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Supporting Information

Metal complexes of Tridentate Schiff base: Synthesis, Characterization, Biological Activity and Molecular Docking Studies with COVID-19 Protein Receptor

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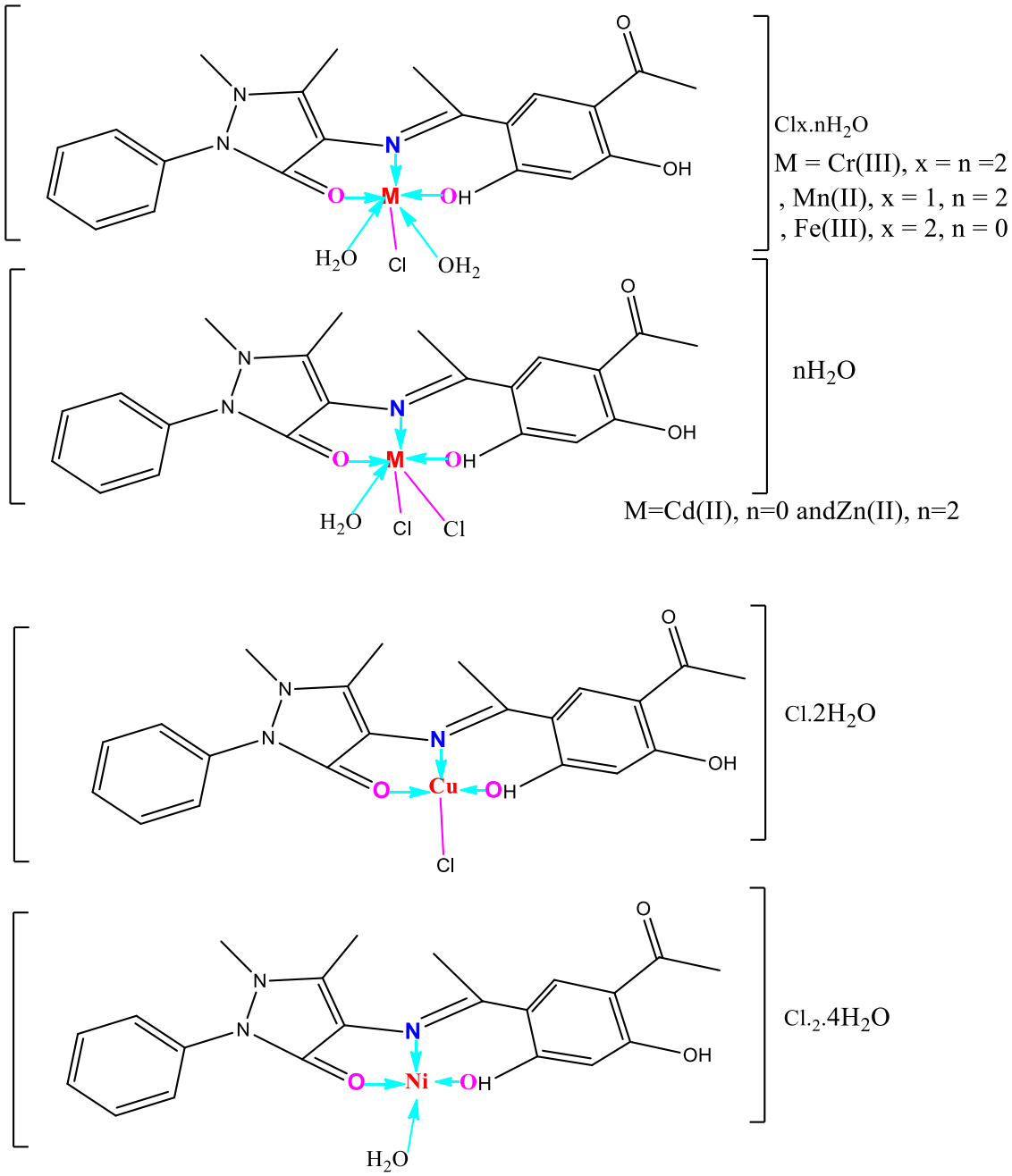


Figure S1. Structures of Schiff base metal complexes.

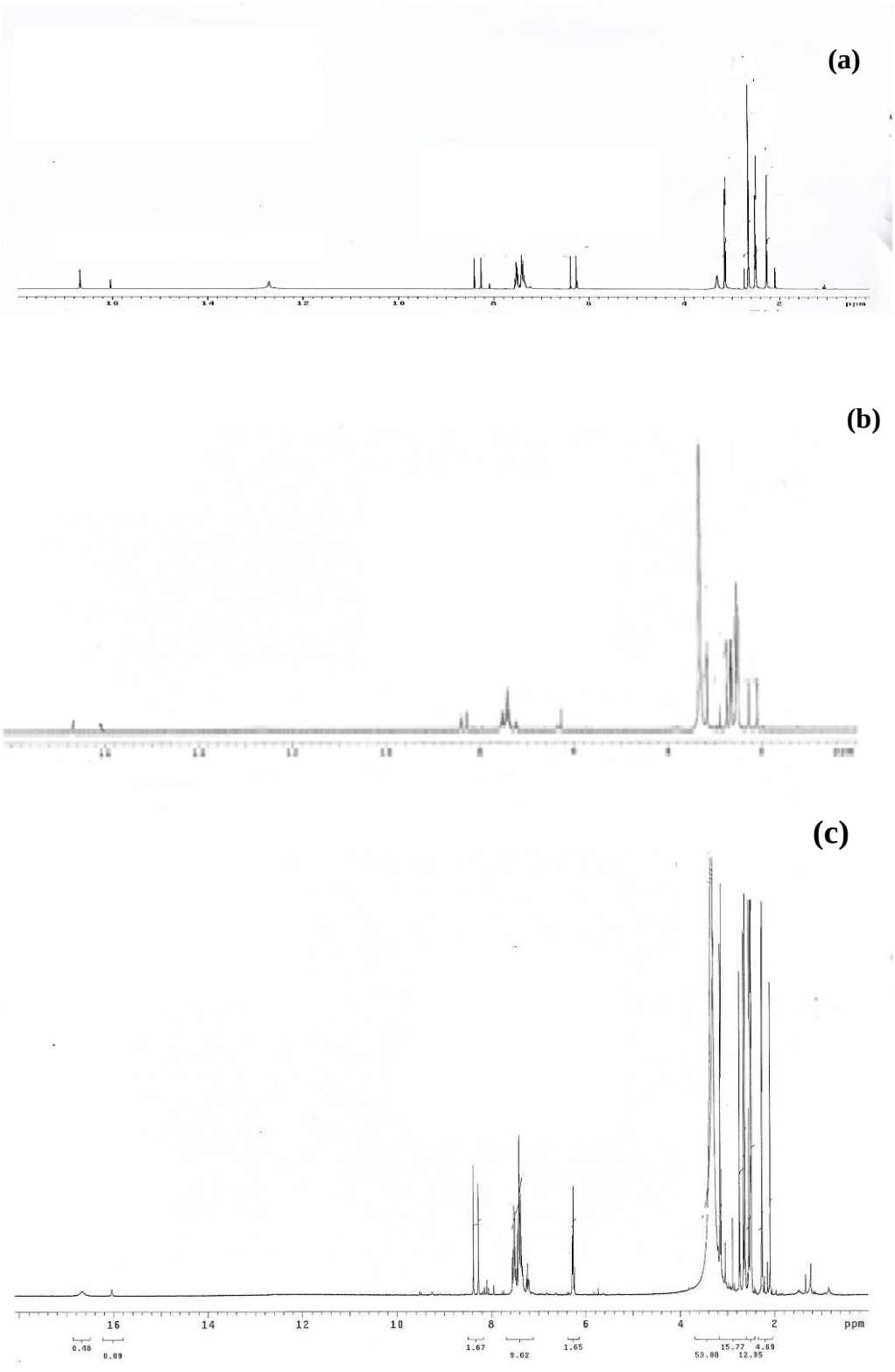


Figure S2. ^{1}H NMR spectra of (a) H_2L, (b) Zn(II) and (c) Cd(II) complexes.

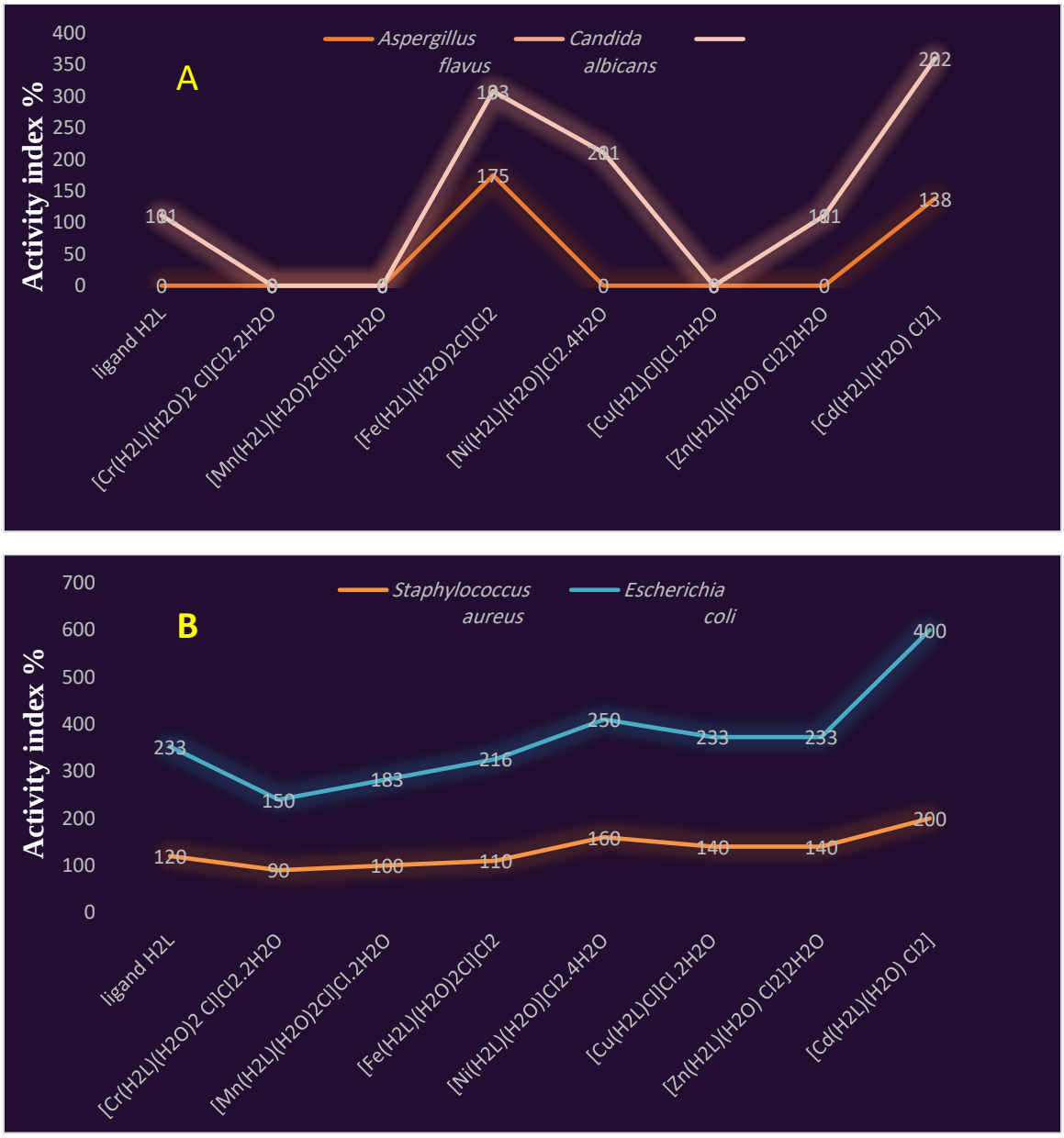


Figure S8. Activity index of Schiff base ligand (H_2L) and its metal complexes against (A) different fungal (B) different Gram (+ve) and Gram (−ve) bacteria.

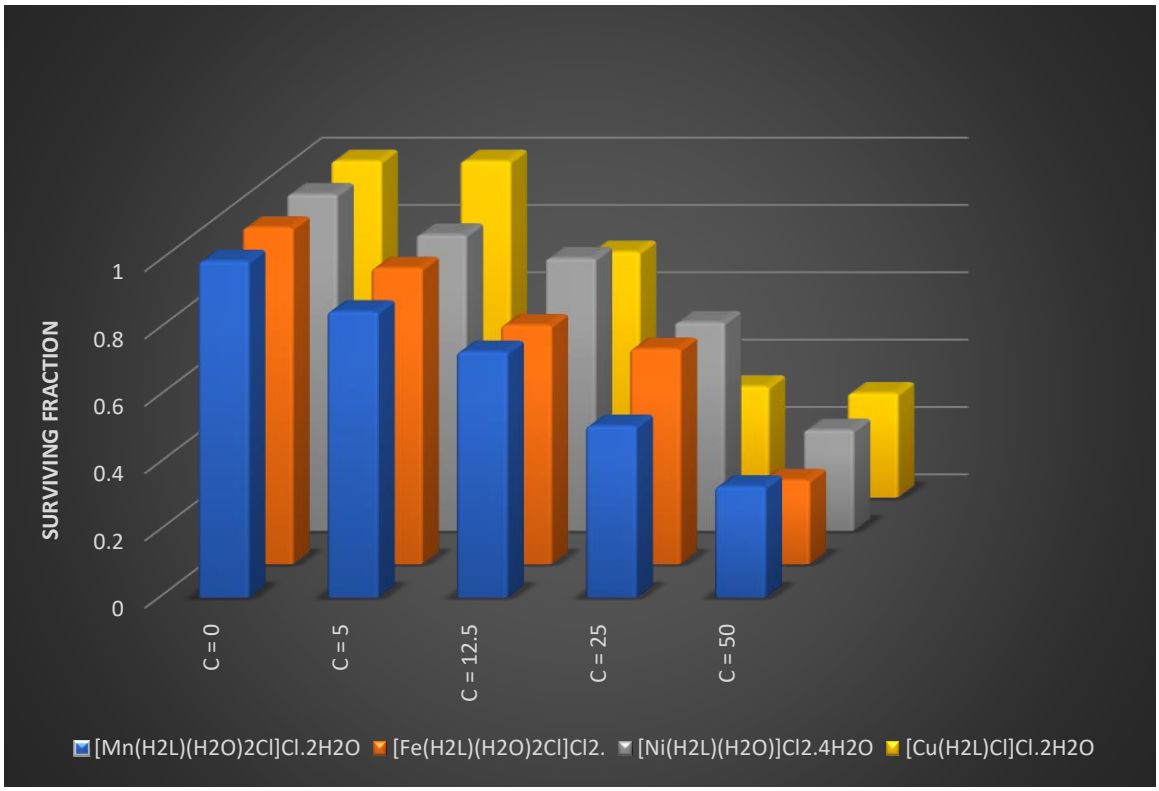
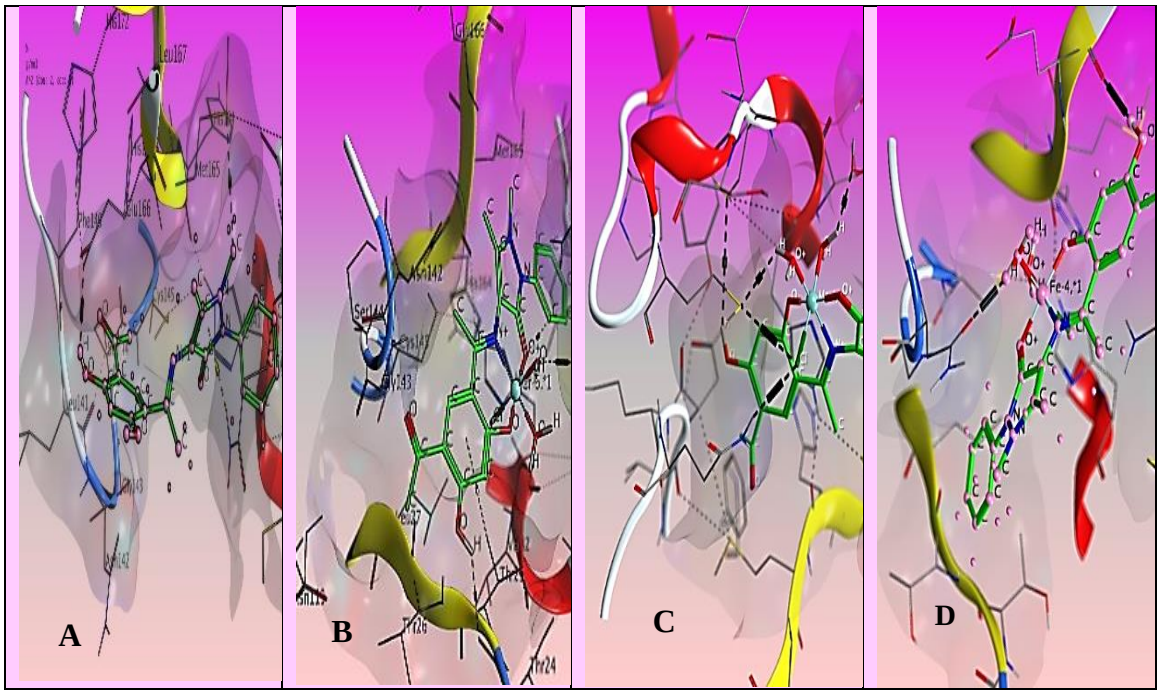


Figure S9 . Anticancer effects of Schiff base ligand and its metal complexes in terms of % cell inhibition at 100 µg/ml concentration.



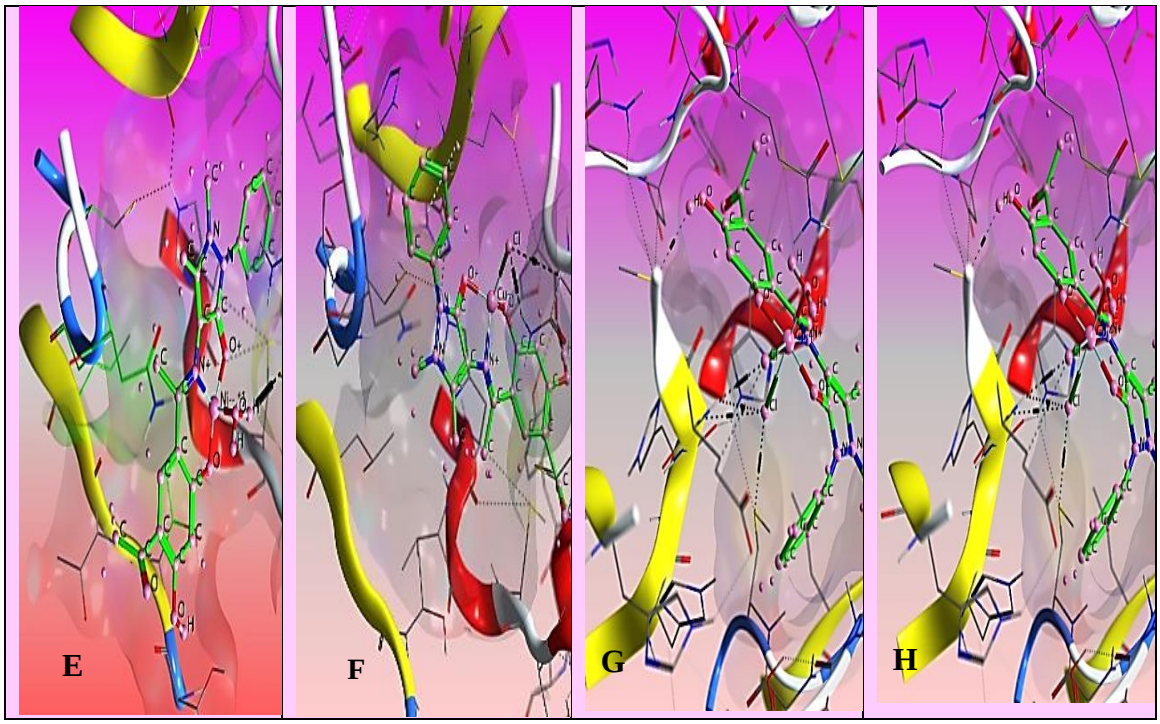


Figure S11. 3D Molecular docking simulation studies of the interaction between (A) Schiff base ligand H_2L and (B) Cr(III), (C) Mn(II), (D) Fe(III), (E) Ni(II), (F) Cu(II), (G) Zn(II) and (H) Cd(II) complexes with the active site of the receptor of PDB ID: 6XBH. The docked conformation of the compound is shown in ball and stick representation.

Table S3. The different optimized and quantum chemical parameters of H_2L and its Cd(II) complex.

Bond lengths (Å)	**H_2L**	$[Cd(H_2L)(H_2O)Cl_2]$
C(1) - N(2)	1.46	1.47
C(1) - O(24)	1.25	1.33
N(2) - N(3)	1.41	1.43
N(2) - C(4)	1.47	1.47
N(3) - C(15)	1.47	1.47
N(3) - C(19)	1.50	1.49
C(25) - N(26)	1.46	1.50
N(26) - C(27)	1.31	1.31
C(29) - O(40)	1.43	1.45
C(34) - O(42)	1.43	1.43
O(40) -,H(41)	0.96	0.96
O(42)- H(43)	0.96	0.96
C(44) - O(45)	1.26	1.26
Cd(50) - Cl(51)	------	2.40
Cd(50) - Cl(52)	----	2.40

Cd(50) - O(53)	----	3.11
O(40) - Cd(50)	----	3.06
N(26) - Cd(50)	----	3.06
O(24) - Cd(50)	----	3.08
Bond angles (º)		
O(24)- Cd(50)- O(40)	----	114
O(24) -Cd(50) - Cl(52)	----	89
N(26) - Cd(50) - Cl(52)	----	93
O(40) - Cd(50) - Cl(51)	----	90
O(40) - Cd(50) - O(53)	----	94
Cl(51) - Cd(50) - O(53)	----	86
The calculated quantum chemical parameters		
E (a.u.)	-1270.99	-7705.93
Dipole moment (Debye)	4.60	13.75
E_{HOMO} (eV)	-5.51	-6.10
E_{LUMO} (eV)	-1.70	-2.30
Δ E (eV)	3.81	3.80
χ(eV)	-3.61	-4.20
η (eV)	1.91	1.90
σ $(eV)^{-1}$	0.52	0.53
Pi (eV)	3.61	4.20
S $(eV)^{-1}$	0.26	0.26
ω (eV)	3.41	4.64
ΔN_{max}	1.89	-2.21

Table S7. Biological activity of Schiff base ligand (H_2L) and its metal complexes.

Sample		Inhibition zone diameter (mm/mg sample)			
		Bacterial species		Fungal species	
		G^+	G^-		
		Staphylococcus aureus	***Escherichia coli***	***Aspergillus flavus***	***Candida albicans***
Control: DMSO		**0.0**	**0.0**	**0.0**	**0.0**
Standard	**Amikacin Antibacterial agent**	**10**	**6**	**--**	**--**
	ketokonazole Antifungal agent	**--**	**--**	**8**	**9**
H_2L		12	14	0	10
$[Cr(H_2L)(H_2O)_2Cl]Cl_2 \cdot 2H_2O$		9	9	0	0
$[Mn(H_2L)(H_2O)_2Cl]Cl \cdot 2H_2O$		10	11	0	0
$[Fe(H_2L)(H_2O)_2Cl]Cl_2$.		11	13	14	12
$[Ni(H_2L)(H_2O)]Cl_2 \cdot 4H_2O$		16	15	0	19
$[Cu(H_2L)Cl]Cl \cdot 2H_2O$		14	14	0	0
$[Zn(H_2L)(H_2O)Cl_2] \cdot 2H_2O$		14	14	0	10
$[Cd(H_2L)(H_2O)Cl_2]$		20	24	11	20