

Table S1 Selected bond lengths (Å) and angles (°) of the ligand.

Ligand			
Bond length		Bond angles	
C(19)-C(20)	1.3895	C(19)-C(20)-C(15)	119.7134
C(18)-C(19)	1.3906	C(20)-C(19)-C(18)	120.4741
C(17)-C(18)	1.3923	C(19)-C(18)-C(17)	119.8737
C(16)-C(17)	1.3876	C(18)-C(17)-C(16)	120.3515
C(15)-C(20)	1.4016	C(17)-C(16)-C(15)	119.8567
C(15)-C(16)	1.4029	C(20)-C(15)-C(16)	119.7298
N(13)-C(15)	1.4380	C(20)-C(15)-N(13)	119.7389
C(12)-N(13)	1.4840	C(16)-C(15)-N(13)	120.3530
C(11)-O(14)	1.2188	C(15)-N(13)-C(12)	115.1311
C(11)-C(12)	1.5130	N(13)-C(12)-C(11)	111.2791
N(9)-C(11)	1.4450	O(14)-C(11)-C(12)	126.0629
N(7)-N(9)	1.3857	O(14)-C(11)-N(9)	114.0590
C(6)-N(7)	1.3093	C(12)-C(11)-N(9)	119.5899
C(5)-C(6)	1.4443	C(11)-N(9)-N(7)	117.9314
S(4)-C(5)	1.7479	N(9)-N(7)-C(6)	120.1928
C(3)-S(4)	1.7211	N(7)-C(6)-C(5)	119.8649
C(2)-C(3)	1.3715	C(6)-C(5)-S(4)	121.3134
C(1)-C(5)	1.3820	C(6)-C(5)-C(1)	127.4346
C(1)-C(2)	1.4296	S(4)-C(5)-C(1)	111.2519
		C(5)-S(4)-C(3)	91.3430
		S(4)-C(3)-C(2)	112.4841
		C(3)-C(2)-C(1)	112.5308
		C(5)-C(1)-C(2)	112.3886

Table S₂. Results and discussion Selected bond lengths (Å) and angles (°) of C₁ complex.

C ₁ Complex		
Bond length		Bond angles
Pd(22)-O(24)	1.9784	O(24)-Pd(22)-Cl(23) 85.1364
Pd(22)-Cl(23)	2.3468	O(24)-Pd(22)-O(14) 84.6444
C(19)-C(20)	1.4213	O(24)-Pd(22)-N(7) 90.9058
C(18)-C(19)	1.3834	Cl(23)-Pd(22)-O(14) 88.2303
C(17)-C(18)	1.3931	Cl(23)-Pd(22)-N(7) 175.9579
C(16)-C(17)	1.3830	O(14)-Pd(22)-N(7) 90.5866
C(15)-C(20)	1.4283	C(19)-C(20)-C(15) 115.3816
C(15)-C(16)	1.4100	C(20)-C(19)-C(18) 123.1711
O(14)-Pd(22)	2.0006	C(19)-C(18)-C(17) 119.7665
N(13)-C(15)	1.4366	C(18)-C(17)-C(16) 119.4226
C(12)-N(13)	1.4868	C(17)-C(16)-C(15) 121.2187
C(11)-O(14)	1.3338	C(20)-C(15)-C(16) 120.5221
C(11)-C(12)	1.5034	C(20)-C(15)-N(13) 124.4550
N(9)-C(11)	1.4570	C(16)-C(15)-N(13) 114.8525
N(7)-Pd(22)	1.9674	Pd(22)-O(14)-C(11) 94.4478
N(7)-N(9)	1.4872	C(15)-N(13)-C(12) 121.9543
C(6)-N(7)	1.4041	N(13)-C(12)-C(11) 109.4735
C(5)-C(6)	1.3996	O(14)-C(11)-C(12) 120.0881
S(4)-C(5)	1.7927	O(14)-C(11)-N(9) 113.5719
C(3)-S(4)	1.7471	C(12)-C(11)-N(9) 123.9940
C(2)-C(3)	1.3823	C(11)-N(9)-N(7) 104.5674
C(1)-C(5)	1.4072	Pd(22)-N(7)-N(9) 100.6995
C(1)-C(2)	1.4204	Pd(22)-N(7)-C(6) 106.0336
		N(9)-N(7)-C(6) 117.3004
		N(7)-C(6)-C(5) 115.9076
		C(6)-C(5)-S(4) 121.7776
		C(6)-C(5)-C(1) 126.5453
		S(4)-C(5)-C(1) 109.8466
		C(5)-S(4)-C(3) 90.9912
		S(4)-C(3)-C(2) 111.4748
		C(3)-C(2)-C(1) 114.1387
		C(5)-C(1)-C(2) 112.5074

Table S3 Selected bond lengths (Å) and angels (°) of C₂ complex.

C ₂ Complex		
Bond length		Bond angles
Cd(22)-Cl(24)	2.2498	Cl(24)-Cd(22)-Cl(23) 154.0146
Cd(22)-Cl(23)	2.2566	Cl(24)-Cd(22)-O(14) 137.7794
C(19)-C(20)	1.3904	Cl(24)-Cd(22)-N(7) 138.8626
C(18)-C(19)	1.3906	Cl(23)-Cd(22)-O(14) 61.7877
C(17)-C(18)	1.3913	Cl(23)-Cd(22)-N(7) 67.1181
C(16)-C(17)	1.3891	O(14)-Cd(22)-N(7) 32.8853
C(15)-C(20)	1.3990	C(19)-C(20)-C(15) 119.8492
C(15)-C(16)	1.4018	C(20)-C(19)-C(18) 120.3702
O(14)-Cd(22)	2.1872	C(19)-C(18)-C(17) 119.8321
N(13)-C(15)	1.4461	C(18)-C(17)-C(16) 120.4259
C(12)-N(13)	1.4822	C(17)-C(16)-C(15) 119.7732
C(11)-O(14)	1.2144	C(20)-C(15)-C(16) 119.7454
C(11)-C(12)	1.5271	C(20)-C(15)-N(13) 121.1971
N(9)-C(11)	1.4564	C(16)-C(15)-N(13) 118.8537
N(7)-Cd(22)	2.2087	Cd(22)-O(14)-C(11) 101.4922
N(7)-N(9)	1.3731	C(15)-N(13)-C(12) 117.1845
C(6)-N(7)	1.3135	N(13)-C(12)-C(11) 113.1074
C(5)-C(6)	1.4428	O(14)-C(11)-C(12) 122.0761
S(4)-C(5)	1.7665	O(14)-C(11)-N(9) 118.8315
C(3)-S(4)	1.7415	C(12)-C(11)-N(9) 118.9308
C(2)-C(3)	1.3692	C(11)-N(9)-N(7) 116.1481
C(1)-C(5)	1.3844	Cd(22)-N(7)-N(9) 133.9912
C(1)-C(2)	1.4310	Cd(22)-N(7)-C(6) 94.2172
		N(9)-N(7)-C(6) 121.7302
		N(7)-C(6)-C(5) 119.1850
		C(6)-C(5)-S(4) 126.5014
		C(6)-C(5)-C(1) 122.9318
		S(4)-C(5)-C(1) 110.5440
		C(5)-S(4)-C(3) 91.2080
		S(4)-C(3)-C(2) 112.2231
		C(3)-C(2)-C(1) 112.7793
		C(5)-C(1)-C(2) 113.2052

Table 12 Antibacterial activity of ligand and its metal complexes.

No.	Compound	Inhibition (%)			
		S.pyogenes		E.coli	
		1mg/mL	5mg/mL	1mg/mL	5mg/mL
	Ligand	50	70	44	65
1	C ₁	75	95	50	75
2	C ₂	70	90	87	92
3	C ₃	65	85	72	83
4	C ₄	53	75	43	65
5	C ₅	60	79	60	80

Table 13 Antioxidant activity of ligand and its metal complexes along with standard ascorbic acid (A).

Compound	100	200	300	IC ₅₀
Ligand	24.10±0.44	32.19±0.29	36.35±0.14	0.514
C ₁	37.51±0.28	46.05±0.14	60.31±0.34	0.217
C ₂	37.47±0.14	46.00±0.28	59.54±0.	0.22
C ₃	41.46±0.28	48.91±0.41	61.13±0.55	0.019
C ₄	38.10±0.59	47.68±0.27	61.08±0.42	0.211
BHA 200 ppm		89.80		
TBHQ 200 ppm		92.87		

