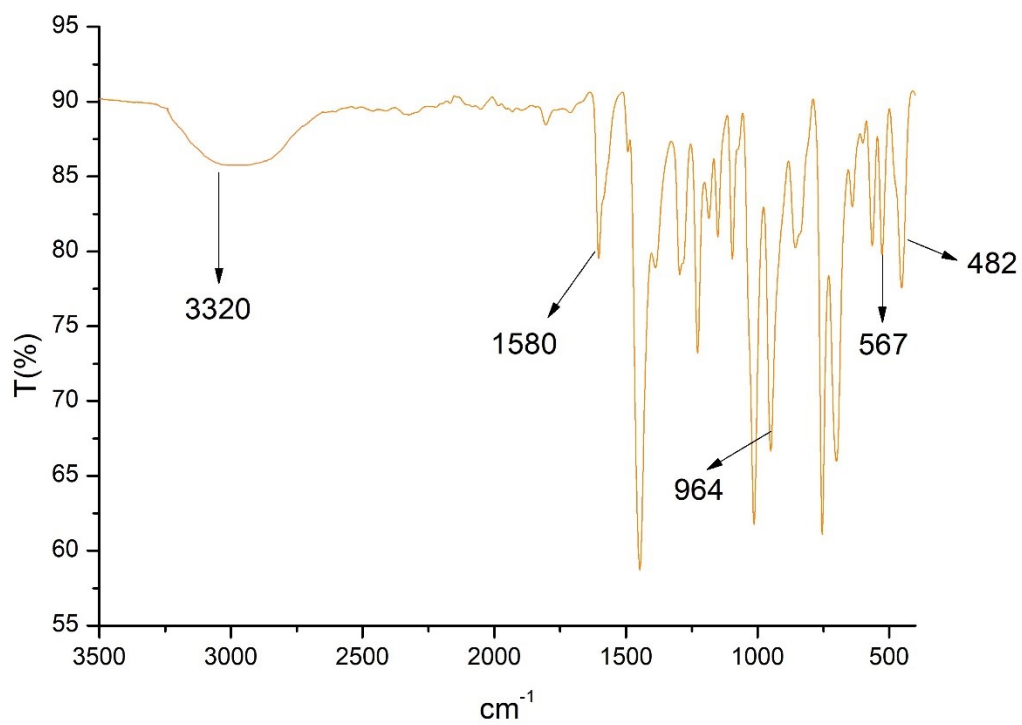


Fig. S7- FT-IR spectrum of complex  $[\text{Co}(\text{L}_1)_2(\text{H}_2\text{O})_2]$

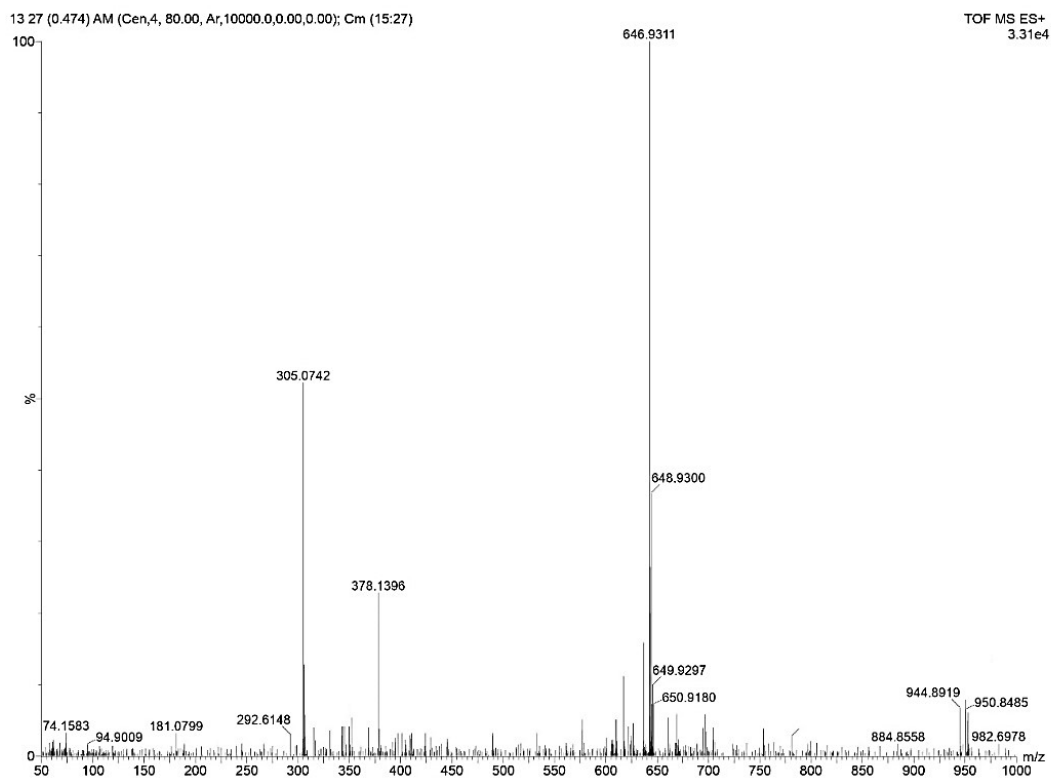


Fig. S8- GSI-MS spectrum of ligand  $\text{L}_1\text{H}$

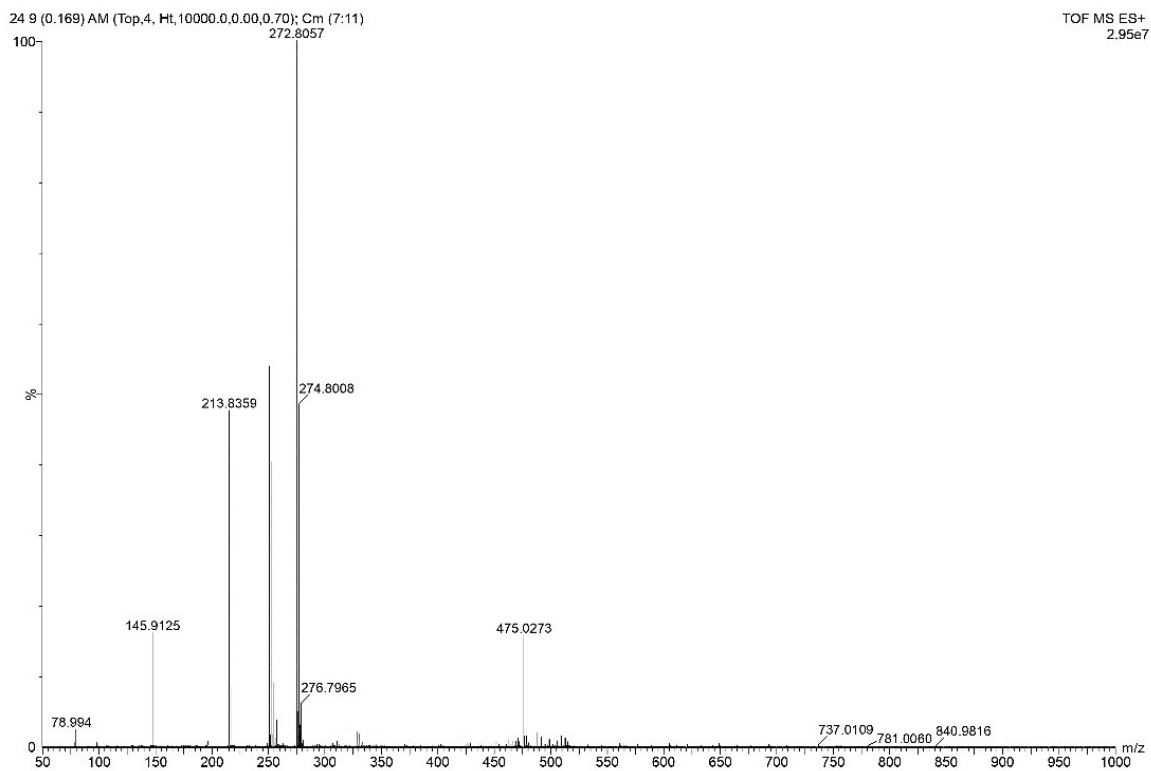


Fig. S9- GSI-MS spectrum of complex  $[\text{Ni}(\text{L}_1)(\text{OAc})(\text{H}_2\text{O})_3]$

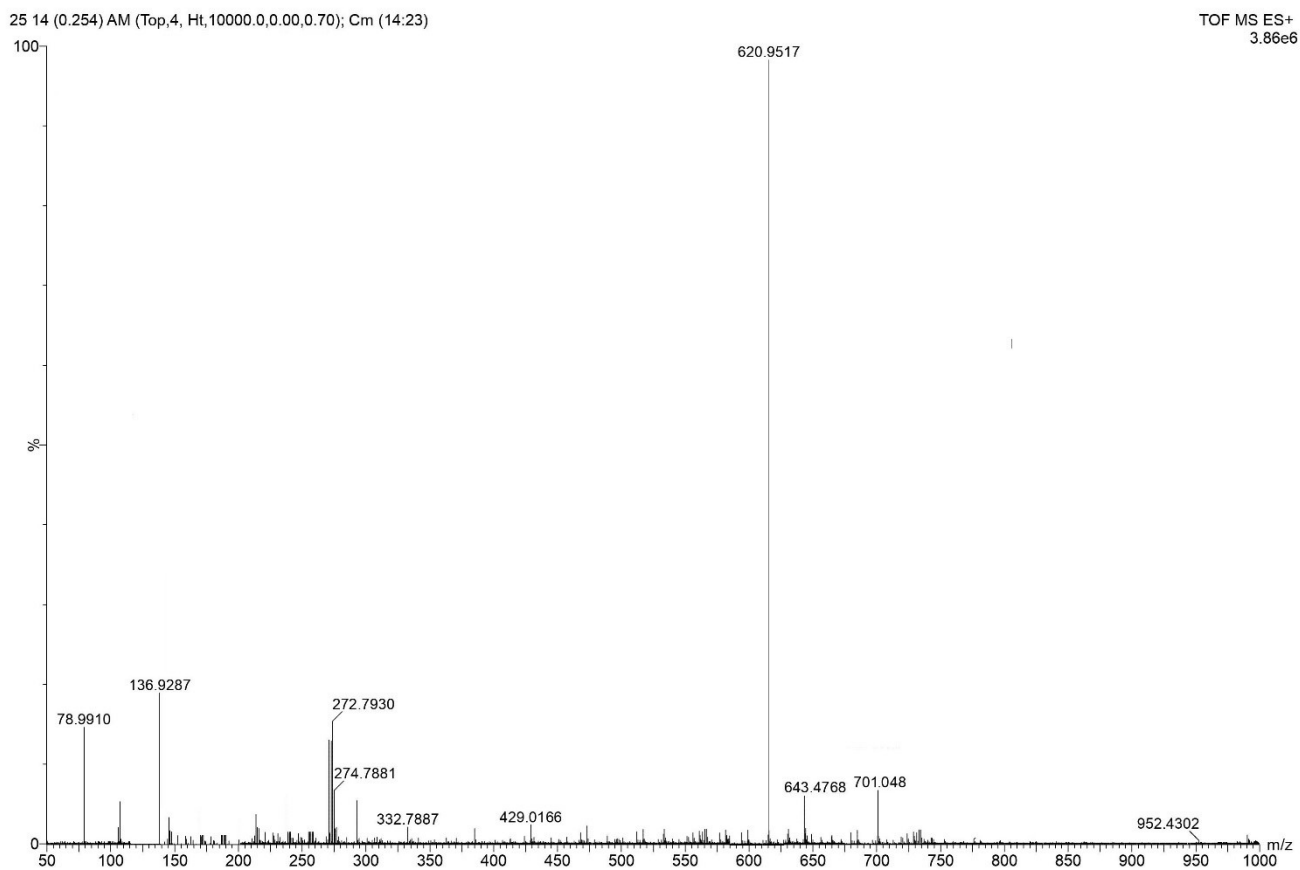


Fig. S10- GSI-MS spectrum of complex  $[\text{Ni}(\text{L}_1)_2(\text{H}_2\text{O})_2]$

26 11 (0.203) AM (Top,4, HI,10000.0,0.00,0.70); Cm (11:15)

TOF MS ES+  
6.79e6

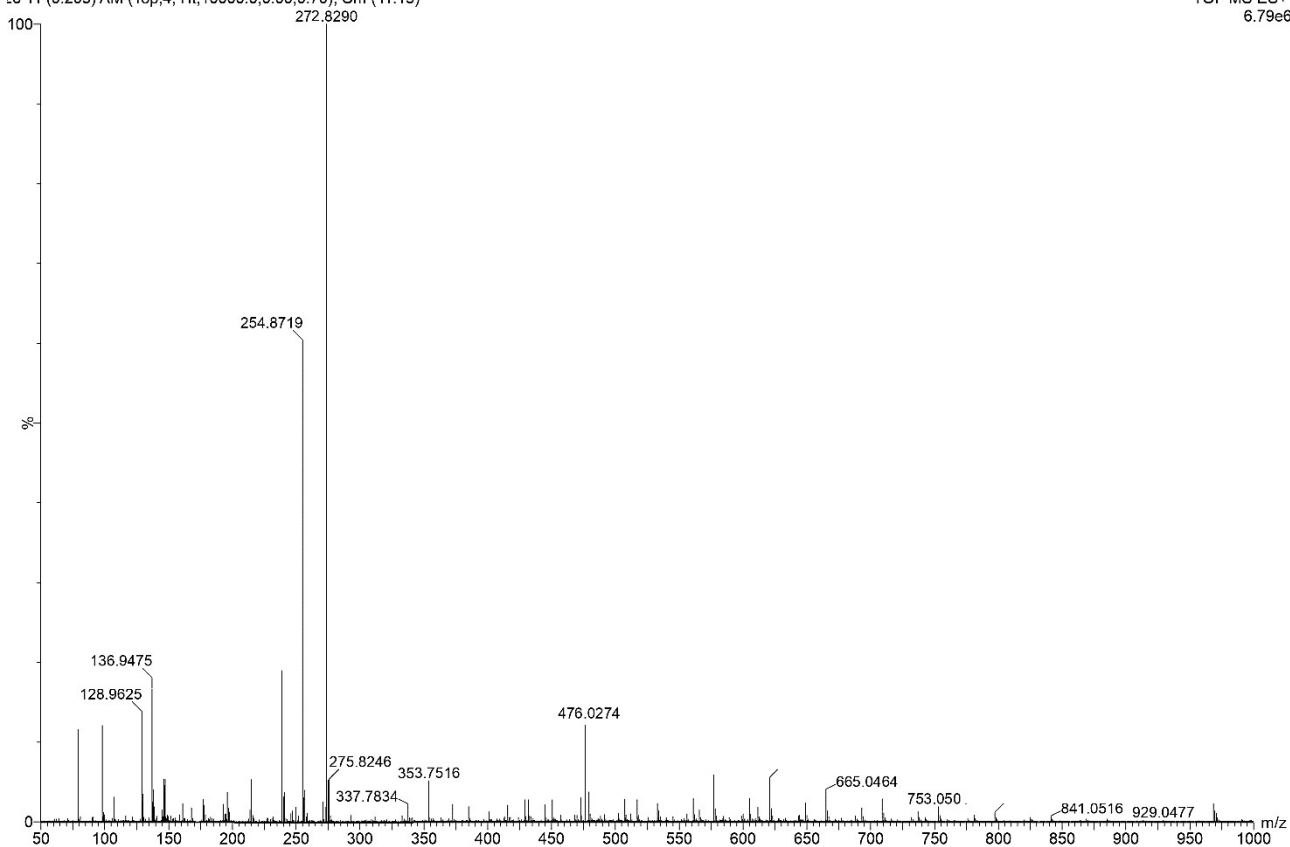


Fig. S11- GSI-MS spectrum of complex  $[\text{Co}(\text{L}_1)(\text{OAc})(\text{H}_2\text{O})_3]$

16 10 (0.186) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.00); Cm (6:17)

TOF MS ES+  
1.99e4

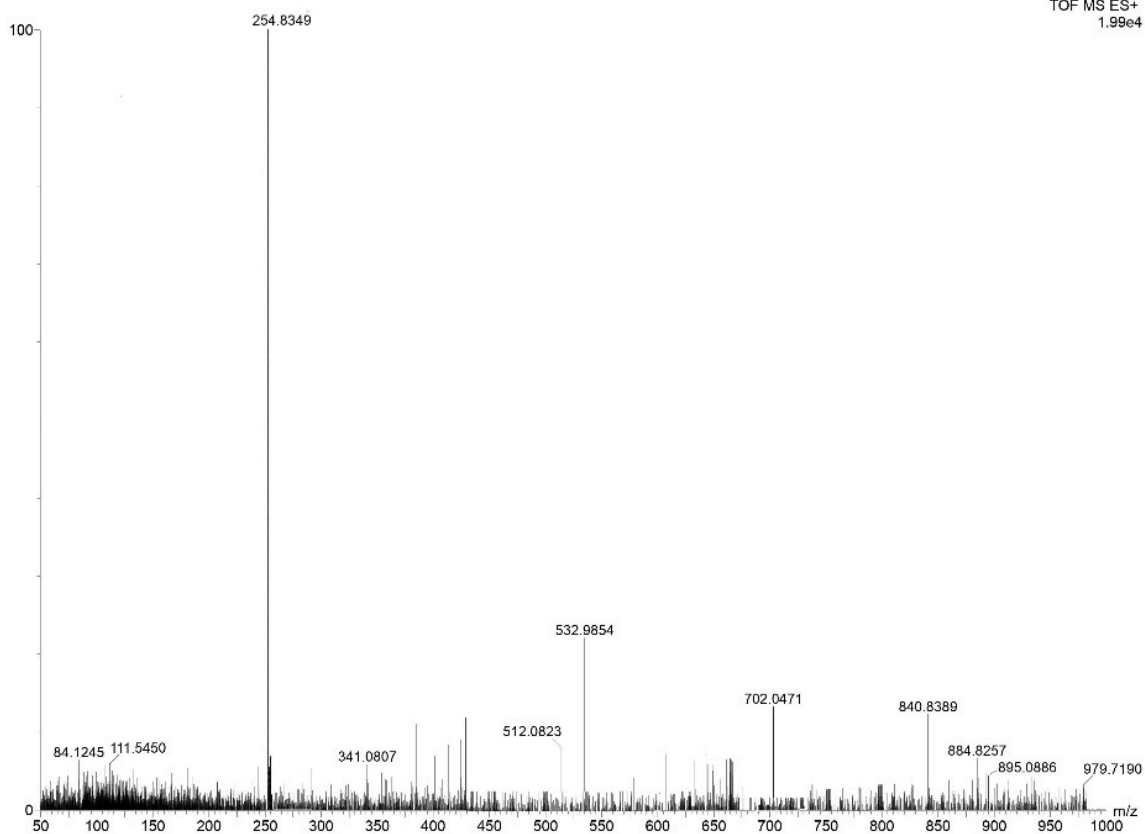


Fig. S12- GSI-MS spectrum of complex  $[\text{Co}(\text{L}_1)_2(\text{H}_2\text{O})_2]$

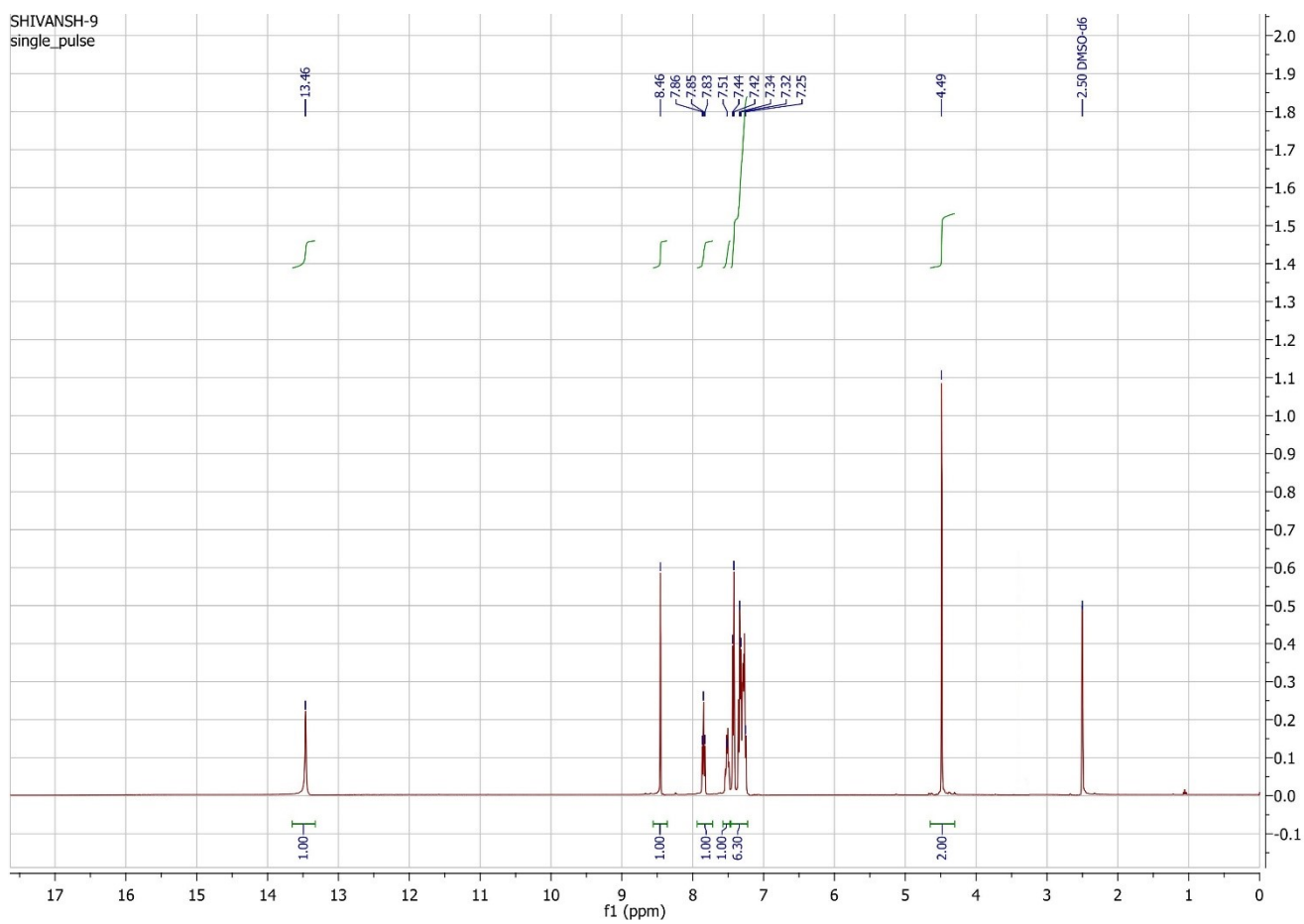


Fig. S13-  $^1\text{H}$ -NMR spectrum of ligand  $\text{L}_1\text{H}$



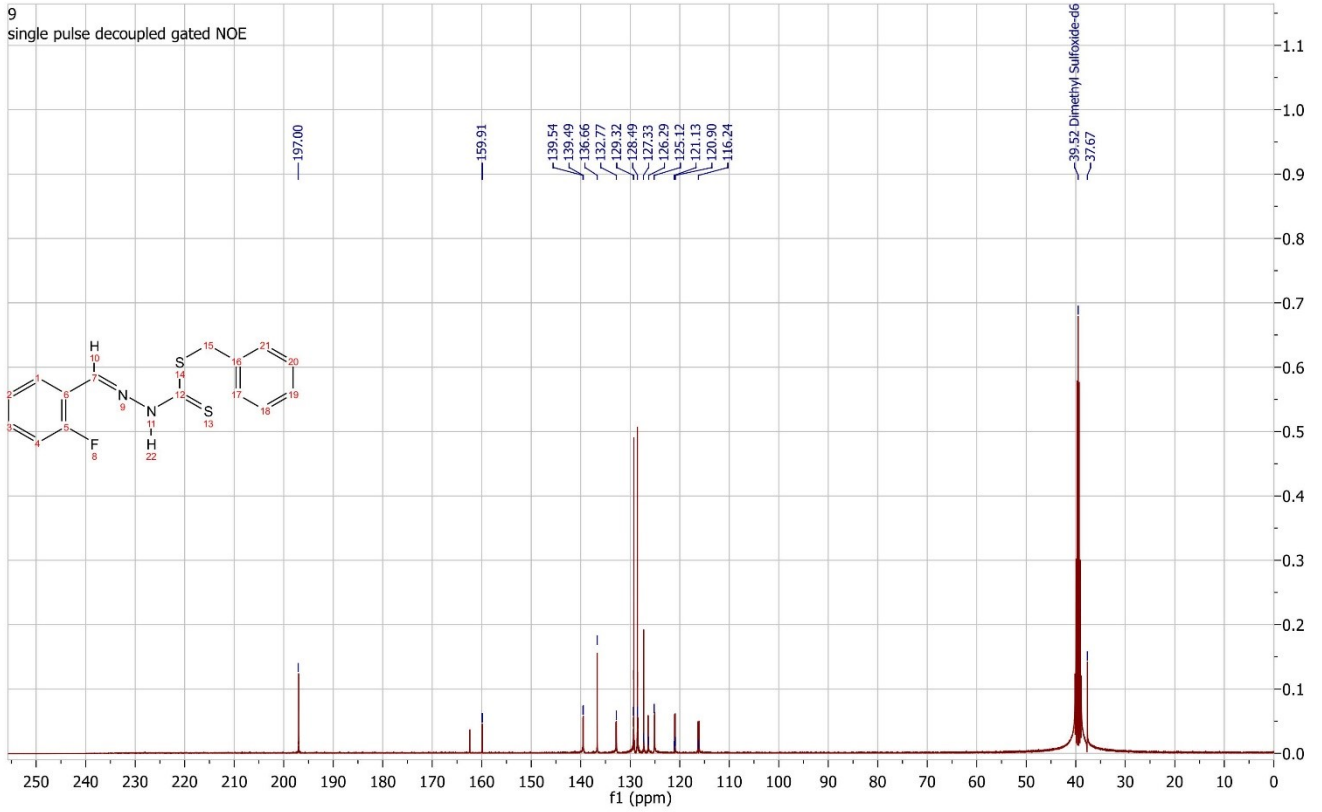


Fig. S14-  $^{13}C$ -NMR spectrum of ligand  $L_1H$

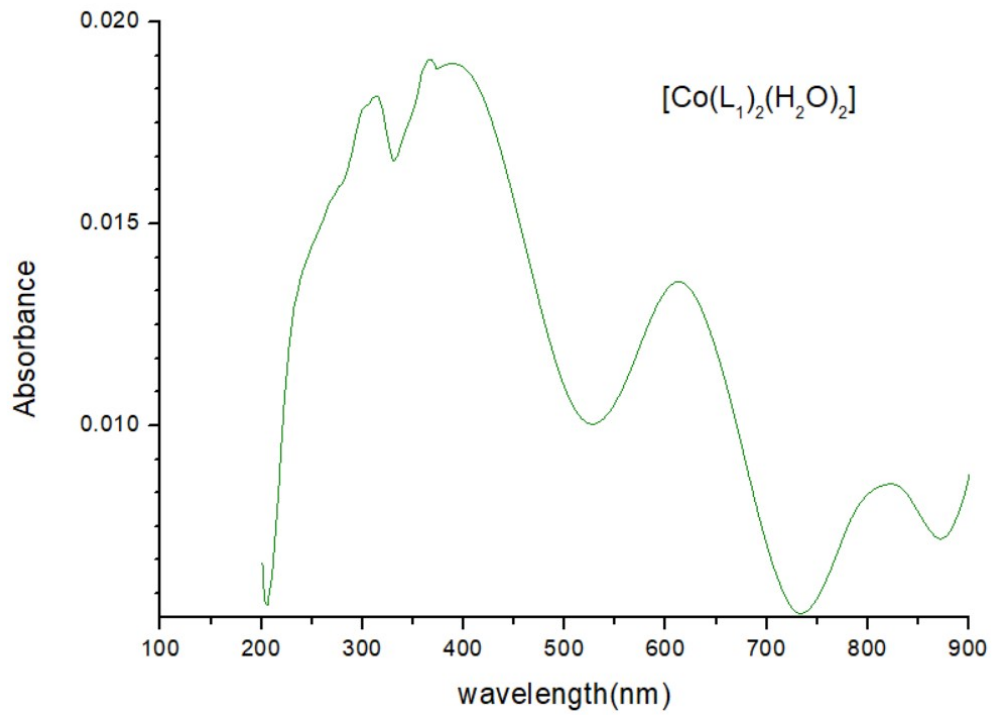


Fig. S15- Electronic absorption spectrum(UV-Visible) of Co(II) complex

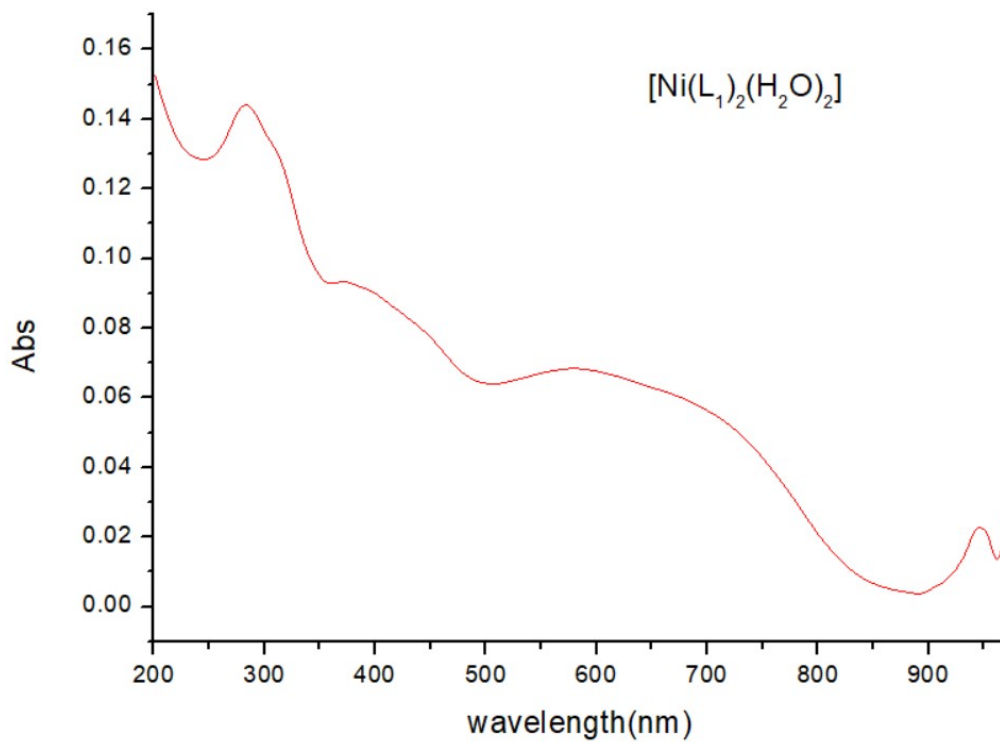


Fig. S16- Electronic absorption spectrum(UV-Visible) of Ni(II) complex

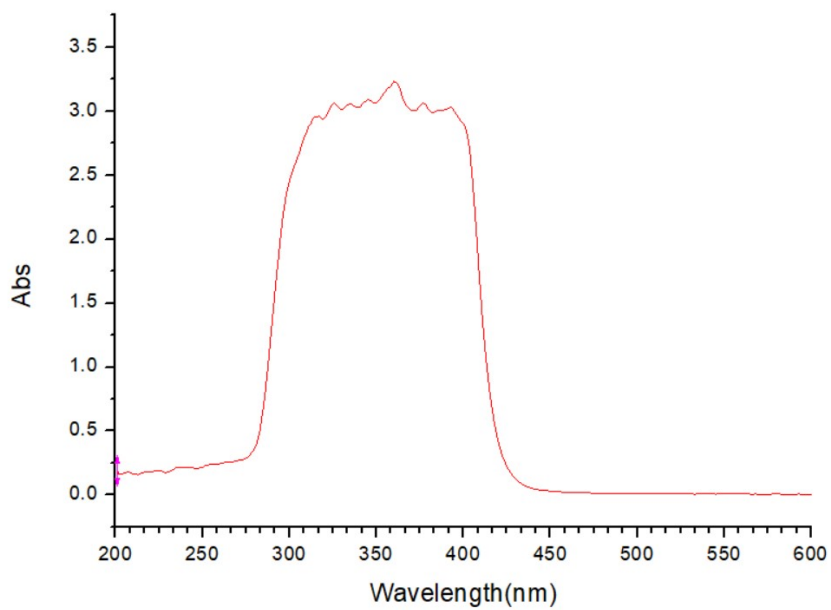


Fig. S17- Electronic absorption spectrum(UV-Visible) of ligand  $\text{L}_1\text{H}$

Concentration (µg)	Absorbance at 570nm	% Inhibition	% Viability	IC50 (µg)
5	0.492	4.65	95.35	89.24
10	0.464	10.07	89.93	
25	0.395	23.44	76.56	
50	0.332	35.65	64.35	
100	0.247	52.13	47.87	
Untreated	0.516	0	100	
Blank	0	0	0	

Table-1 Cytotoxicity screening data for complex L<sub>1</sub>H against MCF-7 cell line

Concentration (µg)	Absorbance at 570nm	% Inhibition	% Viability	IC <sub>50</sub> (µg)
5	0.609	3.02	96.98	86.1
10	0.584	7	93	
25	0.523	16.71	83.29	
50	0.422	32.8	67.2	
100	0.275	56.21	43.79	
Untreated	0.628	0	100	
Blank	0	0	0	

Table-2 Cytotoxicity screening data for complex L<sub>1</sub>H against HeLa cell line

Concentration (µg)	Absorbance at 570nm	% Inhibition	% Viability	IC <sub>50</sub> (µg)
5	0.965	2.12	97.88	344.73
10	0.934	5.27	94.73	
25	0.897	9.02	90.98	
50	0.868	11.96	88.04	
100	0.827	16.12	83.88	
Untreated	0.986	0	100	
Blank	0	0	0	

Table-3 Cytotoxicity screening data for complex L<sub>1</sub>H against normal human HEK293 cell line

Concentration (µg)	Absorbance at 570nm	% Inhibition	% Viability	IC50 (µg)
5	0.496	3.87	96.13	60.48
10	0.457	11.43	88.57	
25	0.385	25.38	74.62	
50	0.254	50.77	49.23	
100	0.129	75	25	
Untreated	0.516	0	100	
Blank	0	0	0	

Table-4 Cytotoxicity screening data for complex  $[\text{Ni}(\text{L}_1)_2 (\text{H}_2\text{O})_2]$  against MCF-7 cell line

Concentration (µg)	Absorbance at 570nm	% Inhibition	% Viability	IC50 (µg)
5	0.585	6.84	93.16	55.28
10	0.546	13.05	86.95	
25	0.419	33.28	66.72	
50	0.273	56.52	43.48	
100	0.145	76.91	23.09	
Untreated	0.628	0	100	
Blank	0	0	0	

Table-5 Cytotoxicity screening data for complex  $[\text{Ni}(\text{L}_1)_2 (\text{H}_2\text{O})_2]$  against HeLa cell line

Concentration (µg)	Absorbance at 570nm	% Inhibition	% Viability	IC50 (µg)
5	0.971	1.52	98.48	399.22
10	0.952	3.44	96.56	
25	0.913	7.4	92.6	
50	0.886	10.14	89.86	
100	0.853	13.48	86.52	
Untreated	0.986	0	100	
Blank	0	0	0	

Table-6 Cytotoxicity screening data for complex  $[\text{Ni}(\text{L}_1)_2 (\text{H}_2\text{O})_2]$  against normal human HEK293 cell line

Concentration (µg)	Absorbance at 570nm	% Inhibition	% Viability	IC50 (µg)
5	0.965	2.12	97.88	344.73
10	0.934	5.27	94.73	
25	0.897	9.02	90.98	
50	0.868	11.96	88.04	
100	0.827	16.12	83.88	
Untreated	0.986	0	100	
Blank	0	0	0	

Table-7 Cytotoxicity screening data for complex  $[\text{Co}(\text{L}_1)_2 (\text{H}_2\text{O})_2]$  against MCF-7 cell line

Concentration (µg)	Absorbance at 570nm	% Inhibition	% Viability	IC50 (µg)
5	0.503	2.51	97.49	88.99
10	0.486	5.81	94.19	
25	0.449	12.98	87.02	
50	0.341	33.91	66.09	
100	0.238	53.87	46.13	
Untreated	0.516	0	100	
Blank	0	0	0	

Table-8 Cytotoxicity screening data for complex  $[\text{Co}(\text{L}_1)_2 (\text{H}_2\text{O})_2]$  against HeLa cell line

Concentration (µg)	Absorbance at 570nm	% Inhibition	% Viability	IC50 (µg)
5	0.593	5.57	94.43	59.67
10	0.566	9.87	90.13	
25	0.437	30.44	69.56	
50	0.294	53.18	46.82	
100	0.168	73.24	26.76	
Untreated	0.628	0	100	
Blank	0	0	0	

Table-9 Cytotoxicity screening data for complex  $[\text{Co}(\text{L}_1)_2 (\text{H}_2\text{O})_2]$  against normal human HEK293 cell line

Concentration(ppm)	L <sub>1</sub> H	[Ni(L <sub>1</sub> )(OAc)(H <sub>2</sub> O) <sub>3</sub> ]	[Ni(L <sub>1</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]	[Co(L <sub>1</sub> )(OAc)(H <sub>2</sub> O) <sub>3</sub> ]	[Co(L <sub>1</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]
20	12.64	36.45	23.78	32.67	17.11
40	16.78	44.67	30.87	37.6	23.01
60	22.67	49.54	36.09	43.58	29.86
80	28.45	54.34	40.05	48.44	34.78
100	32.56	56.23	43.31	51.22	37.63

Table-10 Mean % Radical Scavenging activity of compounds against DPPH free radical

Concentration(ppm)	L <sub>1</sub> H	[Ni(L <sub>1</sub> )(OAc)(H <sub>2</sub> O) <sub>3</sub> ]	[Ni(L <sub>1</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]	[Co(L <sub>1</sub> )(OAc)(H <sub>2</sub> O) <sub>3</sub> ]	[Co(L <sub>1</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]
20	14.26	41.32	25.45	34.54	19.67
40	19.34	46.45	32.54	39.47	25.57
60	25.68	52.54	37.76	45.45	31.64
80	31.38	57.45	42.39	51.56	36.56
100	36.56	61.67	45.65	54.34	39.41

Table-11 Mean % Radical Scavenging activity of compounds against ABTS free radical

Compounds	<i>Penicillium</i> (50ppm)	<i>Penicillium</i> (100ppm)	<i>Penicillium</i> (150ppm)	<i>Penicillium</i> (200ppm)	<i>A.niger</i> (50ppm)	<i>A.niger</i> (100ppm)	<i>A.niger</i> (150ppm)	<i>A.niger</i> (200ppm)
L <sub>1</sub> H	6	9	11	12	6	8	10	12
[Ni(L <sub>1</sub> )(OAc)(H <sub>2</sub> O) <sub>3</sub> ]	10	14	16	19	10	12	16	18
[Ni(L <sub>1</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]	8	11	12	14	6.5	9	11	14
[Co(L <sub>1</sub> )(OAc)(H <sub>2</sub> O) <sub>3</sub> ]	8	10	13	13.5	7	8	9	13
[Co(L <sub>1</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]	11	12	14	15	8	10	13	15

Ketoconazole	24	26	28	30	22	24	26	27
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Table 12- Antifungal screening data of compounds in terms of mean radii of inhibition zone(mm)

Compounds	<i>E.coli</i> (50ppm)	<i>E.coli</i> (100ppm)	<i>E.coli</i> (150ppm)	<i>E.coli</i> (200ppm)	<i>S.aureus</i> (50ppm)	<i>S.aureus</i> (100ppm)	<i>S.aureus</i> (150ppm)	<i>S.aureus</i> (200ppm)
L <sub>1</sub> H	8	10	12	13	6	9	11	13
[Ni(L <sub>1</sub> )(OAc)(H <sub>2</sub> O) <sub>3</sub> ]	14	17	18	20	16	18	19	21
[Ni(L <sub>1</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]	9.5	10	12	13	11	12	13	15
[Co(L <sub>1</sub> )(OAc)(H <sub>2</sub> O) <sub>3</sub> ]	9	10.5	13	15	8	11	12	14
[Co(L <sub>1</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]	11	12	14	18	9	15	16	18
Ciprofloxacin(stand.)	24	27	29	31	26	28	30	32

Table 13- Antibacterial screening data of compounds in terms of mean radii of inhibition zone(mm)

h	K	L	2θ (Exp.) (Degree)	2θ (Calc.) (Degree)	2θ (Diff.) (Degree)	d (Exp.) (Å)	d (Calc.) (Å)	Intensity (Exp.)
0	2	2	22.8565	22.6547	0.2018	3.886128	4.06150	1950
1	1	1	24.4751	24.4231	0.052	3.63267	3.67723	1802
1	2	0	28.8009	28.9876	-0.1867	3.096131	3.11234	1344
1	1	2	29.5314	29.5761	-0.0447	3.021184	3.15432	1292
2	1	0	30.7633	30.8765	-0.1132	2.902951	2.91611	1434
1	3	0	32.7543	32.4567	0.2976	2.730895	2.70767	1640
2	2	1	39.1571	39.3256	-0.1685	2.297829	2.26341	1222
3	1	2	45.0702	45.1234	-0.0532	1.982378	1.98421	1345
2	3	2	56.1998	56.3067	-0.1069	1.63240	1.64047	1113
4	0	0	56.9889	56.7689	0.2200	1.61579	1.62460	1324

Table 14- h,k,l value and other lattice parameters for complex [Co(L<sub>1</sub>)<sub>2</sub> (H<sub>2</sub>O)<sub>2</sub>]

<b>h</b>	<b>K</b>	<b>L</b>	<b>2θ (Exp.) (Degree)</b>	<b>2θ (Calc.) (Degree)</b>	<b>2θ (Diff.) (Degree)</b>	<b>d (Exp.) (Å)</b>	<b>d (Calc.) (Å)</b>	<b>Intensity (Exp.)</b>
1	0	0	13.0016	13.3456	0.344	6.801094	6.68251	1178
1	0	1	14.9210	14.7654	-0.1556	5.930255	5.910255	2011
1	1	0	17.6855	17.8965	0.211	5.009005	5.109002	1350
1	1	1	19.6766	19.4356	-0.241	4.506398	4.406396	941
2	0	0	20.3498	20.4567	0.1069	4.358814	4.258812	1242
2	1	0	22.1689	22.2345	0.0656	4.005084	4.002085	1544
2	1	1	24.0284	24.2345	0.2061	3.699182	3.38324	1222
2	2	0	26.4948	26.7345	0.2397	3.360153	3.260156	1278
2	2	1	28.8296	28.6978	-0.1318	3.093114	3.043116	1113
2	2	2	29.6894	28.8976	-0.7918	3.005465	3.005503	1324
3	0	0	30.8976	30.5783	0.1193	2.890638	2.712215	1950
3	1	0	35.0605	35.2315	0.1710	2.556362	2.456363	450
3	2	0	41.1481	41.4567	0.3086	2.191125	2.091126	490

Table 15- h,k,l value and other lattice parameters for complex  $[\text{Ni}(\text{L}_1)_2(\text{H}_2\text{O})_2]$