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J. Serb. Chem. Soc. *89* (2) S76–S86 (2024) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Anticancer acitivity of Schiff base ligand (*E*)-4-((5-chloro-2--hydroxybenzylidene)amino)-1,5-dimethyl-2-phenyl-1*H*-pyrazol--3(2*H*)-one and its Co(II), Cu(II) and Zn(II) metal complexes

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TABLE I. Physical and analytical data of ligand and its metal complexes; M.P.: melting point

No.	Compound	Colour	Yield (%)	M.P. (°C)	Elemental analysis Found % (Calcd.%)		
					C	H	N
1.	L	Yellow	71	275	62.85(63.25)	4.92(4.72)	11.90(12.29)
2.	Mn(II) complex	Pink	68	>300	48.92(49.86)	4.50(4.98)	8.50(8.31)
3.	Co(II) complex	Brown	75	>300	48.85(49.47)	4.15(4.94)	8.65(8.24)
4.	Ni(II) complex	Light yellow	64	>300	48.75(49.50)	4.30(4.94)	7.95(8.25)
5.	Cu(II) complex	Green	72	>300	49.50(49.03)	4.80(4.90)	7.55(8.17)
6.	Zn(II) complex	Yellow	62	>300	48.03(48.85)	4.75(4.88)	7.58(8.14)
7.	VO(II) complex	Light brown	69	>300	48.10(48.72)	3.95(4.32)	8.96(9.47)

TABLE S-II. XRD spectral data of metal complexes

Compounds	Mn(II)	Co(II)	Ni(II)	Cu(II)	Zn(II)	VO(II)
No. of reflections	12	10	19	25	29	23
Maxima(2θ)	49.56^0	54.51^0	32.13^0	72.00^0	35.20^0	60.19^0
Intensity	82.5 a.u.	100 a.u.	21.4 a.u.	14.2a.u.	59.6 a.u.	100a.u.
d value	9.762 Å	12.106 Å	18.560 Å	7.983Å	15.808 Å	7.470 Å
Lattice constant (Å)	a = 7.8130 b = 8.0580 c = 10.2120	a = 12.4230 b = 4.7220 c = 16.1100	a = 8.4047 b = 25.3897 c = 18.6676	a = 15.9658 b = 15.9658 c = 7.1487	a = 8.9034 b = 10.0168 c = 16.7090	a = 5.9645 b = 12.5730 c = 9.4371
Unit cell volume	590.695	920.888	2952.077	1578.117	1281.614	696.431
Axis and axis angle	a ≠ b ≠ c and α ≠ β ≠ γ	a ≠ b ≠ c and α = γ	a ≠ b≠ c and α = γ =90^0	a = b ≠ c and α = β =	a ≠ b ≠ c and α ≠ β	a ≠ b ≠ c and α = γ =

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		$= 90^0 \neq \beta$	$\neq \beta$	$90^0 \neq \gamma$	$\neq \gamma$	$90^0 \neq \beta$
Z Value	1	2	6	1	2	4
Crystal system	Orthorhom.	Monoclinic	Monoclinic	Hexagonal	Orthorhom.	Monoclinic

MASS SPECTRUM OF SCHIFF BASE LIGAND

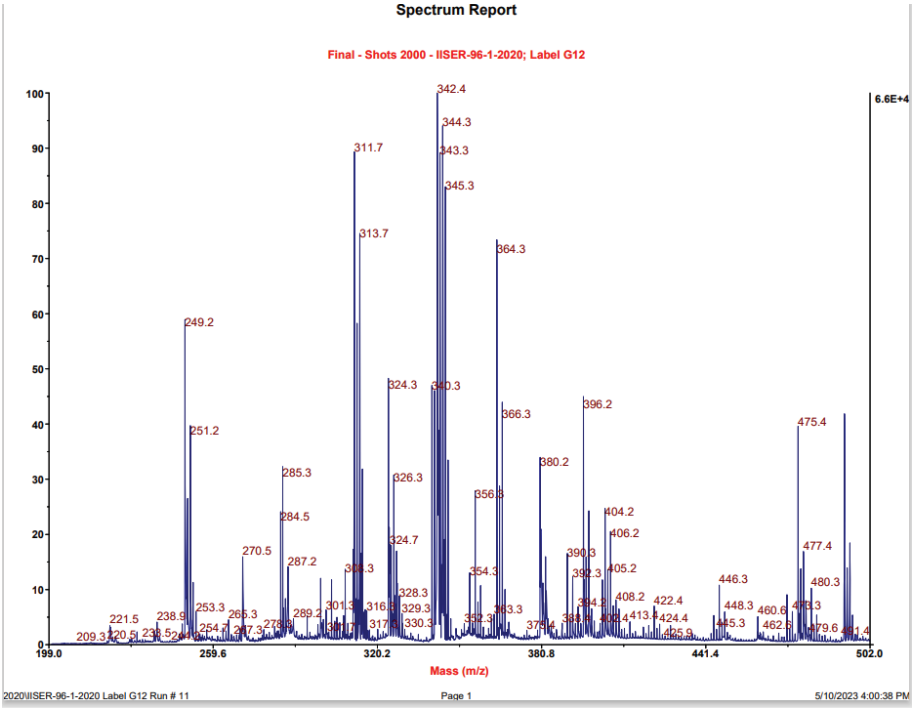


Fig. S-1. The mass spectrum of Schiff base ligand was expected to show the peak at 342 and in spectrum it showed 342 and 343(M+1).

^{1}HNMR SPECTRUM OF SCHIFF BASE LIGAND

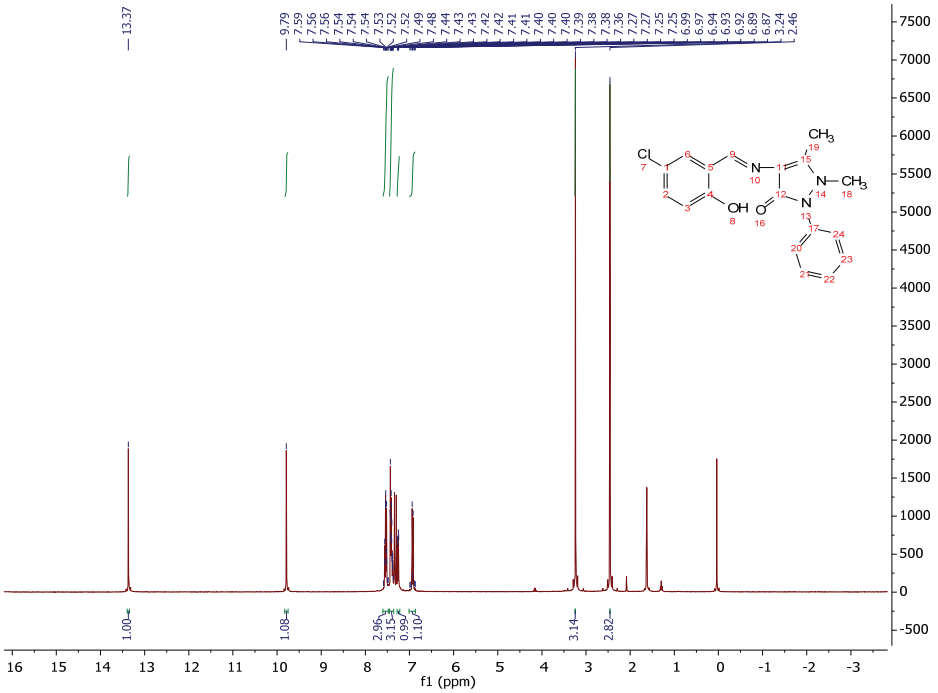


Fig. S-2. In the ^{1}H-NMR the above figure shows peaks at δ 13.36(s, 1H), 9.78(s, 1H), 7.58 – 7.49 (m, 2H), 7.46 – 7.35 (m, 3H), 7.33 (d, J = 2.6 Hz, 1H) meta coupling, 7.36 – 7.25 (m, 1H), 6.92 (d, J = 8.8 Hz, 1H), 3.24 (s, 3H) it goes to N-CH_3, 2.46 (s, 3H) it belongs to C-CH_3.

FTIR SPECTRUM OF SCHIFF BASE LIGAND

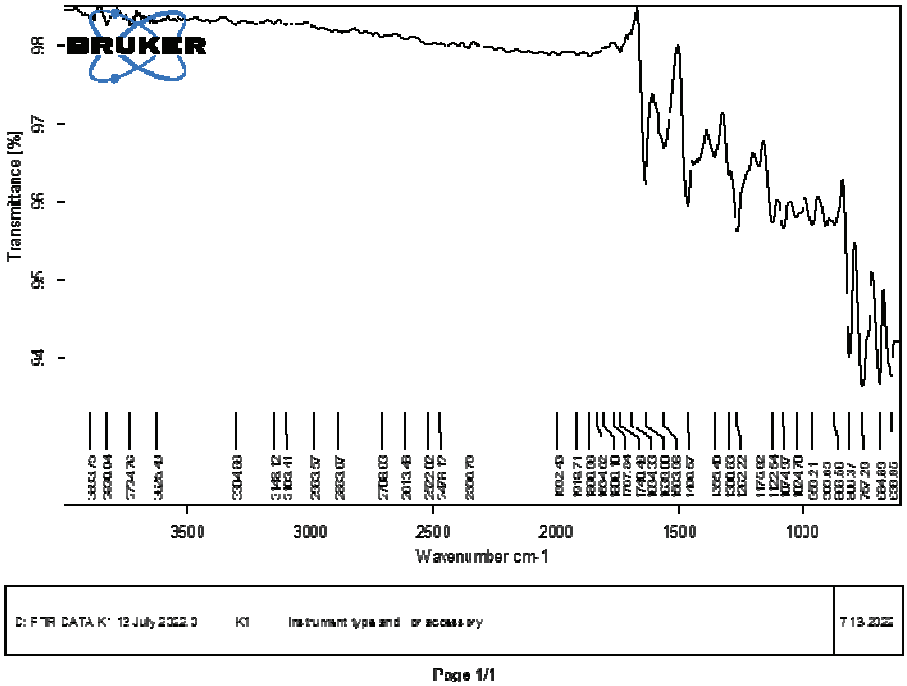


Fig. S-3. FTIR Spectrum of Schiff base ligand shows bands at 1639cm^{-1}.

FTIR SPECTRUM OF METAL COMPLEXES

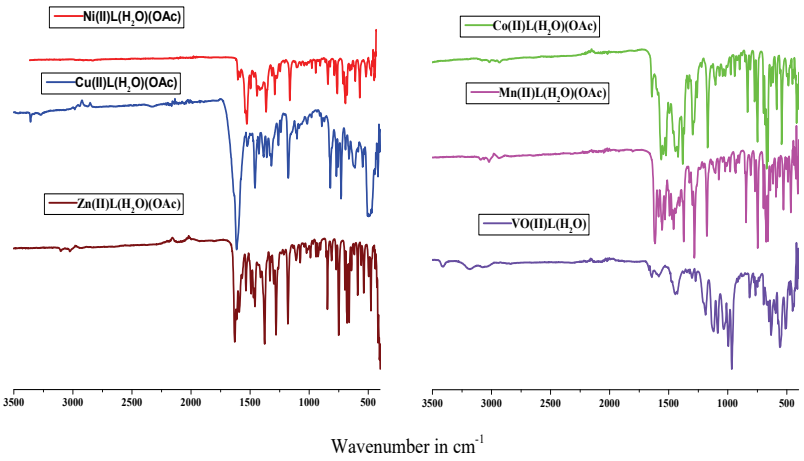


Fig. S-4. The FTIR spectrum of metal complexes decreased by 30-35cm^{-1} it is primary suggestion that metal complexes may be formed.

ELECTRONIC SPECTRA

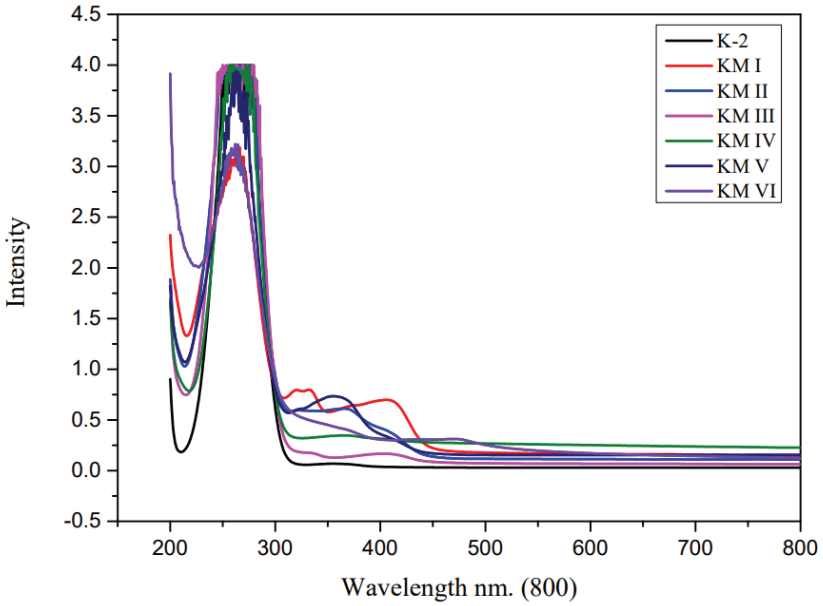


Fig. S-5. The electronic spectra of Schiff base and metal complexes is represented as above.

TGA-DTA OF METAL COMPLEXES

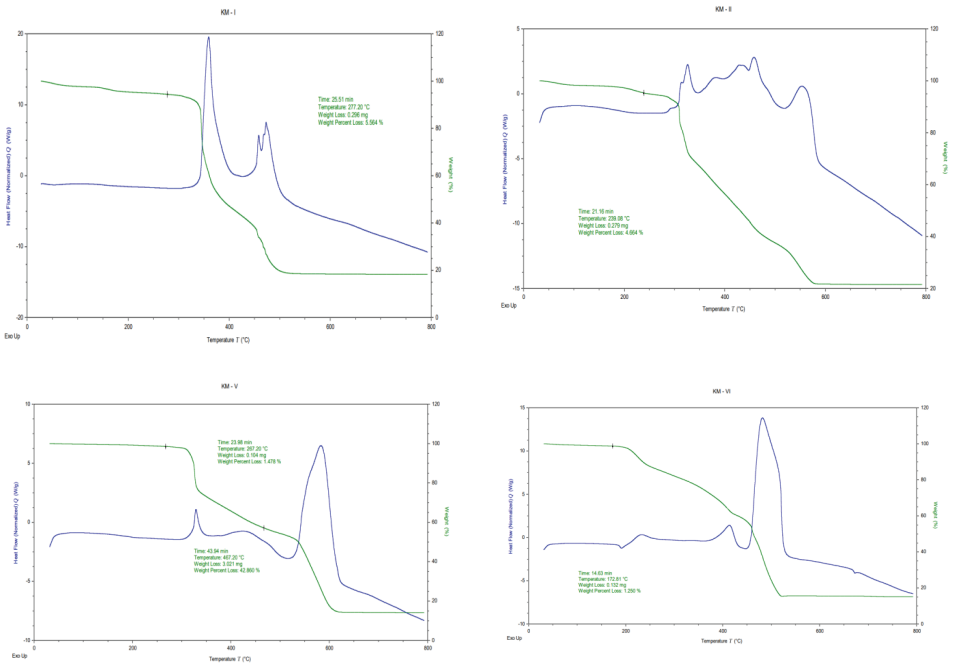


Fig. S-6. The TGA-DTA shows the formation of metal oxide which give the confirmation regarding the formation of metal complexes by loss of coordinated molecules.

POWDER XRD

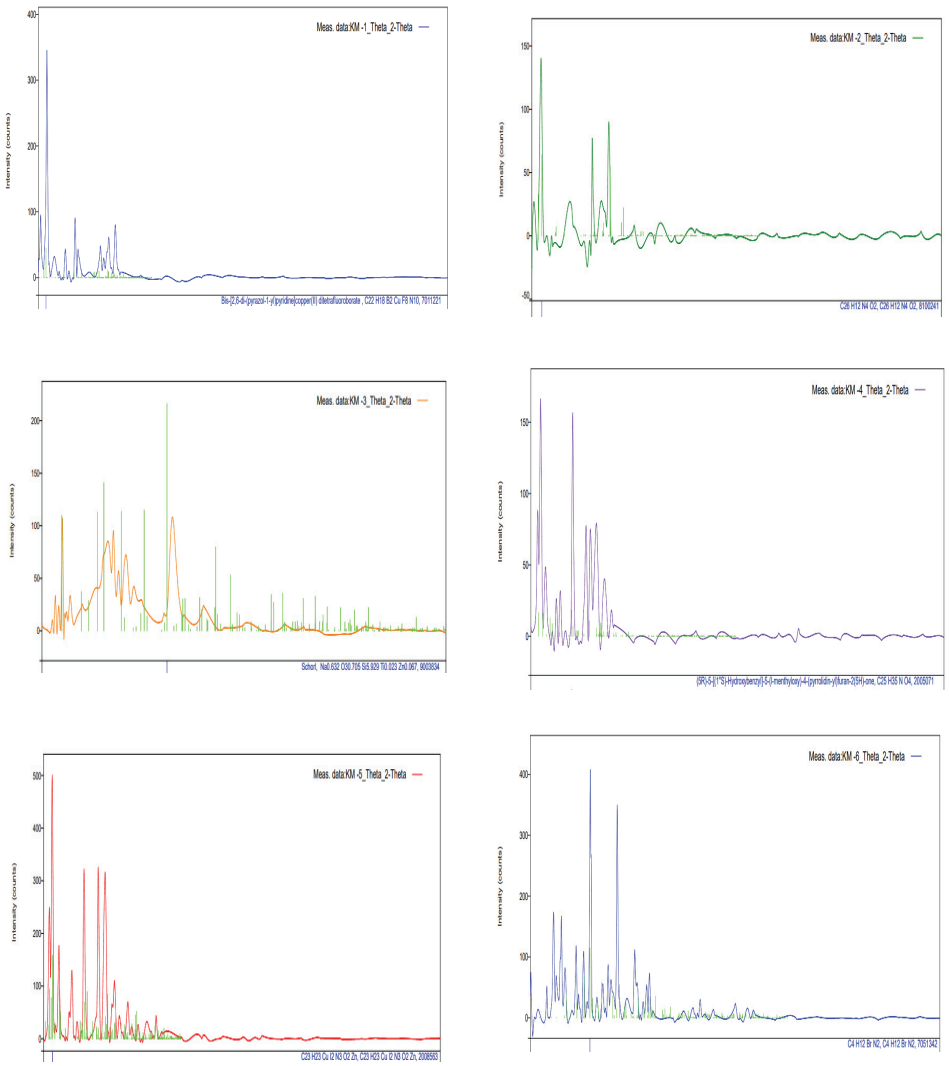


Fig. S-7. The powder XRD gives the information regarding the crystal systems of metal complexes.

ANTIBACTERIAL ACTIVITY

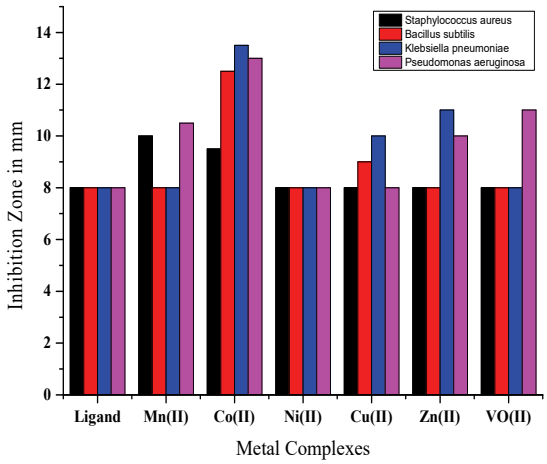


Fig. S-8. The antibacterial activity of Schiff base ligand and metal complexes shows that metal complexes are more active than that of ligand.

ANTIFUNGAL ACTIVITY

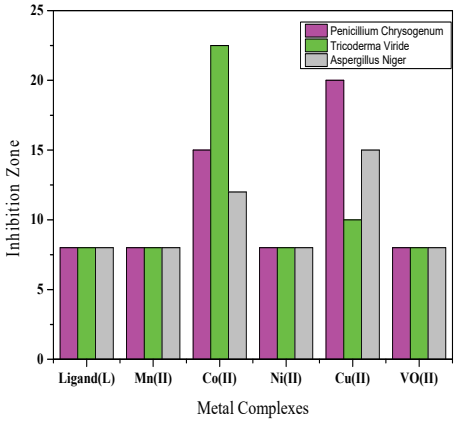


Fig. S-9. The antifungal activity of Schiff base ligand and metal complexes shows that metal complexes are more active than that of ligand.

ANTICANCER ACTIVITY

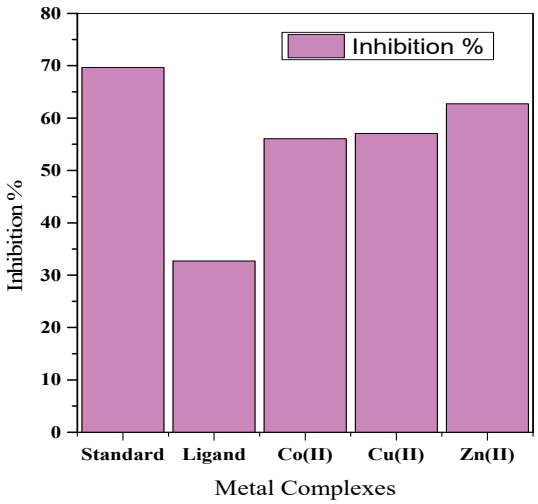
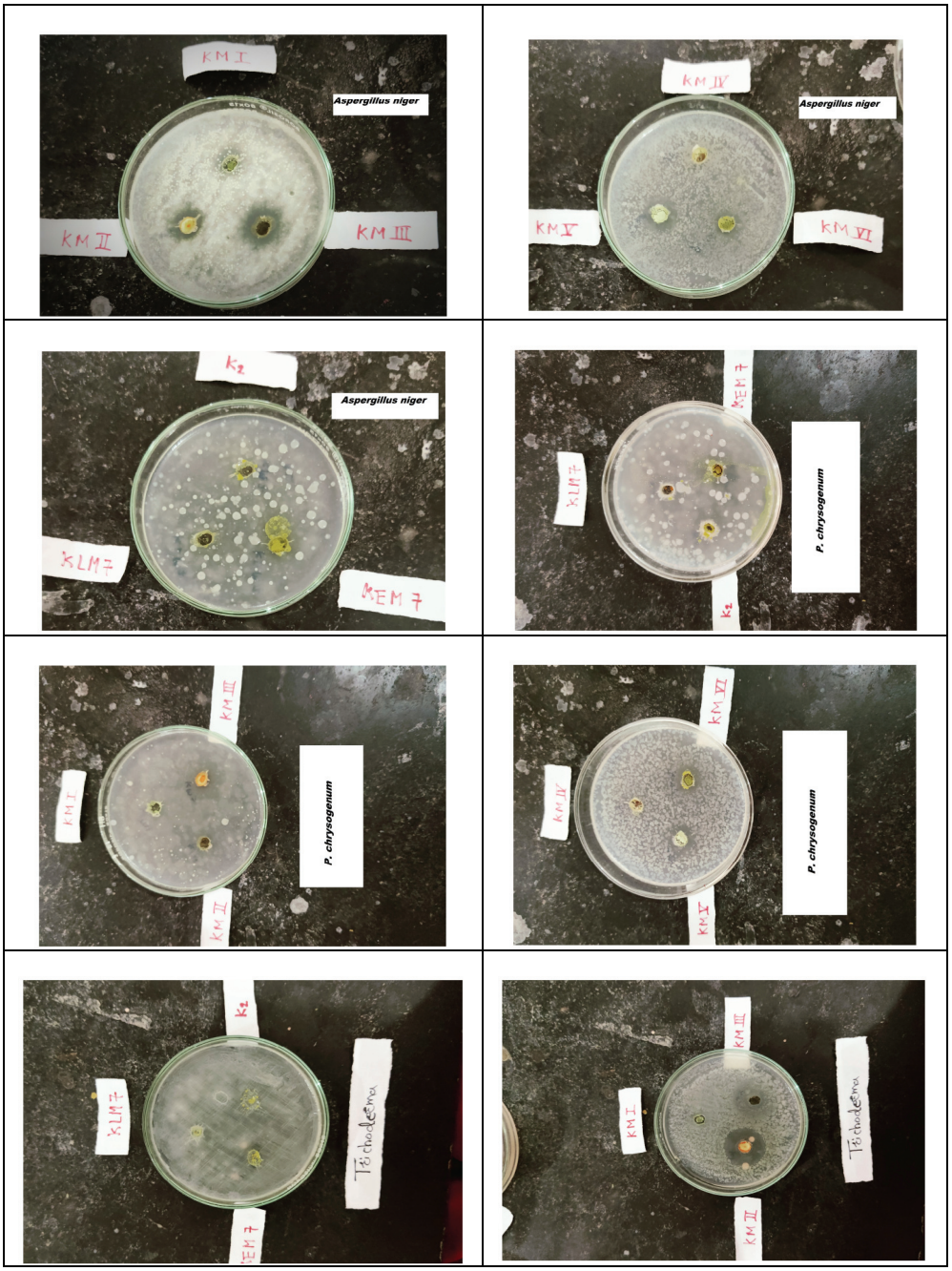


Fig. S-10. The Anticancer Activity of Schiff base ligand and metal complexes shows that metal complexes are more active than that of ligand.

PHOTOGRAPHS OF BIOLOGICAL ACTIVITY



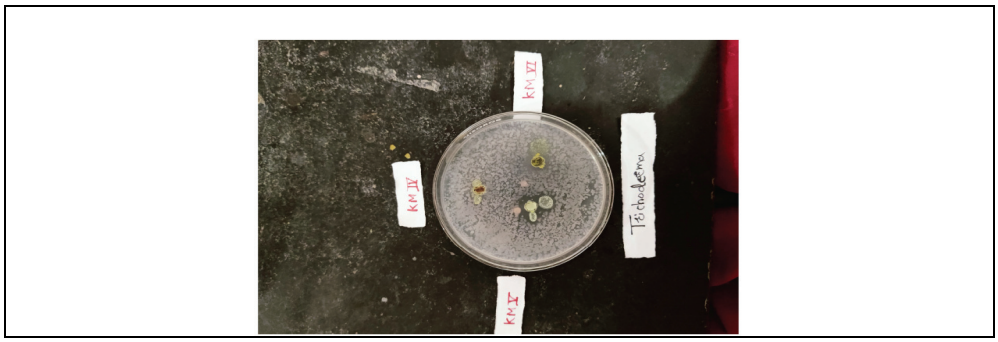


Fig S-11. These photograph shows the biological activities of Schiff base ligand and metal complexes.