Chapter 1 includes a literature review on amine functionalized ligands and 1,1-dithio ligand systems and their importance in the coordination chemistry of transition metals that display a wide range of applications. The biological applications, particularly, anticancer properties of the newly synthesised molecules have been further emphasised. The main objectives of the present investigation are also described in this chapter.

Chapter 2 describes the synthesis of a new series of amide functionalized 2º- and 3º-aminomethylferrocene derived from ferrocenylmethylamine. The compounds were characterized by microanalysis, ^{1}H, ^{13}C NMR, UV-visible, fluorescence, FTIR, thermogravimetric and crystallographic techniques. All the compounds were evaluated against MCF 7, IMR 32, HepG2 and immortal L132 cell lines by MTT assay and the results were compared with cisplatin. The majority of the newly synthesized compounds fluorescence in the visible region of upon excitation in the ultraviolet region with a concomitant Stokes shift of 60-100 nm. X-ray crystallography revealed the propensity of amidic and amine groups of newly synthesized amines to form intermolecular hydrogen bonding. The western blot, gene expression, mitochondrial membrane potential and flow cytometry study were used to investigate the mode of action of these derivatives as antitumor agents. The results showed apoptotic property of the compounds by modulating inflammatory pathway against human tumor cells of different origin. Moreover, a detailed in-silico study on the compounds have been carried out to rationalize the experimental results.

Chapter 3 deals with the derivatization of ferrocenylmethylamine into a novel series of ferrocene functionalized chiral tertiary/ secondary amine ligand precursors. The compounds were characterized by microanalysis, HPLC, ^{1}H, ^{13}C NMR, UV-visible, fluorescence, FTIR, thermogravimetric and crystallographic techniques. Further, compounds have been screened for their potential cytotoxicity by MTT assay against human carcinoma cell lines MCF 7, IMR 32, HepG2, and immortal L132 cell lines and the results were compared with cisplatin. Chirality-related influence on the antiproliferative activity of some enantiomeric pairs and at the supramolecular level is

elaborated. The electrochemical, DFT calculations and molecular docking study have been performed to justify the experimental outcomes.

Chapter 4 chiral secondary amines holding ferrocene functionality (presented in the previous chapter) were taken for the development of new Ni^{+2}-bis-dithiocarbamates complexes. Compounds were characterized by microanalysis, ^{1}H, ^{13}C NMR, UV-visible, fluorescence, FTIR, thermogravimetric techniques. Single crystal X-ray crystallographic study have been performed on some of the representative compounds to elucidate their molecular structures. The molecular electrostatic potential clearly demonstrates the presence of polar amide subunits projected towards the outside in these molecules. This would provide H-bond donor-acceptor sites to facilitate the interactions of these molecules with biomolecules through increased concentration of complexes at the site of action via an effective cellular membrane transportation.

Chapter 5 demonstrates the synthesis of a number of benzyl functionalized chiral 2^0 and 3^0 amines. All the compounds were thoroughly characterized by microanalysis, ^{1}H, ^{13}C NMR, UV-visible, fluorescence, FTIR and CD-spectral studies. Single crystal X-ray crystallographic study have been performed on some of the representative compounds to elucidate their molecular structures and crystal packing patterns. Preliminary investigation of the tertiary amine compounds **5-13** holding a greater number of biologically relevant groups for their cytotoxicity potentials against MDA-MB-231 carcinoma cell line have been caried out by MTT assay and the results showed cytotoxic activity of these compounds against in low micro-molar concentrations. However, further explorations are needed to establish the mode of action of these molecules.

Chapter 6 is devoted to the utilization of benzyl functionalized chiral secondary amines (presented in chapter 5) in the development of new Cu^{+2} and Ni^{+2} dithiocarbamates complexes. The potassium salt of dithiocarbamate (dtc) ligands have been prepared *in situ* by the reaction of chiral secondary amines with CS_2 in the presence of base. The newly synthesized compounds were characterized by mass, IR, NMR (^{1}H, ^{13}C), UV-visible absorption, fluorescence, and magnetic susceptivity studies. The experimental data are well supported by theoretical study. The thermal stability of these compounds has been investigated by thermogravimetric analysis. Notably, Ni^{II}-/ Cu^{II}-

dithiocarbamates complexes reported in this chapter have shown their potentials to form metal sulphide nanoparticles, as revealed by thermogravimetric study.

Chapter 7, deals with the synthesis, characterization and i*n-silico* study of a new series of naphthoquinone functionalized Chiral and achiral 2^0 amine ligand precursors. The overall synthetic procedure is outlined in the scheme given below. All the compounds have been suitably characterized by standard spectroscopic and thermogravimetric techniques. The unprecedented molecular structures (Fig. 12) of some of the representative ligands have been established by single crystal XRD. Notably, compounds exhibit medium to strong fluorescence emission bands in the visible region with concomitant Stokes shifts of ≈ 280 nm. Supramolecular structures of some of the compounds have been studied by means of single-crystal X-ray diffraction to determine the influence of N-alkyl substituents and chirality on the association of molecules in the solid state. Moreover, the in-silico study was performed to reinforce the experimental data and to observe the influence of various N-alkyl substituents and chirality on the protein-ligand interactions with ATPase domain of Topoisomerase-II (PDB:1ZXM).

In **Chapter 8,** Xanthate ligand based complexes based metallomacrocyclic complexes of Ni^{II}, Cu^{II} and Zn^{+2} holding pendent amido groups have been synthesized by utilizing metal directed self-assembly of novel diol precursors L^1-L^3 , CS_2 and metal ion under basic reaction condition. All the diol precursors L^1-L^3 and their metallomacrocyclic 1,1-dithio complexes 1-9 have been characterized by thermogravimetric analysis and relevant spectroscopic techniques. Spectral data reveals the structural features of the newly synthesized compounds. The structures of these macrocyclic complexes 1-9 have been optimized by DFT calculations performed at B3LYP/lan2dz and the theoretical data are compared well with the experimental results. The mapping of molecular electrostatic potential (MESP) of all the compounds revealed that positive charges are mainly accumulated amidic NH whereas negative charges are localized at amidic CO. This shows the potentials of these molecules to involve in an effective H-bonding interactions in the biological systems.