8. SUMMARY AND CONCLUSION

The Schiff base compounds L1, L2 and L3 were prepared by the condensation of 2,6-dimethyl-5-heptenaldehyde, commonly known as melonal, which is present in watermelon with aniline/chloroaniline/fluoroaniline in 1:1 molar ratio and they were characterized by GC-MS, IR spectra, $^1$H NMR, UV-Visible spectra and TGA.

Schiff base compounds were used as ligands to synthesize metal-complexes using the transition metals- copper, nickel, cobalt and chromium and inner transition metal samarium. The complexes were characterized by Maldi-TOF, TGA, IR, UV-Visible and EDX.

Spectral study and thermal data of the Schiff base and metal complexes derived from L1 and L2 indicated that Cu(II), Ni(II), Co(II), Cr(III) and Sm(III) form mononuclear complexes. In case of Schiff base metal complexes derived from L3, Cu(II),Ni(II) and Sm(III) form mononuclear complexes whereas Co(II) and Cr(III) formed binuclear bridging complexes.

Schiff base ligands L1, L2 and L3 and their respective metal complexes were screened for antibacterial activity. The studies were conducted against gram−negative strains, viz., E. coli (ETEC), S. typhi, P. aeruginosa and gram−positive bacterial strains viz., s. aureus, B. subtilis, B. megaterium bacterial strains and fungi (C. albicans, P. chrysogenum, A. niger, A. flavus, A. fumigatus, C. oxysproum). The minimum inhibition concentration (MIC) obtained were compared with that of standard drug gentamycin for bacteria and amphotericin for fungi.

Metal complexes derived from L1, exhibited moderate anti-bacterial activity against E. coli and particularly Cr(III) complex exhibited better anti-fungal activity.
Schiff base ligand L2 and its Cr(III) complex were exhibiting antifungal activity equivalent to that of reference Amphotericin against *P. chrysogenum*. Co(II) complex showed better activity against *Pencillium chrysogenum* compared to reference amphotericin.

The thermal stability of the shiff base ligand increased due to halogen substitution.

The complexes derived from ligands L2 & L3 have better antimicrobial activity due to the presence of electronegative groups (Cl & F) compared to unsubstituted aniline complexes. This also helps to conclude that electron withdrawing group enhances the antimicrobial activity.

The anti-oxidant studies revealed that, among the L1 complexes, except Cu(II) complex the other metal complexes exhibited moderate scavenging activity against DPPH. Complexes of L2 with Co(II) and Ni(II) exhibited moderate anti-oxidant activities. Complexes of L3 with Co(II) and Cr(III) however exhibited moderate anti-oxidant activities.

The binuclear complexes have distinct advantage over mononuclear counterparts in their cytotoxicity. Binuclear cobalt and chromium complexes of L3 exhibit better cytotoxicity than their mononuclear counterparts.

Computational studies were carried out to support the structural elucidation. Molecular docking studies were undertaken to evaluate the possible binding for biomolecules. The structures obtained from ab initio DFT were consequently docked against the appropriate proteins. This supported the mechanistic rationale behind the interaction between the selected protein and the synthesized complexes. The docking studies supports best poses of binding unto the protein.

Sm(III)–L2 complex exhibited very good cytotoxicity of 47%. Co(II)-L2 and Co(II)-L3 complexes showed better activity against *Pencillium chrysogenum* compared to reference amphotericin. They also exhibited moderate antioxidant and anticancer properties. From the foregoing
discussions it is clear that Co(II)-L2 and Co(II)-L3 complexes are rare a combination of antifungal, anticancer and antioxidant properties and Sm(III)–L2 complex had very good anti-cancer activity.