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Supplementary Materials

Synthesis, Structural Determination, Electrochemical Investigation of Metal Complexes of Novel 4-[3-Hydroxypyridin-2-yl)diazenyl]-5-methyl-2-phenyl-2,4-dihydro-3H-pyrazol-3-one; Biological Evaluations

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Supplementary Figures

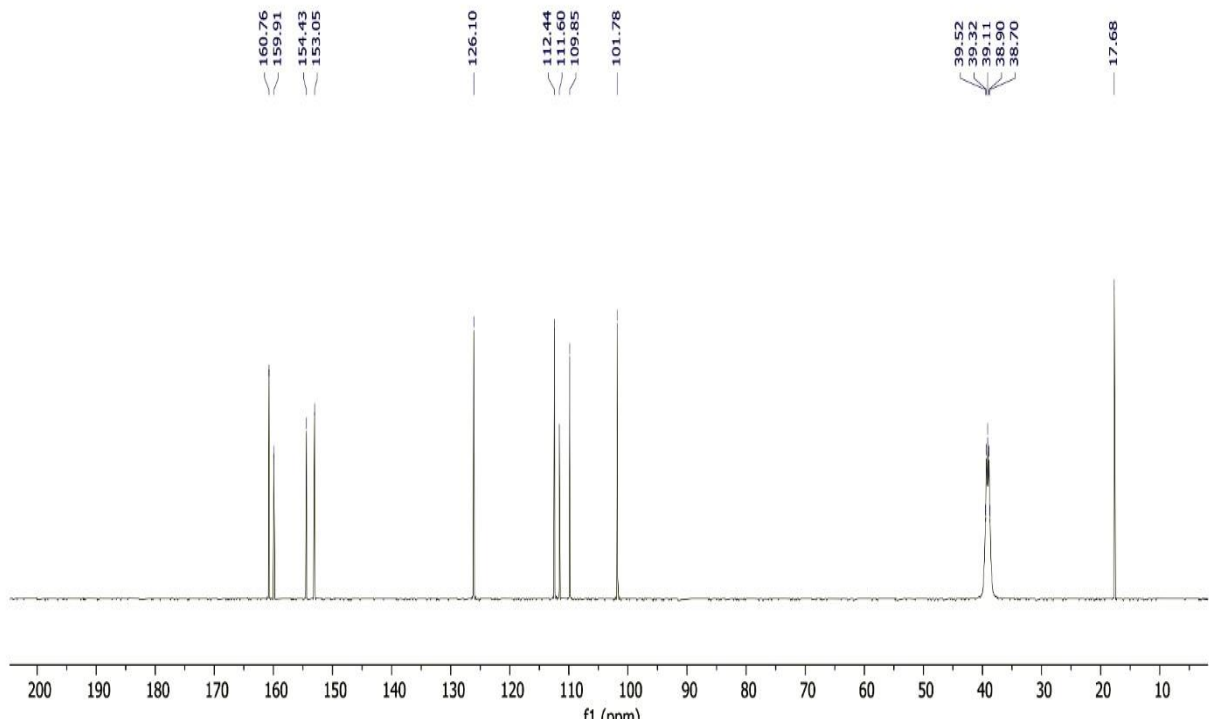

Figure S1. ^{13}C NMR spectrum of PDP

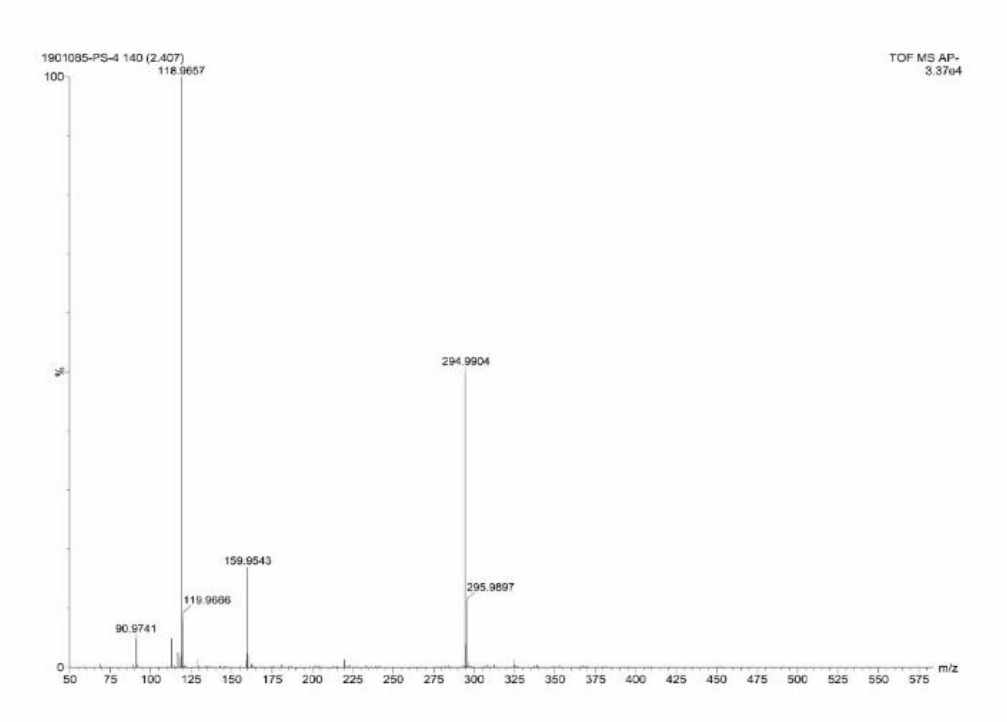

Figure S2. Mass spectrum of PDP

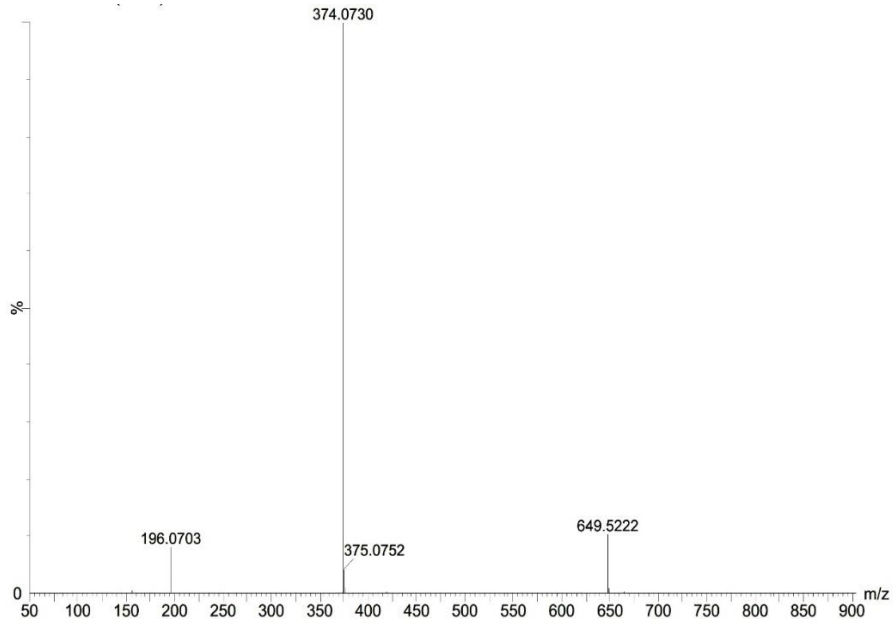

Figure S3. Mass spectrum of $[Co(PDP)_2]Cl_2.2H_2O$

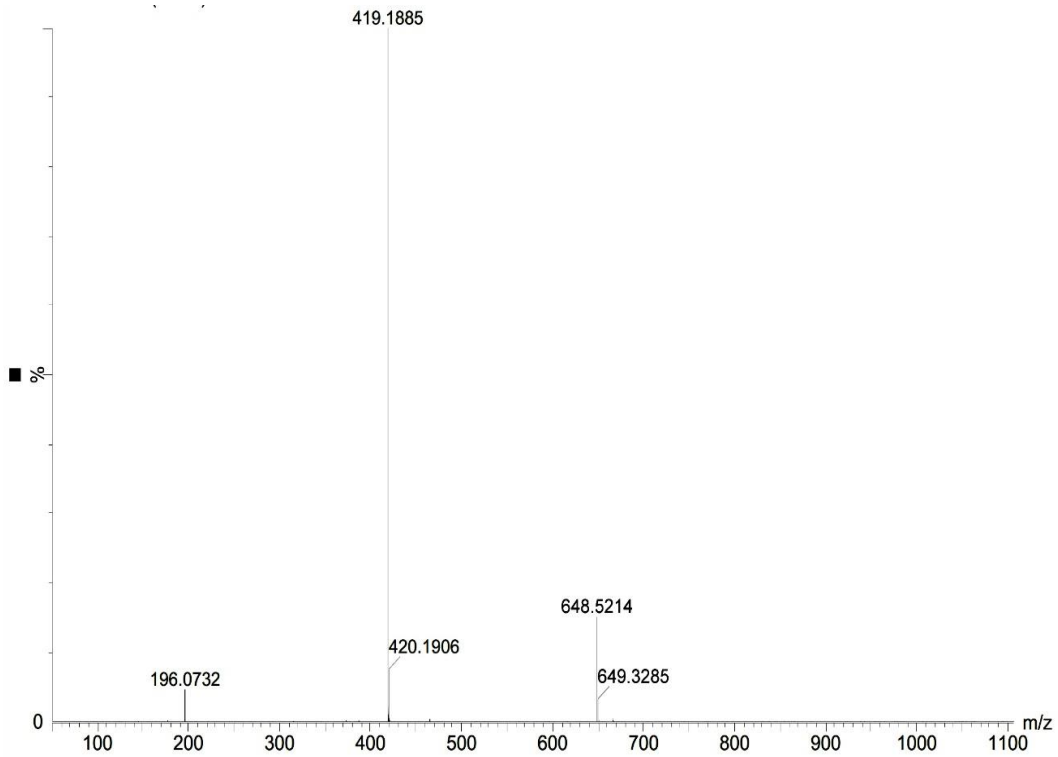

Figure S4. Mass spectrum of $[Ni(PDP)_2]Cl_2.2H_2O$

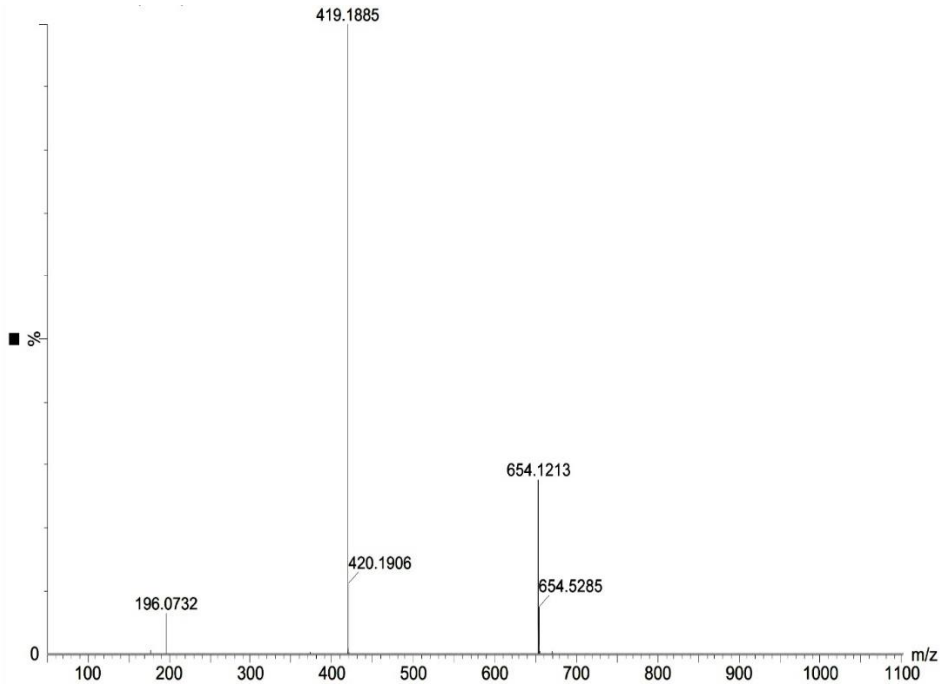

Figure S5. Mass spectrum of $[Cu(PDP)_2]Cl_2.2H_2O$

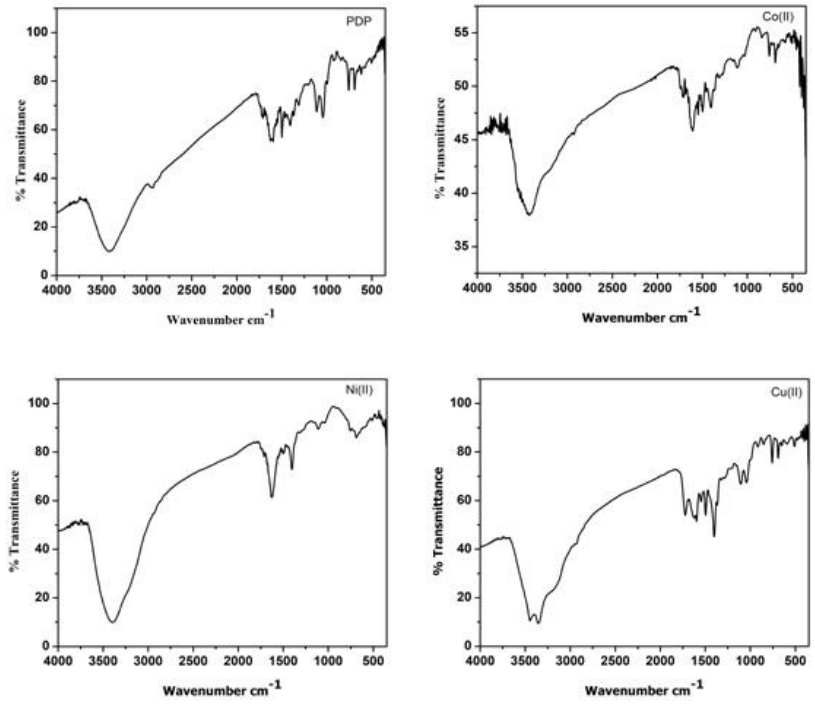

Figure S6. FT-IR spectra of PDP and their metal complexes

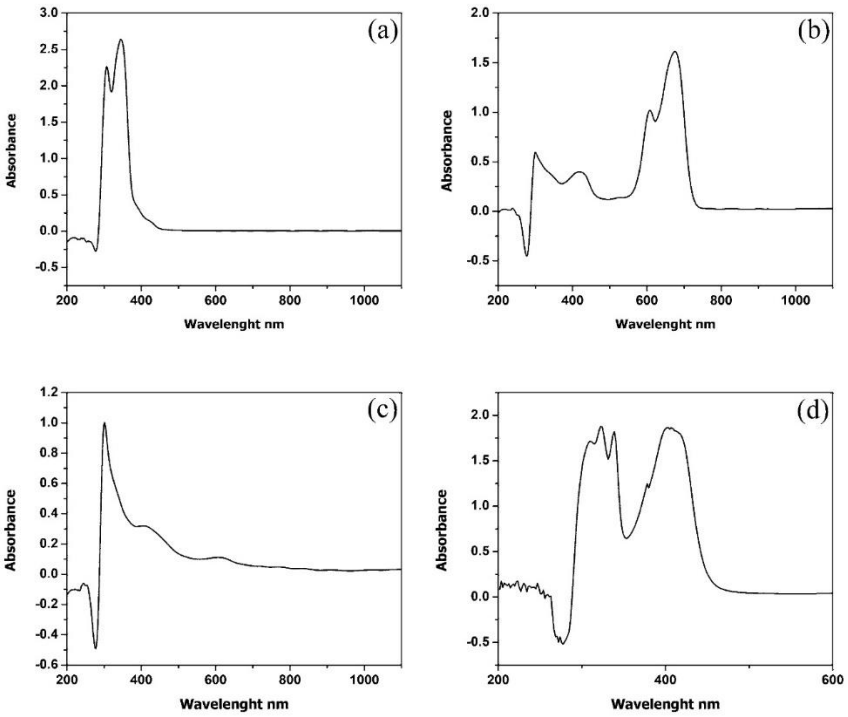

Figure S7. Electronic absorption spectra of (a) PDP (b) $[Co(PDP)_2]Cl_2.2H_2O$ (c) $[Ni(PDP)_2]Cl_2.2H_2O$ (d) $[Cu(PDP)_2]Cl_2.2H_2O$

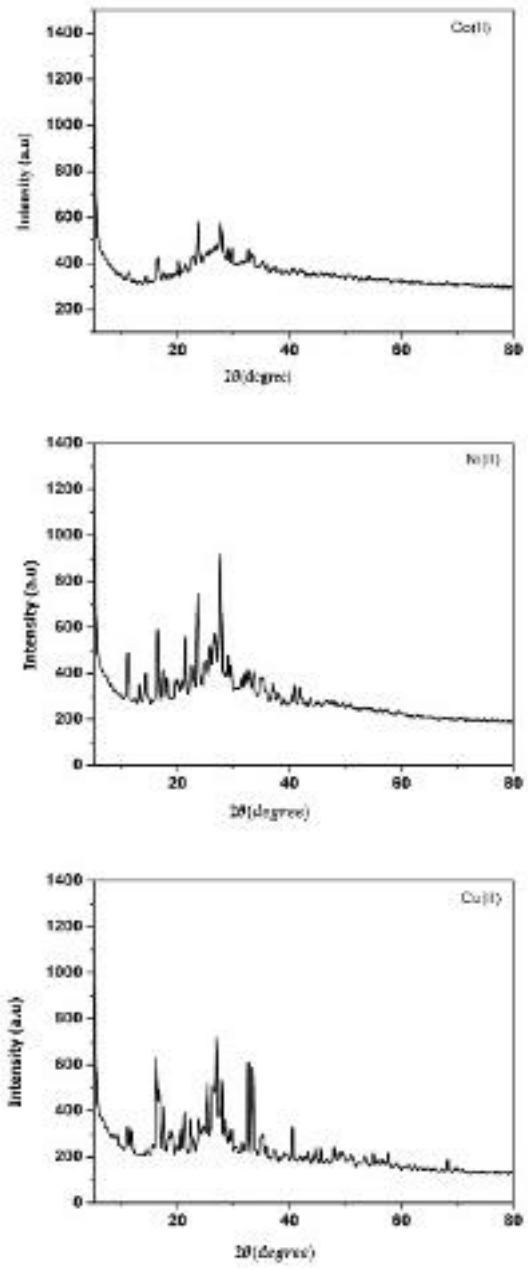

Figure S8. Powder XRD pattern of (a) $[Co(PDP)_2]Cl_2.2H_2O$ (b) $[Ni(PDP)_2]Cl_2.2H_2O$ (c) $[Cu(PDP)_2]Cl_2.2H_2O$

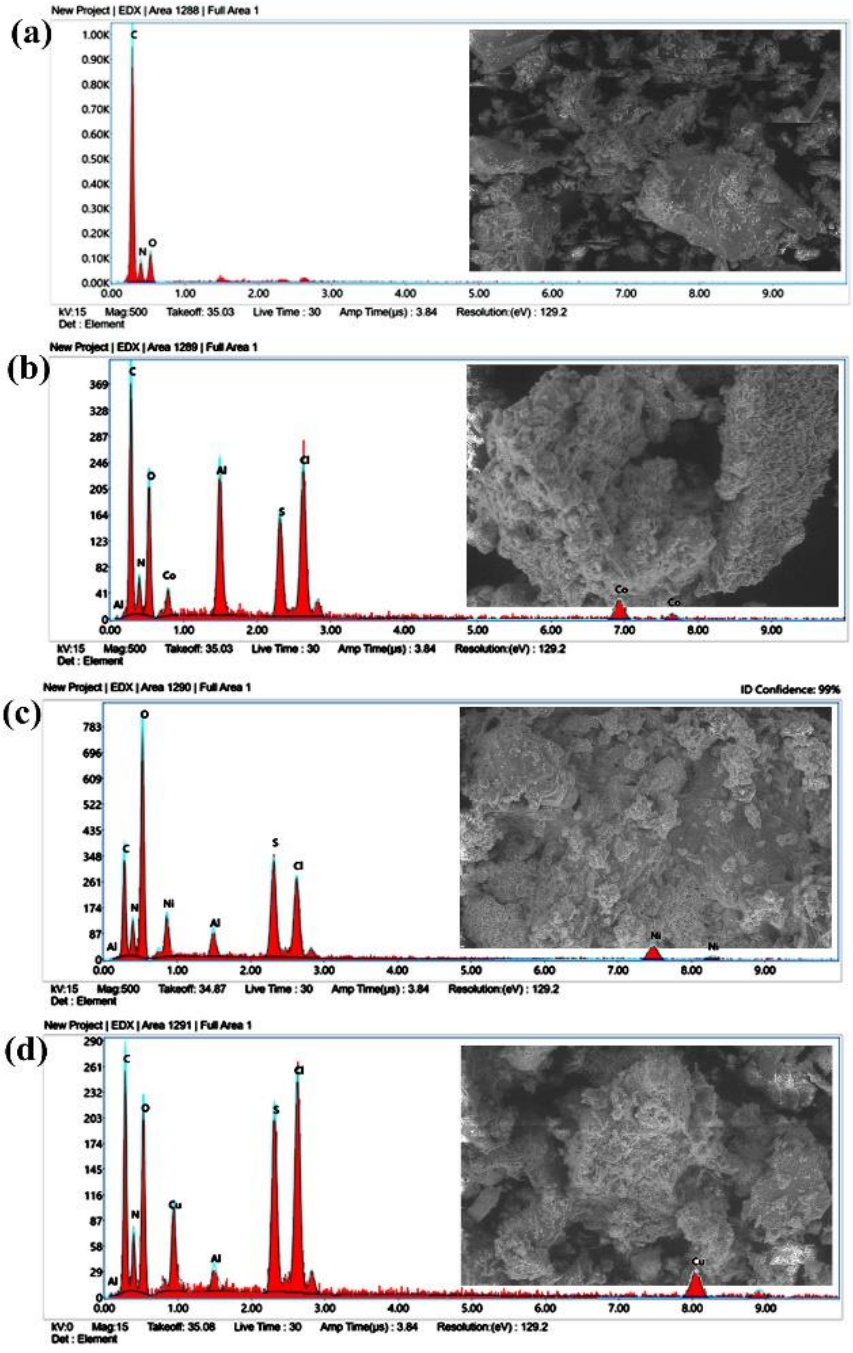

Figure S9. SEM and EDX images of (a) PDP (b) $[Co(PDP)_2]Cl_2.2H_2O$ (c) $[Ni(PDP)_2]Cl_2.2H_2O$ (d) $[Cu(PDP)_2]Cl_2.2H_2O$

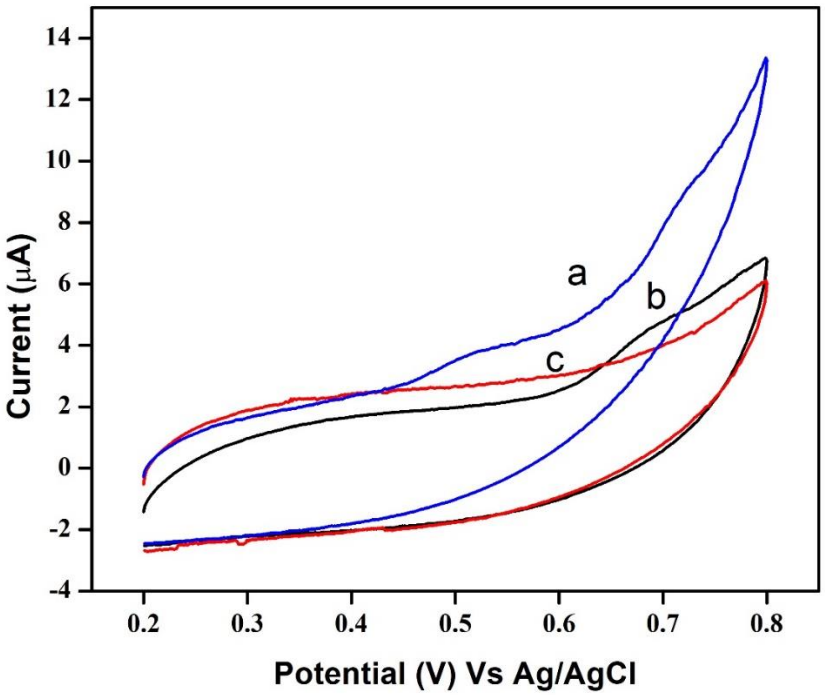

Figure S10. Cyclic voltammogram of FA at (a) pH-7 (b) pH-4 (c) pH-9 in buffer solution at scan rate 50 mV/S

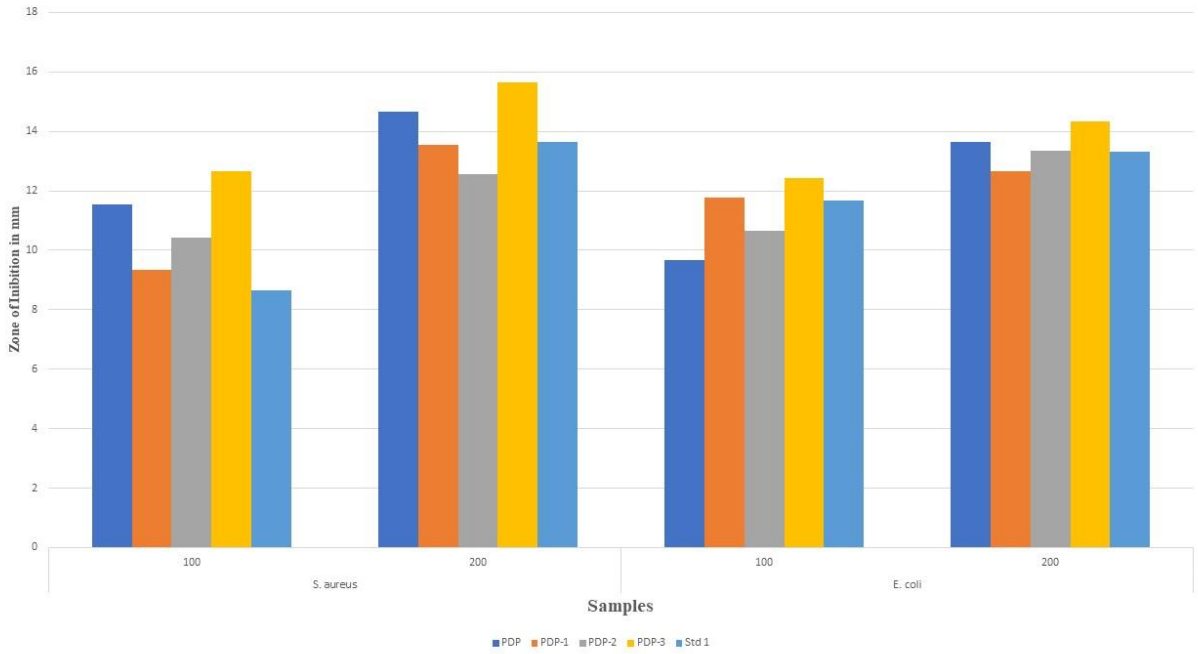

Figure S11. Antibacterial activity of PDP and its metal complexes

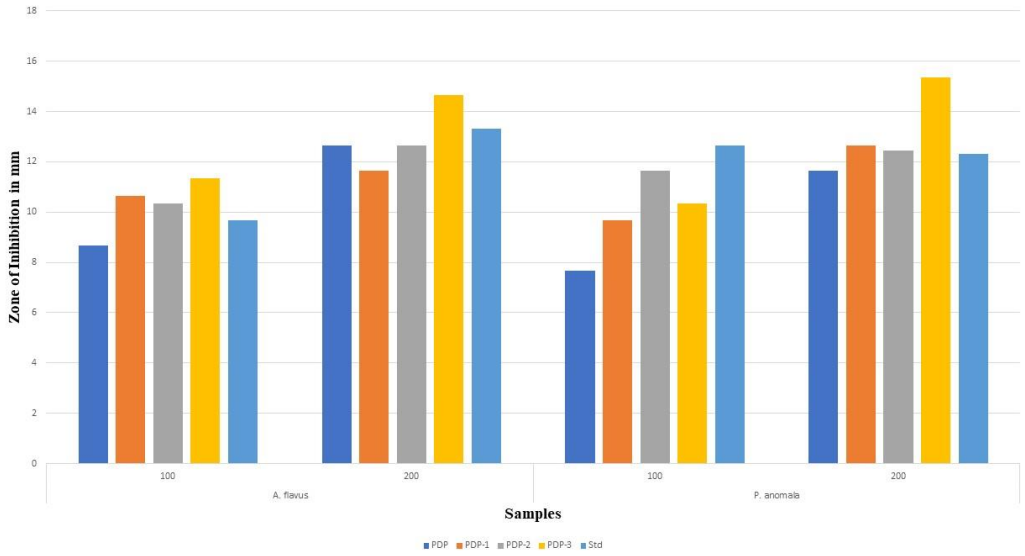

Figure S12. Antifungal activity of PDP and its metal complexes

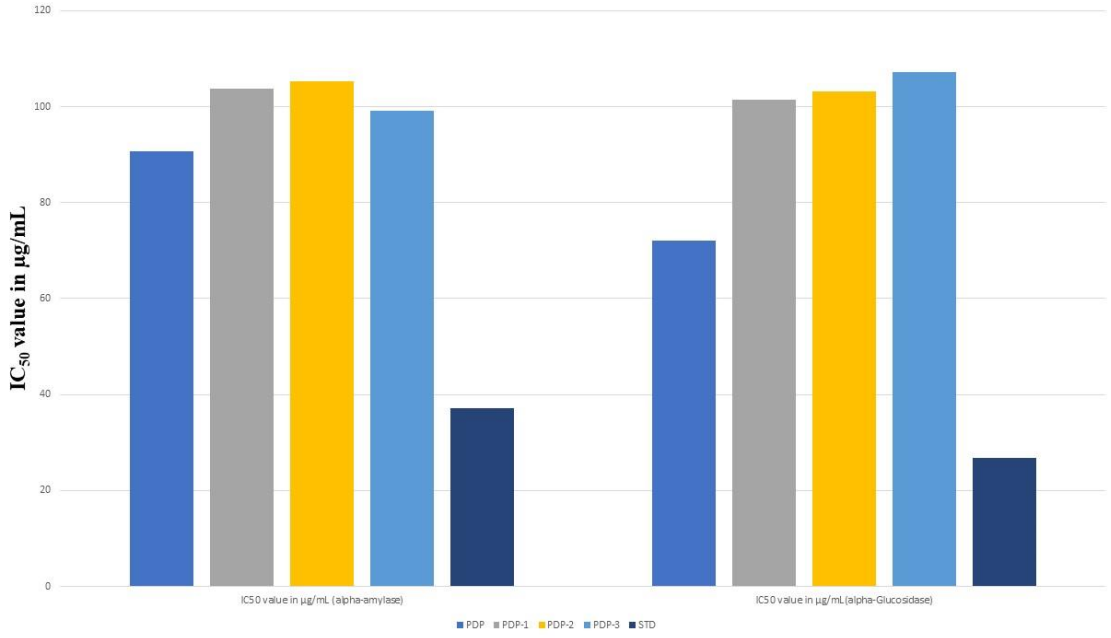

Figure S13. IC_{50} of PDP and its metal complexes

Supplementary Tables

Table S1. FT-IR spectral data (cm^{-1}) of PDP and its metal complexes

Comp. No.	*V*(OH)	*V*(C=O)	*V*(C=N)	*V*(N=N)	*V*(M-O)	*V*(M-N)
PDP	3416	1745	1615	1368	-	-
$[Co(PDP)_2]Cl_2.2H_2O$	3440	1730	1610	1394	530	436
$[Ni(PDP)_2]Cl_2.2H_2O$	3455	1725	1618	1390	544	428
$[Cu(PDP)_2]Cl_2.2H_2O$	3443	1730	1614	1392	538	440

Table S2. Electronic absorption spectral bands of metal complexes

Comp. No.	λ (nm)	Transitions (cm^{-1})	Magnetic moment
PDP	350	28,571	
$[Co(PDP)_2]Cl_2.2H_2O$	450 600 670	22,222 16,666 14,925	4.73
$[Ni(PDP)_2]Cl_2.2H_2O$	410 680 780	24,390 14,705 12,826	2.75
$[Cu(PDP)_2]Cl_2.2H_2O$	410	24,390	1.70

Table S3a. Powder XRD spectral data of $[Co(PDP)_2]Cl_2.2H_2O$

Peak No.	**2θ**	**θ (degree)**	**θ (radian)**	**Sinθ**	**hkl**	**D**		**a in Å**
						Cal	**Obs**	
1	8.95	4.47	0.078	0.077	1 1 1	10.45	10.20	10.78
2	12.39	6.19	0.108	0.107	2 0 0	8.89	8.46	10.75
3	15.42	7.71	0.134	0.134	2 2 0	7.30	7.08	10.78
4	18.72	9.36	0.163	0.162	3 1 1	5.45	5.12	10.78
5	21.99	10.99	0.191	0.190	2 2 2	4.90	4.34	10.77
6	24.03	12.01	0.209	0.208	4 0 0	3.87	3.32	10.77
7	27.54	13.77	0.240	0.239	3 3 1	3.28	2.97	10.76
8	29.25	14.62	0.255	0.254	0 2 4	2.77	2.31	10.78
9	30.44	15.22	0.265	0.264	4 2 2	2.56	2.08	10.77

Table S3b. Powder XRD spectral data of $[Ni(PDP)_2]Cl_2.2H_2O$

Peak No.	**2θ**	**θ (degree)**	**θ (radian)**	**Sinθ**	**hkl**	**D**		**a in Å**
						Cal	**Obs**	
1	8.91	4.45	0.077	0.076	1 1 1	9.24	9.15	9.20
2	10.11	5.05	0.088	0.087	1 0 1	7.78	7.43	9.20
3	13.76	6.88	0.120	0.120	0 1 2	6.90	6.30	9.20
4	16.84	8.42	0.146	0.145	1 2 2	5.75	5.39	9.21
5	20.65	10.32	0.180	0.180	2 1 0	5.15	4.78	9.22
6	24.76	12.38	0.216	0.125	2 0 0	4.11	3.87	9.20

Table S3c. Powder XRD spectral data of $[Cu(PDP)_2]Cl_2.2H_2O$

Peak No.	**2θ**	**θ (degree)**	**θ (radian)**	**Sinθ**	**Hkl**	**D**		**a in Å**
						Cal	**Obs**	
1	9.88	4.94	0.086	0.086	1 0 0	9.56	9.32	9.45
2	9.10	4.55	0.079	0.078	1 1 0	8.21	7.90	9.45
3	11.98	5.99	0.104	0.103	1 1 2	7.76	7.23	9.45
4	13.65	6.82	0.119	0.119	1 1 3	6.73	6.20	9.43
5	15.69	7.84	0.136	0.135	1 2 2	5.32	5.03	9.44
6	18.87	9.43	0.164	0.163	2 0 0	4.98	4.25	9.46
7	20.54	10.27	0.179	0.178	1 1 2	4.21	3.94	9.45
8	22.80	11.40	0.198	0.197	2 2 0	3.56	3.22	9.45
9	26.43	13.21	0.230	0.229	0 1 2	2.27	2.11	9.44