**ABSTRACT**

A new series of transition metal complexes of mercapto pyrimidine Schiff base complexes has been studied and characterized using various spectral techniques like single crystal XRD, FT-IR, electronic, EDX and TGA. The molecular properties of the ligand and the complexes have been derived from HOMO-LUMO calculations using Gaussian software. The biological evaluation of the ligands and the complexes has been studied and compared. The DNA binding studies of the complexes has been carried out and the binding constants are in the order of 104 M−1. The DNA cleavage activity of the complexes proves the mechanism of cleavage is through non-hydrolytic pathway.