Table S1: Selected bond lengths (Å) of ligand.

Sr.No	Atoms	Actual bond lenghts	Optimal bond lenghts
1	C(11)-N(3)	1.269	1.260
2	N(12)-C(28)	1.264	1.260
3	N(12)-C(13)	1.271	1.456
4	C(2)-N(3)	1.275	1.456
5	C(29)-O(39)	1.366	1.355
6	C(48)-O(50)	1.361	1.355

Table S2: Various bond length (Å) of $[Co(L)(H_2O)_2].3H_2O$ complex (**1**).

Sr. No	Atoms	Actual bond length	Optimal bond length	Sr. No.	Atoms	Actual bond length	Optimal bond length
1	O(52)-H(84)	1.185	0.942	48	C(44)-C(39)	1.336	1.420
2	O(52)-H(83)	1.084	0.942	49	C(43)-C(44)	1.372	1.420
3	O(51)-H(82)	1.094	0.942	50	C(42)-C(43)	1.334	1.420
4	O(51)-H(81)	1.221	0.942	51	C(41)-C(42)	1.365	1.420
5	C(46)-H(80)	1.107	1.100	52	C(40)-C(41)	1.365	1.420
6	C(45)-H(79)	1.118	1.100	53	C(39)-C(40)	1.341	1.420
7	C(44)-H(78)	1.093	1.100	54	C(38)-C(33)	1.359	1.420
8	C(41)-H(77)	1.127	1.100	55	C(37)-C(38)	1.352	1.420
9	C(40)-H(76)	1.120	1.100	56	C(36)-C(37)	1.344	1.420
10	C(39)-H(75)	1.145	1.100	57	C(35)-C(36)	1.344	1.420
11	C(38)-H(74)	1.093	1.100	58	C(32)-C(35)	1.351	1.420
12	C(37)-H(73)	1.118	1.100	59	C(34)-C(29)	1.381	1.420
13	C(36)-H(72)	1.115	1.100	60	C(33)-C(34)	1.371	1.420
14	C(35)-H(71)	1.105	1.100	61	C(32)-C(33)	1.349	1.420
15	C(31)-H(70)	1.100	1.100	62	C(31)-C(32)	1.344	1.420
16	C(30)-H(69)	1.125	1.100	63	C(30)-C(31)	1.351	1.420
17	C(28)-H(68)	1.128	1.100	64	C(29)-C(30)	1.350	1.420
18	C(27)-H(67)	1.094	1.100	65	C(28)-N(12)	1.295	1.260
19	C(26)-H(66)	1.091	1.100	66	N(21)-C(24)	1.414	1.345
20	C(25)-H(65)	1.085	1.100	67	N(4)-C(22)	1.464	1.345
21	N(21)-H(64)	1.065	1.012	68	C(27)-C(22)	1.331	1.420
22	C(17)-H(63)	1.105	1.100	69	C(26)-C(27)	1.347	1.420
23	C(16)-H(62)	1.100	1.100	70	C(25)-C(26)	1.352	1.420
24	C(15)-H(61)	1.115	1.100	71	C(24)-C(25)	1.331	1.420
25	C(14)-H(60)	1.113	1.100	72	N(23)-C(24)	1.268	1.358
26	C(11)-H(59)	1.008	1.100	73	C(22)-N(23)	1.339	1.358
27	C(9)-H(58)	1.117	1.100	74	C(19)-N(21)	1.452	1.369
28	C(8)-H(57)	1.116	1.100	75	C(19)-O(20)	1.212	1.208
29	C(7)-H(56)	1.114	1.100	76	C(18)-C(19)	1.392	1.517
30	C(6)-H(55)	1.104	1.100	77	C(18)-C(13)	1.371	1.420
31	N(4)-H(54)	1.013	1.012	78	C(17)-C(18)	1.340	1.420
32	Co(50)-N(3)	1.867	-	79	C(16)-C(17)	1.341	1.420
33	Co(50)-N(12)	1.925	-	80	C(15)-C(16)	1.340	1.420
34	Co(50)-O(52)	1.282	0.600	81	C(14)-C(15)	1.340	1.420
35	Co(50)-O(51)	1.150	0.600	82	C(13)-C(14)	1.359	1.420
36	O(49)-Co(50)	1.157	0.600	83	N(12)-C(13)	1.265	1.456
37	O(53)-C(29)	1.487	1.355	84	C(5)-O(10)	1.194	1.208
38	O(53)-Co(50)	1.147	0.600	85	C(9)-C(2)	1.360	1.420
39	C(11)-N(3)	1.284	1.260	86	C(8)-C(9)	1.338	1.420
40	C(28)-C(34)	1.370	1.503	87	C(7)-C(8)	1.343	1.420
41	C(48)-C(11)	1.335	1.503	88	C(6)-C(7)	1.351	1.420
42	C(47)-O(49)	1.696	1.355	89	C(1)-C(6)	1.357	1.420
43	C(48)-C(43)	1.363	1.420	90	C(5)-C(1)	1.424	1.517
44	C(47)-C(48)	1.318	1.420	91	N(4)-C(5)	1.547	1.369
45	C(46)-C(47)	1.388	1.420	92	C(2)-N(3)	1.262	1.456
46	C(45)-C(46)	1.407	1.420	93	C(1)-C(2)	1.349	1.420
47	C(42)-C(45)	1.356	1.420				

Table S3: Various bond angle (˚) of $[Co(L)(H_2O)_2].3H_2O$ complex (**1**).

Sr. No	Atoms	Actual bond angles	Optimal bond angles	Sr. No	Atoms	Actual bond angles	Optimal bond angles
1	C(29)-O(53)-Co(50)	125.532	103.260	46	H(77)-C(41)-C(40)	114.925	120.000
2	H(84)-O(52)-H(83)	72.872	-	47	C(42)-C(41)-C(40)	122.796	-
3	H(84)-O(52)-Co(50)	112.234	-	48	H(76)-C(40)-C(41)	121.014	120.000
4	H(83)-O(52)-Co(50)	126.022	-	49	H(76)-C(40)-C(39)	116.795	120.000
5	H(82)-O(51)-H(81)	58.418	-	50	C(41)-C(40)-C(39)	121.982	-
6	H(82)-O(51)-Co(50)	142.001	-	51	H(75)-C(39)-C(44)	120.704	120.000
7	H(81)-O(51)-Co(50)	107.780	-	52	H(75)-C(39)-C(40)	127.270	120.000
8	N(3)-Co(50)-N(12)	153.770	-	53	C(44)-C(39)-C(40)	112.025	-
9	N(3)-Co(50)-O(52)	124.547	-	54	H(74)-C(38)-C(33)	120.062	120.000
10	N(3)-Co(50)-O(51)	86.567	-	55	H(74)-C(38)-C(37)	113.556	120.000
11	N(3)-Co(50)-O(49)	78.332	-	56	C(33)-C(38)-C(37)	124.743	-
12	N(3)-Co(50)-O(53)	86.689	-	57	H(73)-C(37)-C(38)	120.525	120.000
13	N(12)-Co(50)-O(52)	81.556	-	58	H(73)-C(37)-C(36)	119.882	120.000
14	N(12)-Co(50)-O(51)	67.595	-	59	C(38)-C(37)-C(36)	118.961	-
15	N(12)-Co(50)-O(49)	100.791	-	60	H(72)-C(36)-C(37)	120.935	120.000
16	N(12)-Co(50)-O(53)	99.598	-	61	H(72)-C(36)-C(35)	120.712	120.000
17	O(52)-Co(50)-O(51)	148.723	-	62	C(37)-C(36)-C(35)	118.271	-
18	O(52)-Co(50)-O(49)	90.909	-	63	H(71)-C(35)-C(36)	116.501	120.000
19	O(52)-Co(50)-O(53)	84.636	-	64	H(71)-C(35)-C(32)	121.202	120.000
20	O(51)-Co(50)-O(49)	99.531	-	65	C(36)-C(35)-C(32)	120.196	-
21	O(51)-Co(50)-O(53)	95.178	-	66	C(28)-C(34)-C(29)	114.785	120.000
22	O(49)-Co(50)-O(53)	158.243	-	67	C(28)-C(34)-C(33)	121.634	120.000
23	Co(50)-O(49)-C(47)	135.574	103.260	68	C(29)-C(34)-C(33)	119.852	120.000
24	C(11)-C(48)-C(43)	120.196	120.000	69	C(38)-C(33)-C(34)	123.862	120.000
25	C(11)-C(48)-C(47)	89.831	120.000	70	C(38)-C(33)-C(32)	113.431	120.000
26	C(43)-C(48)-C(47)	141.792	120.000	71	C(34)-C(33)-C(32)	119.925	120.000
27	O(49)-C(47)-C(48)	118.280	124.300	72	C(35)-C(32)-C(33)	123.542	120.000
28	O(49)-C(47)-C(46)	142.669	124.300	73	C(35)-C(32)-C(31)	115.858	120.00
29	C(48)-C(47)-C(46)	95.562	120.000	74	C(33)-C(32)-C(31)	119.53	120.00
30	H(80)-C(46)-C(47)	118.555	120.000	75	H(70)-C(31)-C(32)	118.962	120.00
31	H(80)-C(46)-C(45)	113.048	120.000	76	H(70)-C(31)-C(30)	118.841	120.00
32	C(47)-C(46)-C(45)	127.782	-	77	C(32)-C(31)-C(30)	119.428	-
33	H(79)-C(45)-C(46)	126.353	120.000	78	H(69)-C(30)-C(31)	121.234	120.000
34	H(79)-C(45)-C(42)	109.449	120.000	79	H(69)-C(30)-C(29)	115.254	120.000
35	C(46)-C(45)-C(42)	124.127	-	80	C(31)-C(30)-C(29)	122.496	-
36	H(78)-C(44)-C(39)	95.497	120.000	81	O(53)-C(29)-C(34)	125.404	124.300
37	H(78)-C(44)-C(43)	135.213	120.000	82	O(53)-C(29)-C(30)	117.857	124.307
38	C(39)-C(44)-C(43)	128.540	-	83	C(34)-C(29)-C(30)	116.347	120.00
39	C(48)-C(43)-C(44)	129.620	120.000	84	H(68)-C(28)-C(34)	122.679	120.00
40	C(48)-C(43)-C(42)	113.232	120.000	85	H(68)-C(28)-N(12)	114.764	116.500
41	C(44)-C(43)-C(42)	116.560	120.000	86	C(34)-C(28)-N(12)	120.176	123.506
42	C(45)-C(42)-C(43)	111.366	120.000	87	H(67)-C(27)-C(22)	119.175	120.00
43	C(45)-C(42)-C(41)	131.876	120.000	88	H(67)-C(27)-C(26)	122.648	120.00
44	C(43)-C(42)-C(41)	116.758	120.000	89	C(22)-C(27)-C(26)	117.922	-
45	H(77)-C(41)-C(42)	122.270	120.000	90	H(66)-C(26)-C(27)	120.540	120.00

Table S3: Continued

Sr. No	Atoms)	Actual bond angles	Optimal bond angles	Sr. No	Atoms	Actual bond angles	Optimal bond angles
91	H(66)-C(26)-C(25)	115.918	120.000	136	H(57)-C(8)-C(9)	119.492	120.000
92	C(27)-C(26)-C(25)	121.895	-	137	H(57)-C(8)-C(7)	121.516	120.000
93	H(65)-C(25)-C(26)	129.753	120.00	138	C(9)-C(8)-C(7)	118.910	-
94	H(65)-C(25)-C(24)	110.44	120.00	139	H(56)-C(7)-C(8)	118.087	120.000
95	C(26)-C(25)-C(24)	119.686	-	140	H(56)-C(7)-C(6)	120.451	120.000
96	N(21)-C(24)-C(25)	140.560	120.000	141	C(8)-C(7)-C(6)	121.019	-
97	N(21)-C(24)-N(23)	110.956	120.000	142	H(55)-C(6)-C(7)	113.008	120.000
98	C(25)-C(24)-N(23)	108.155	120.000	143	H(55)-C(6)-C(1)	123.848	120.00
99	C(24)-N(23)-C(22)	138.618	115.000	144	C(7)-C(6)-C(1)	123.087	-
100	N(4)-C(22)-C(27)	121.026	120.000	145	O(10)-C(5)-C(1)	102.501	123.00
101	N(4)-C(22)-N(23)	130.565	120.000	146	O(10)-C(5)-N(4)	117.134	122.600
102	C(27)-C(22)-N(23)	107.667	120.000	147	C(1)-C(5)-N(4)	138.513	112.740
103	H(64)-N(21)-C(24)	105.293	110.000	148	H(54)-N(4)-C(22)	108.068	110.000
104	H(64)-N(21)-C(19	114.866	117.400	148	H(54)-N(4)-C(5)	94.428	117.400
105	C(24)-N(21)-C(19)	135.334	-	149	C(22)-N(4)-C(5)	141.592	-
106	N(21)-C(19)-O(20)	124.442	122.600	150	Co(50)-N(3)-C(11)	110.867	-
107	N(21)-C(19)-C(18)	121.672	112.740	151	Co(50)-N(3)-C(2)	123.060	-
108	O(20)-C(19)-C(18)	112.900	123.000	152	C(11)-N(3)-C(2)	102.461	-
109	C(19)-C(18)-C(13)	125.687	117.600	153	C(9)-C(2)-N(3)	127.829	120.000
110	C(19)-C(18)-C(17)	118.134	117.600	154	C(9)-C(2)-C(1)	127.349	120.000
111	C(13)-C(18)-C(17)	115.575	120.000	155	N(3)-C(2)-C(1)	104.750	120.000
112	H(63)-C(17)-C(18)	120.486	120.00	156	C(6)-C(1)-C(5)	125.944	117.600
113	H(63)-C(17)-C(16)	119.254	120.000	157	C(6)-C(1)-C(2)	112.134	120.000
114	C(18)-C(17)-C(16)	120.208	-	158	C(5)-C(1)-C(2)	121.723	117.600
115	H(62)-C(16)-C(17)	116.529	120.000				
116	H(62)-C(16)-C(15)	119.563	120.000				
117	C(17)-C(16)-C(15)	123.903	-				
118	H(61)-C(15)-C(16)	119.334	120.000				
119	H(61)-C(15)-C(14)	123.498	120.000				
120	C(16)-C(15)-C(14)	117.114	-				
121	H(60)-C(14)-C(15)	113.950	120.000				
122	H(60)-C(14)-C(13)	126.936	120.000				
123	C(15)-C(14)-C(13)	119.094	-				
124	C(18)-C(13)-C(14)	123.325	120.000				
125	C(18)-C(13)-N(12)	110.224	120.000				
126	C(14)-C(13)-N(12)	126.438	120.000				
127	Co(50)-N(12)-C(28)	121.346	-				
128	Co(50)-N(12)-C(13)	114.217	-				
129	C(28)-N(12)-C(13)	124.410	-				
130	H(59)-C(11)-N(3)	98.077	116.500				
131	H(59)-C(11)-C(48)	87.626	120.000				
132	N(3)-C(11)-C(48)	137.194	123.500				
133	H(58)-C(9)-C(2)	129.548	120.000				
134	H(58)-C(9)-C(8)	113 .466	120.000				
135	C(2)-C(9)-C(8)	116.98	-				

Table S4: X-ray diffraction data of ligand and its Cu(II) complexes (**3,4**).

Compounds	**Peak**	**2Th°**	**d-sp**	**Rel. Int %**	**D (nm)**
H_2L	1	35.385	2.53467	100	3.0
	2	62.622	1.48225	68.3	11.8
	3	57.105	1.61163	42.4	18.6
	4	43.061	2.09891	33.6	17.6
	5	30.236	2.9535	44.4	15.2
	6	74.444	1.27342	21.2	15.2
Mean D					13.7
3-[Cu (L)]	1	62.765	1.47921	55.4	3.0
	2	53.379	1.715	44.6	60.7
	3	35.395	2.53395	100	9.0
	4	57.161	1.61018	45.2	7.7
Mean D					20.1
4-[Cu (H_2L)(OH) Br]	1	62.765	1.47921	63.4	10.5
	2	56.89	1.61721	54.6	35.1
	3	35.538	2.52406	100	42.8
	4	30.165	2.96035	69.9	11.4
Mean D					24.95

Table S5: Antimicrobial screening of the compounds at 10 mg mL^{-1}.

No.	Compound	Inhibition diameter (mm)			
		Bacterial strains		Fungal strains	
		E.coli(G^-)	*S.aureus*(G^+)	*A.flavus*	*C.albicans*
	H_2L	12.0	12.0	-	10.0
1	$[Co(L)(H_2O)_2].3H_2O$	14.0	15.0	-	-
2	$[Ni(L)(H_2O)_2].1½H_2O$	11.0	13.0	-	-
3	[Cu(L)]	-	-	-	-
4	$[Cu(H_2L)(OH)Br]$				-
	Ampicillin	-	11.0	-	-
		22.0	18.0	-	
	Amphotericin B	-	-	14.0	-

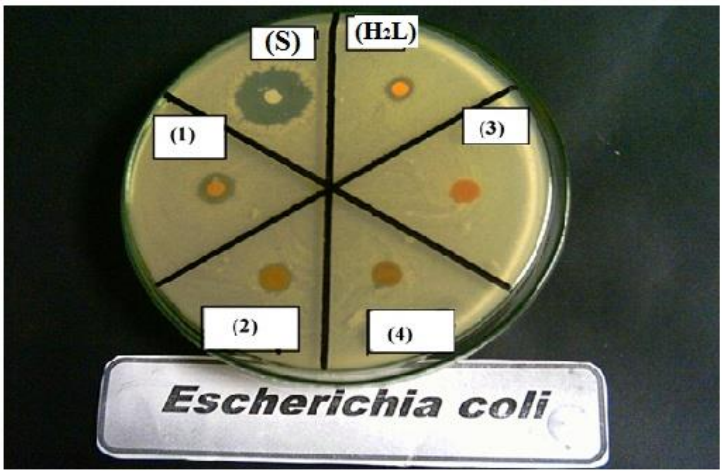

Fig. S1: Photograph showing the antibacterial (*E. coli*) screening of ligand (H_2L) and its metal(II) complexes (**1-4**) with standard (Ampicillin) (S).

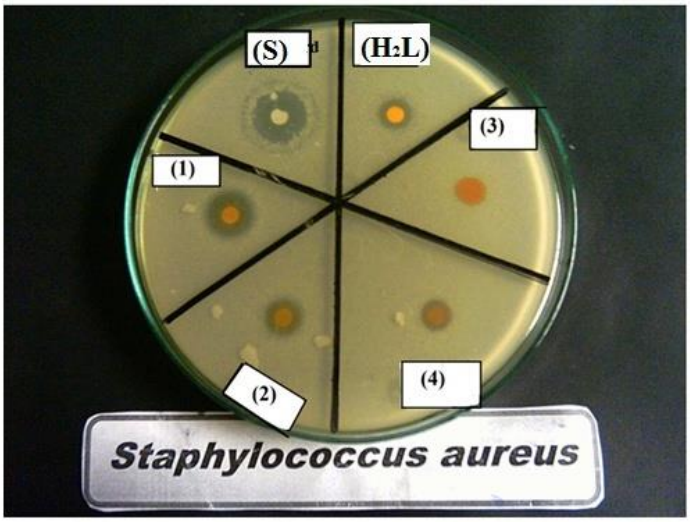

Fig. S2: Photograph showing the antibacterial (*S. aureus*) screening of ligand (H_2L) and its metal(II) complexes (**1-4**) with standard (Ampicillin) (S).