The thesis entitled “Synthesis, Characterization and Structures of Organotin and Organoiron complexes” describes the chemistry of organotin(IV) and organoiron appended organotin(IV) complexes.

The sequence of the chapters reflect the synthesis of arylazo ligands, metallo pro-ligands (containing iron) and their subsequent reactions with organotin precursors followed by their characterization with the help of analytical and spectroscopic data. The solid state structures of some representative compounds were determined using single crystal X-ray crystallography. The work has been divided in six chapters.

Chapter 1

This is a general introductory chapter which highlights a brief account of organotin(IV) and ferrocene appended organotin(IV) compounds.

Chapter 2

This chapter describes the synthesis and characterization of multinuclear organostannoxanes containing drum- or ladder-type structural motifs, the former with aminobenzoate ligands and the latter with related framework ligands where an azo group (–N=N–ArNMe₂) has been replaced the amino group. In the case of ladders, a systematic variation of the carboxylate anchoring positions was accomplished. The pro-ligands used in this work comprise 2- and 3-aminobenzoic acids (L₁H and L₂H, respectively), the 2-, 3- and 4-{(E)-2-[4-(dimethylamino)phenyl]diazenyl}benzoic acid, (L₃H, L₄H and L₅H in this order), and also the 2-{(E)-[4-(dimethylamino)benzylidene] amino}benzoic acid (L₆H). Drum type structural motifs were prepared by reacting respective ligands (L₁H, L₂H, L₃H and L₆H) with BuSn(O)OH in anhydrous toluene in a 6:6 molar ratio to give compounds of the compositions [₆⁶Sn₆O₆(Lₙ)₆]. On the other hand, ladder type structural motifs were prepared by reacting respective ligands (L₃H, L₄H and L₅H) with Bu₂SnO in anhydrous toluene in a 4:4 molar ratio to give compounds of the compositions [₄₄Sn₄O₂(Lₙ)₄]. The compounds were fully characterized by elemental analysis, IR, ¹H, and ¹³C NMR spectroscopy and the geometry of the complexes in solution was
ascertained from $^{119}$Sn NMR spectroscopic techniques. The solid state structures were confirmed by single crystal X-ray crystallography, where possible.

**Chapter 3**

This chapter describes the synthesis and characterization of triphenyltin(IV) compounds of six pro-ligands (i) isomeric 2-, 3- and 4- \{ (E) \}-2-[4-(dimethylamino)phenyl]diazenyl]benzoic acids and their isoelectronic imino counterparts, i.e. (ii) 2-, 3- and 4- \{ (E) \}-[4-(dimethylamino)phenyl]methylidene]-amino]benzoic acid. Triphenyltin(IV) compounds were prepared by reacting respective ligands (L$_3$-$^8$H) with Ph$_3$SnOH in anhydrous toluene in a 1:1 molar ratio to give compounds of the compositions Ph$_3$Sn(L$_3$-$^8$). The compounds were fully characterized by elemental analysis, IR, $^1$H, and $^{13}$C NMR spectroscopy and the geometry of the complexes in solution was ascertained from $^{119}$Sn NMR spectroscopic techniques. The solid state structures were confirmed by single crystal X-ray crystallography, where possible. This chapter describes in vitro cytotoxicity study for some of the compounds and it was tested across a panel of human cell lines viz. cancer cells (MDAMB-231 and HeLa cells) and normal cell (HEK 293), along with standard drug which is used clinically. To realize the mechanistic/mode of cell death objective, an additional series of experiments were conducted: (i) the cytotoxic activity was examined by MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay (ii) the ability of the test compounds to generate ROS (reactive oxygen species) in the cells (iii) apoptosis or mode of cell death was detected by Hoechst 33342/PI (propidium iodide) and annexin V-PI assay and (iv) cell cycle arrest by the compounds were examined by FACS (fluorescence-activated cell sorting) studies.

**Chapter 4**

This chapter describes the synthesis and characterization of multinuclear organostannoxanes with ladder-type structural motif derived from 2- \{ (E) \}-4-hydroxy-3-[(E)-phenyliminomethyl]phenyldiazenyl]benzoic acid (L$_{9-15}^9$H'). Ladder type structural motifs were prepared by reacting respective ligands (L$_{9-15}^9$H') with Bu$_2$SnO in anhydrous toluene in a 4:4 molar ratio to give compounds of the compositions (viii)
The compounds were fully characterized by elemental analysis, IR, $^1$H, and $^{13}$C NMR spectroscopy and the geometry of the complexes in solution was ascertained from $^{119}$Sn NMR spectroscopic techniques. The solid state structures were confirmed by single crystal X-ray crystallography, where possible. This chapter describes in vitro cytotoxicity study for some of the compounds and it was tested across a panel of human cell lines viz. cancer cells (A375 and HCT116) and normal cell (PBMC), along with standard drug which is used clinically. To realize the mechanistic/mode of cell death objective, an additional series of experiments were conducted: (i) the cytotoxic activity was examined by MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay (ii) live and dead assay for cytolysis (iii) PARP cleavage (iv) action of p53 and (v) measurement of membrane fluorescence studies.

**Chapter 5**

This chapter describes the synthesis and characterization of triphenyltin(IV) complexes of polyaromatic benzoate ligands. In this endeavour, pro-ligands (i) 2-((E)-(4-hydroxy-3-((4-methoxycarbonyl)phenyl)imino)methyl)phenyldiazenyl))benzoic acid (L$^{16}$H$'$$'$) (ii) 4-((E)-(2-hydroxy-5-((E)-(2-(methoxycarbonyl)phenyl)diazenyl)benzylideneamino))benzoic acid (L$^{17}$H$'$$'$) (ii) 2-((E)-(3-((E)-((4-carboxyphenyl)imino)methyl)-4-hydroxyphenyl)diazenyl))benzoic acid (L$^{18}$H$_2$$'$$'$) have been designed and their triphenyltin(IV) esters prepared. Triphenyltin(IV) compounds were prepared by reacting respective ligands with Ph$_3$SnOH in anhydrous toluene in a suitable molar ratio to give compounds of the compositions Ph$_3$Sn(L$^{16-17}$H) or (Ph$_3$Sn)$_2$L$^{18}$H. The compounds were fully characterized by elemental analysis, IR, and $^1$HNMR spectroscopy and the geometry of the complexes in solution was ascertained from $^{119}$Sn NMR spectroscopic techniques. The solid state structure for (Ph$_3$Sn)$_2$L$^{18}$H was confirmed by single crystal X-ray crystallography. This chapter describes in vitro cytotoxicity study for all the compounds and it was tested across a panel of human cell lines viz., A498, EVSA-T, H226, IGROV, M19 MEL, MCF-7, and WIDR along with standard drugs which are used clinically. The encouraging cytotoxicity for these test compounds prompted us to perform the molecular docking studies to understand the complex-protein interactions.
Chapter 6

The final chapter describes the synthesis and characterization of ferrocene appended organotin(IV) compounds. The metallo pro-ligands (FcL$^{19-21}$H) were prepared by diazo-coupling reaction of 2-, 3- and 4-aminobenzoic acids with ferrocene in presence of phase transfer catalyst. Heterobimetallic compounds were prepared by reacting respective metallo pro-ligands (FcL$^{19-21}$H) with suitable organotin precursors in anhydrous toluene/methanol in a suitable molar ratio to give compounds of the compositions R$_3$SnFcL$^{19-21}$. The compounds were fully characterized by elemental analysis, IR,$^1$H and $^{13}$C NMR spectroscopy and the geometry of the complexes in solution was ascertained from $^{119}$Sn NMR spectroscopic techniques. The solid state structures were confirmed by single crystal X-ray crystallography, where possible.