

Potential Bioactive ligand and its divalent M (II) complexes: Synthesis, physicochemical characterization, DFT calculations and biological applications

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Supplementary Data

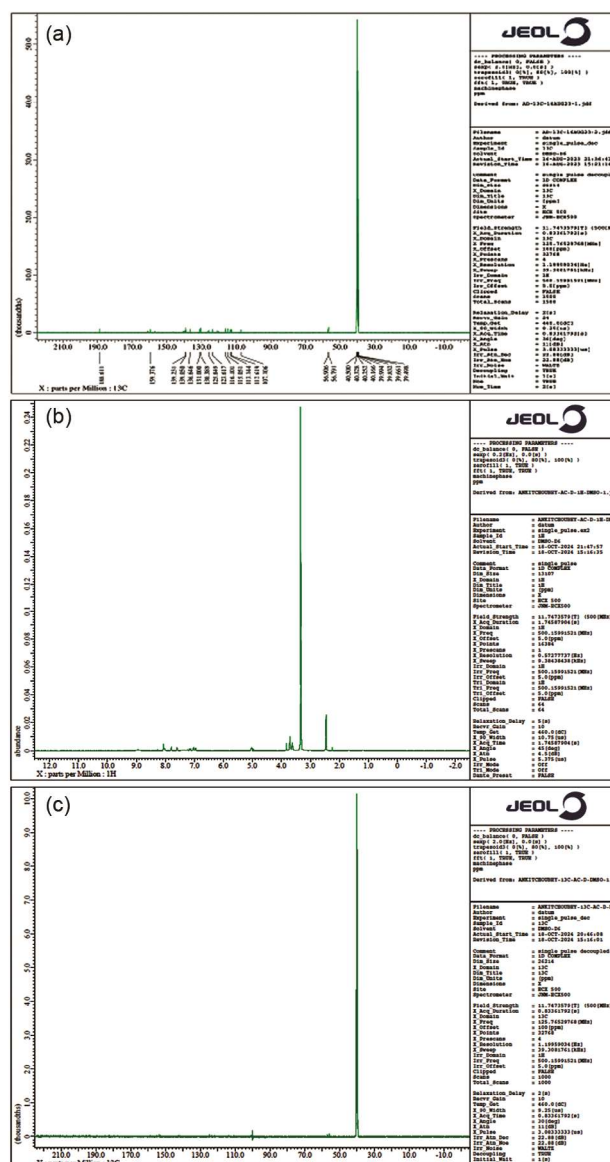


Fig. S1 — (a) ¹³C NMR of bioactive ligand L; (b) ¹H NMR of ZnL; and (c) ¹³C NMR of ZnL

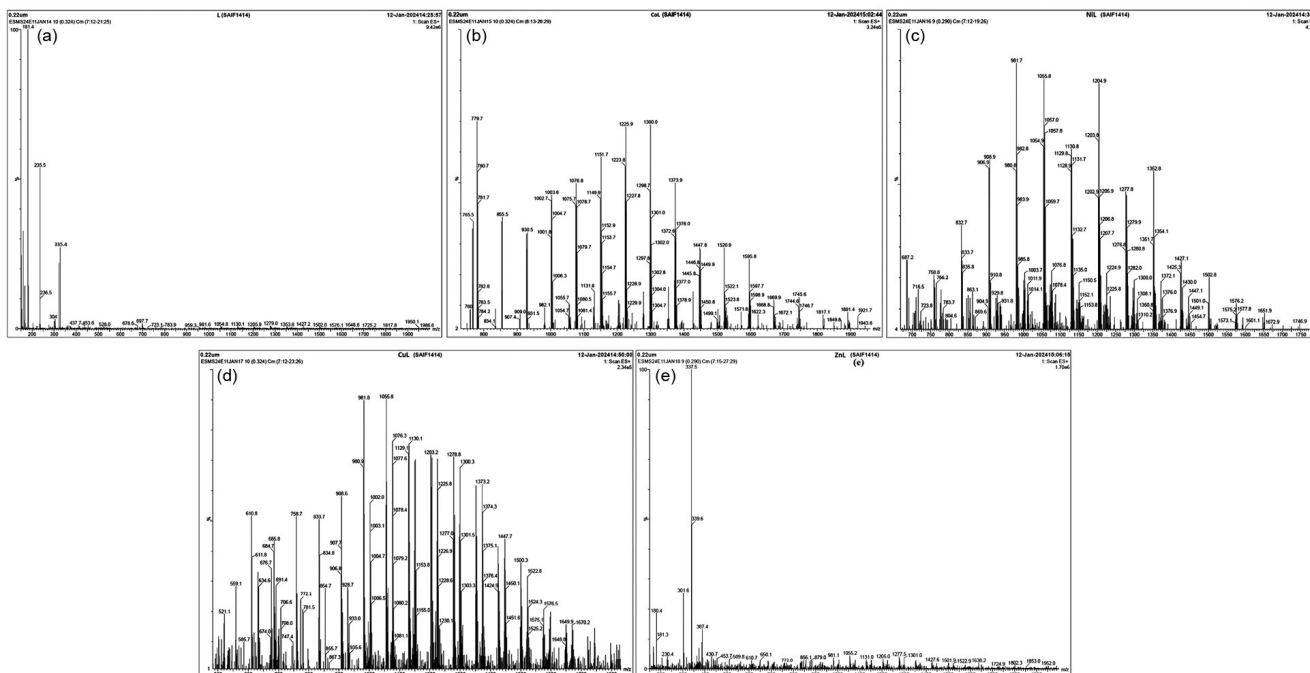


Fig. S2 — (a) ESI-MS of Bioactive ligand L; (b) ESI-MS of CoL; (c) ESI-MS of NiL; (d) ESI-MS of CuL; and (e) ESI-MS of ZnL

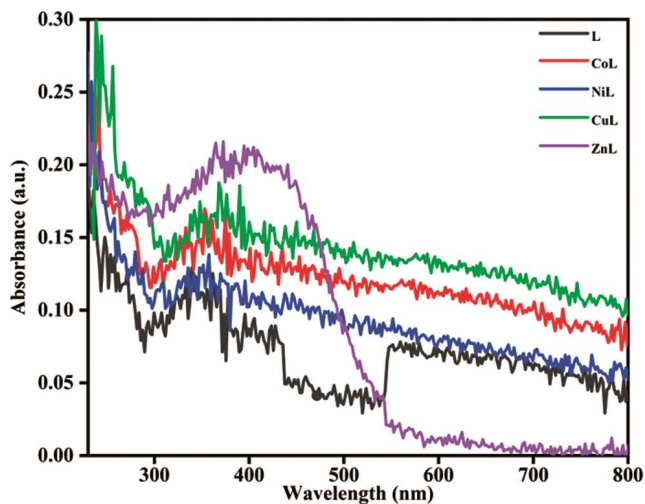


Fig. S3 — UV-DRS of bioactive ligand L and its metal complexes

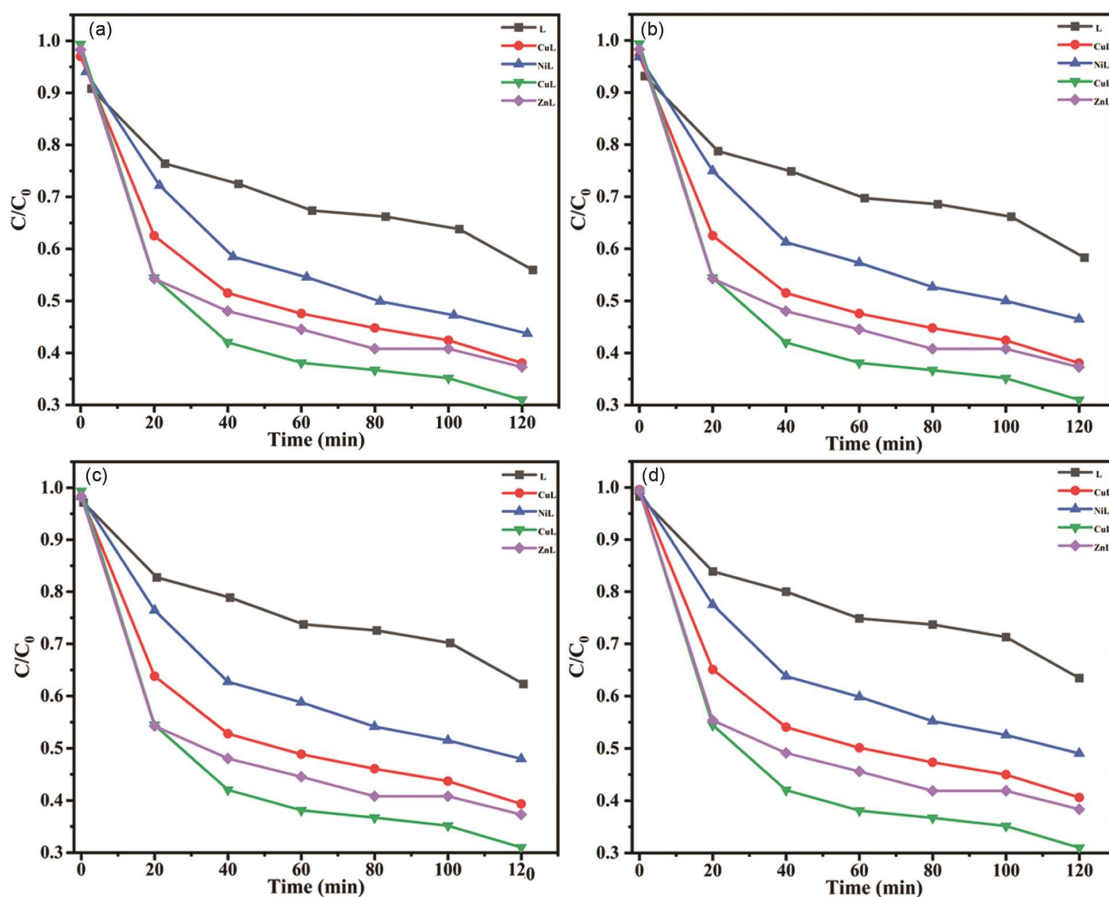


Fig. S4 — Degradation of MB at various concentrations (a) 10 mg/L; (b) 20 mg/L; (c) 30 mg/L; and (d) 40 mg/L of the bioactive ligand L and its metal complexes at room temperature

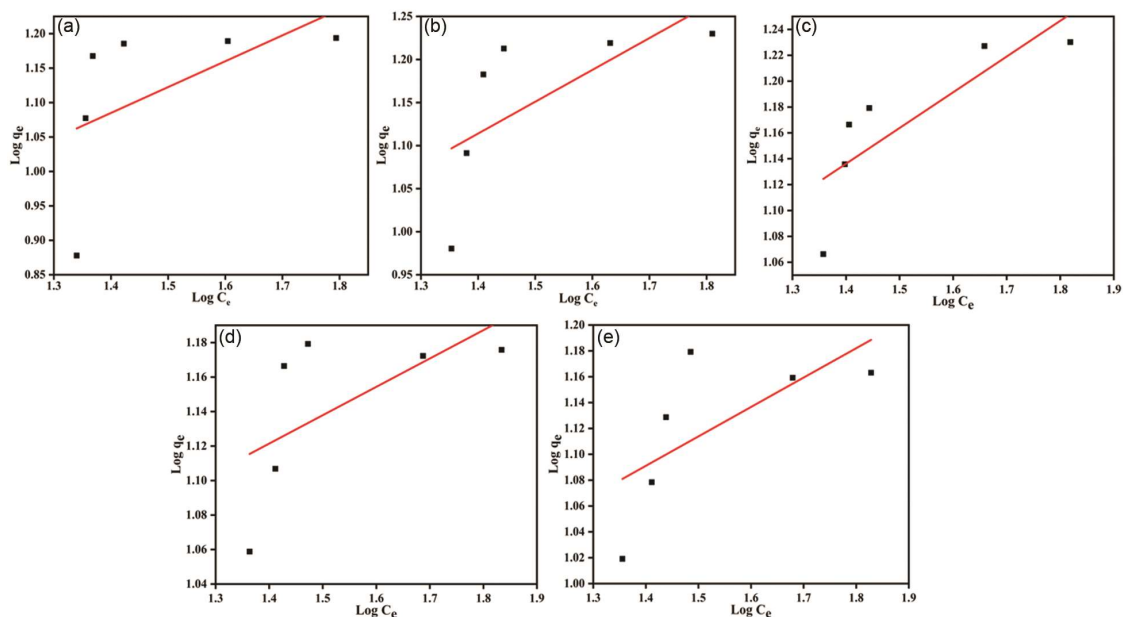


Fig. S5 — Freundlich adsorption isotherm for bioactive ligand and metal complexes

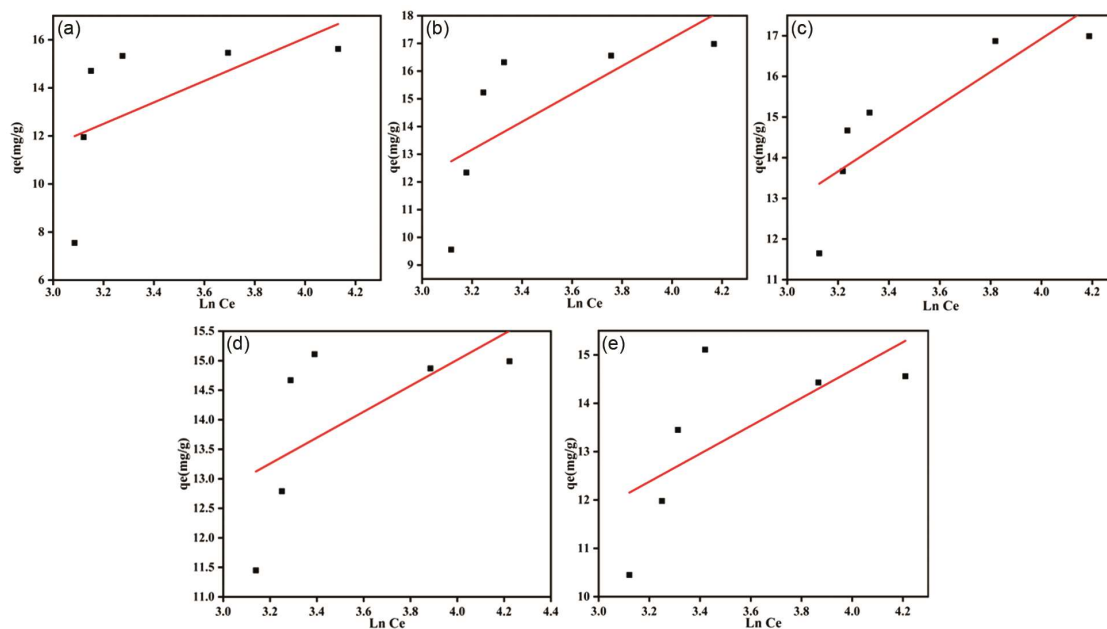


Fig. S6 — Temkin adsorption isotherm for bioactive ligand and metal complexes

Table S1 (a) — Crystal parameters of bioactive ligand L

2θ	β	d-spacing	Crystalline size
23.43	0.18	3.79	43.68
25.96	0.30	3.42	26.43
28.85	0.13	3.09	59.34
31.23	0.38	2.86	21.15
45.03	0.28	2.01	30.16
56.19	20.73	1.63	0.43

Table S1 (b) — Crystal parameters of CoL

2θ	β	d-spacing	Crystalline size
28.56	0.29	3.12	28.15
31.27	6.47	2.85	1.27
40.77	0.32	2.21	26.36
50.33	0.54	1.81	16.02
66.49	0.59	1.40	15.96

Table S1 (c) — Crystal parameters of NiL

2θ	β	d-spacing	Crystalline size
8.28036	0.29475	10.66943	27.02315414
21.30736	0.26936	4.166663	30.0105063
24.97691	0.31944	3.562198	25.47210486
29.75889	0.34892	2.999773	23.55817122
30.81131	0.41402	2.899666	19.90331932
43.35355	0.47894	2.085442	17.84950703
58.60431	0.45577	1.573919	19.98791448
69.37224	0.46965	1.353587	20.571216

Table S1 (d) — Crystal parameters of CuL

$2\theta(^{\circ})$	β	d-spacing	Crystalline size(nm)
13.33	0.22	6.63	34.80
26.14	0.35	3.40	23.13
28.32	0.51	3.14	15.99
40.52	0.46	2.22	18.06
50.14	0.42	1.81	20.71
66.42	0.37	1.40	25.63

Table S1 (e) — Crystal parameters of ZnL

$2\theta(^{\circ})$	β	d-spacing	Crystalline size(nm)
8.44	0.52	10.46	15.13
9.78	0.22	9.03	35.23
15.62	0.23	5.66	34.25
22.20	0.21	4.00	37.61
29.99	0.58	2.97	14.10
30.05	0.28	2.70	29.38
58.60	0.59	1.57	15.23