

Electronic Supplementary Data

Theoretical and experimental studies of novel histidine derived Schiff base metal complexes, active towards biomedical and MCF 7 cell lines

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Table S1 — Antibacterial results of complexes 1-5

| Ligands | Zone inhibition in mm | | | |
|-------------------|-----------------------|-----------------|----------------|------------------------|
| | <i>E.coli</i> | <i>S.aureus</i> | <i>A.niger</i> | <i>Penicillium sp.</i> |
| Copper complex | 29 | 25 | 17 | 26 |
| Cobalt complex | 24 | 22 | 15 | 24 |
| Manganese complex | 19 | 18 | 13 | 19 |
| Zinc complex | 18 | 19 | 12 | 14 |
| Nickel complex | 13 | 18 | 9 | 14 |

Table S2 — IC₅₀ values of DPPH scavenging activity of L and its complexes (1-3)

| Compound | IC ₅₀ (mg/mL) |
|----------|--------------------------|
| L | 0.398 |
| 1 | 0.217 |
| 2 | 0.180 |
| 3 | 0.196 |
| 4 | 0.253 |
| 5 | 0.231 |

Table S3 — Anti-cancer activity of Metal complexes against MCF – 7

| Concentration μg/mL | Copper Complex | Cobalt Complex | Manganese Complex | Zinc Complex | Nickel Complex |
|------------------------|-------------------|-------------------|----------------------|-----------------|-------------------|
| 250 | 14.58 | 29.17 | 19.58 | 36.25 | 25.83 |
| 100 | 33.75 | 39.79 | 38.33 | 53.75 | 44.58 |
| 50 | 50.21 | 54.38 | 54.38 | 67.5 | 58.13 |
| 25 | 55.42 | 59.38 | 61.25 | 72.08 | 66.88 |
| 12.5 | 61.04 | 63.75 | 66.46 | 78.96 | 75.42 |
| 6.25 | 67.29 | 69.17 | 72.08 | 84.58 | 82.29 |
| IC 50 μg/mL | 45.89 | 59.83 | 60.39 | 114.43 | 75.74 |

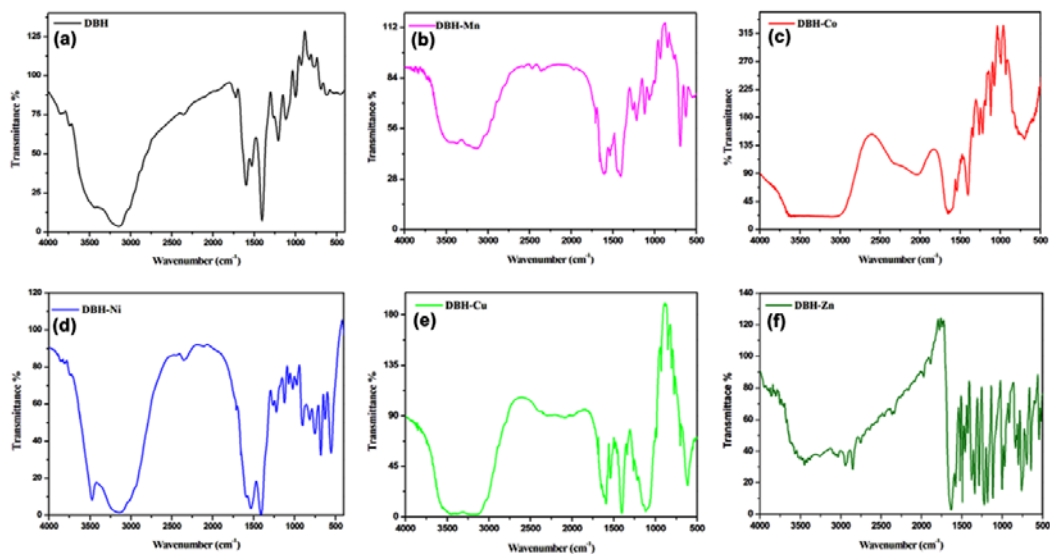


Fig.S1 — FT-IR spectrum of Ligand and complexes 1-5 respectively in a-f

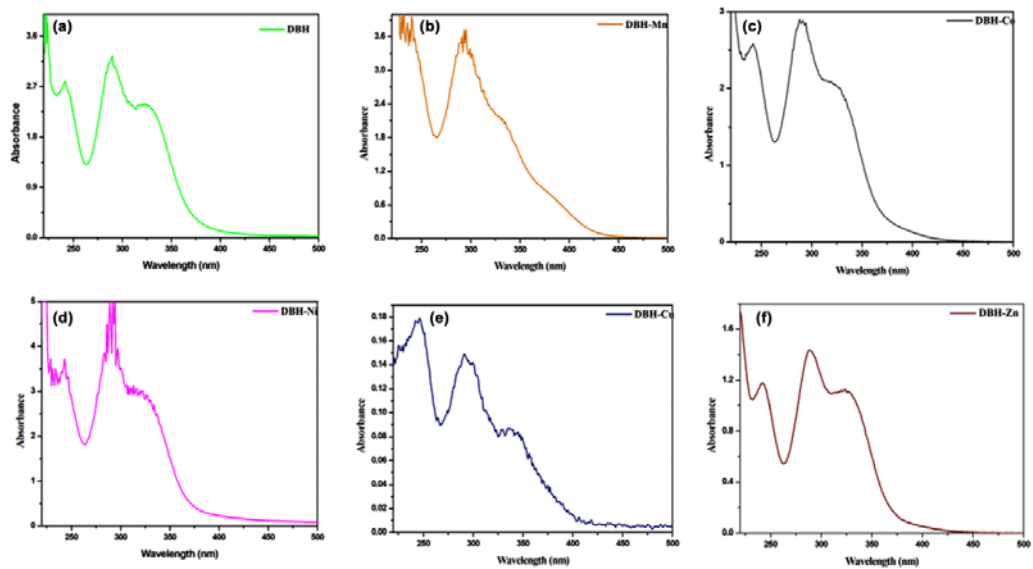


Fig. S2 — Absorption spectra of L and complexes 1-5 respectively in a-f

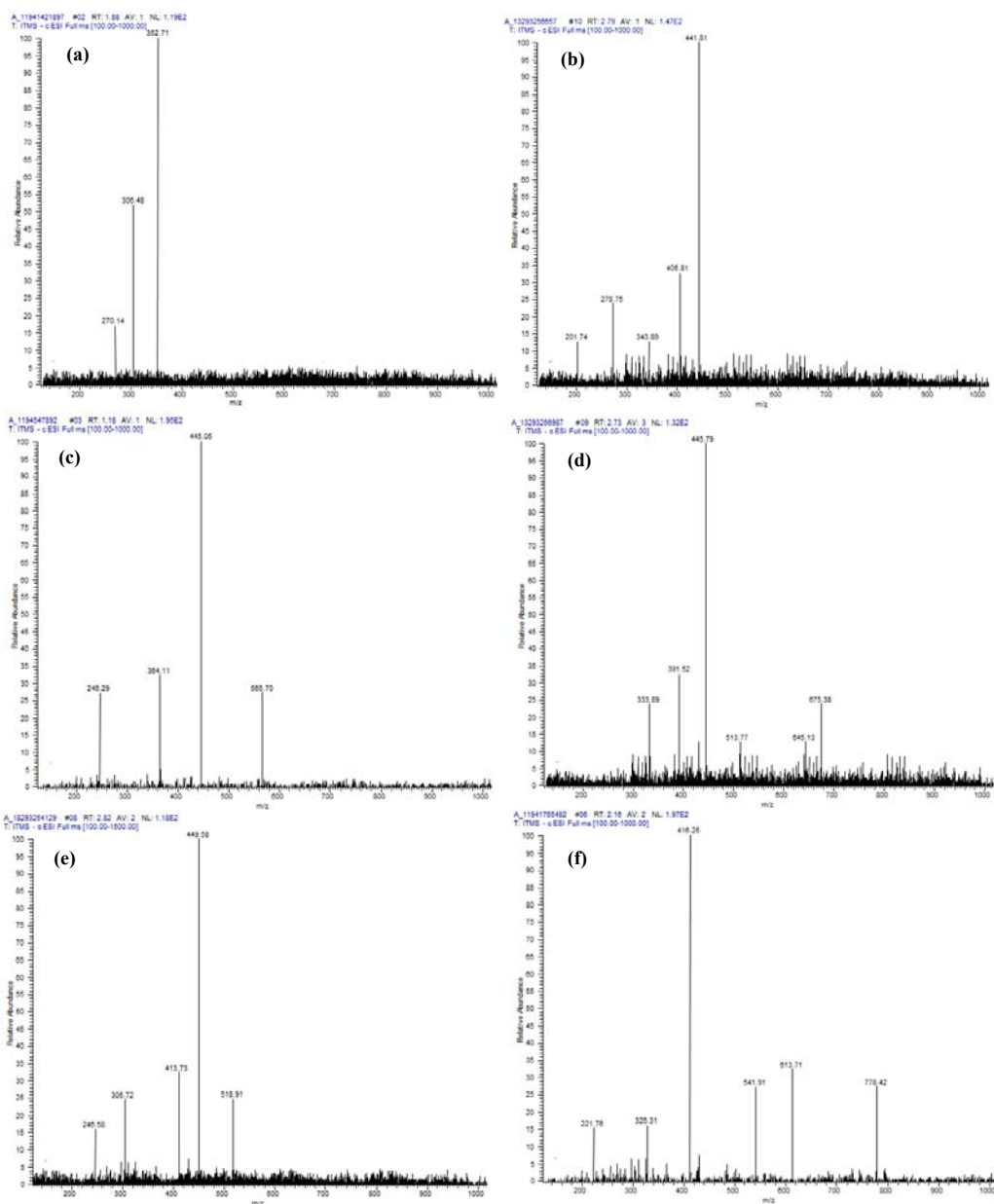


Fig. S3 — ESI-MS spectra of L and complexes 1-5 respectively in a-f

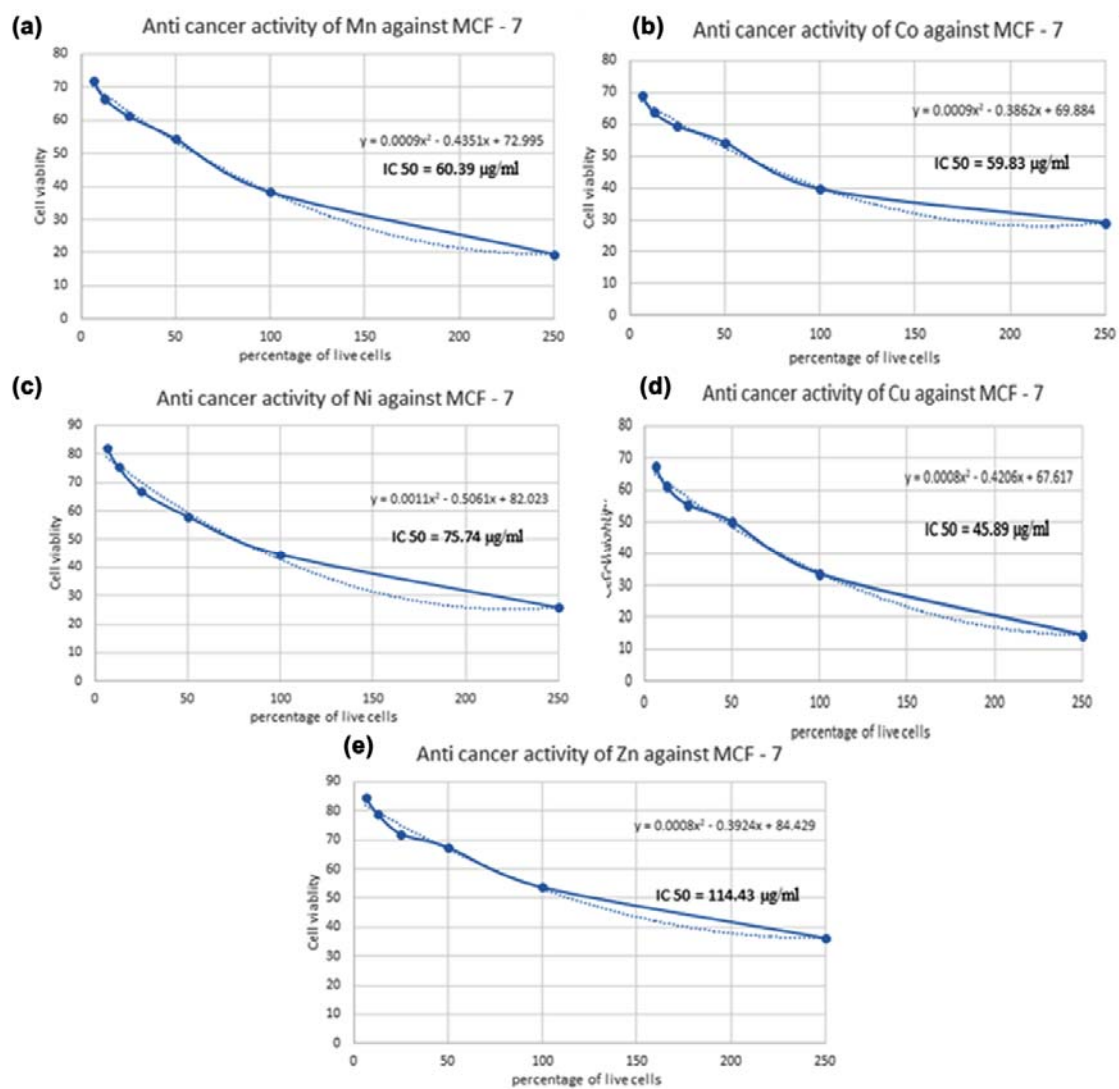


Fig. S4 — Cytotoxicity of complexes 1-5 represent in a-e