Acknowledgements
Contents
List of Abbreviations
PREFACE

Chapter 1	**Introduction: Exploring Novel Metallomacrocyclic Dithiocarbamate Complexes: Applications and Insights into Host-Guest Binding Studies**		
	Abstract		1
	1.1	Self-Assembly	2
	1.2	1,1 -Dithio Ligands	5
	1.2.1	Dithiocarbamate	5
	1.2.1.1	Binding Modes	7
	1.2.2	Applications of Dithiocarbamates	9
	1.2.2.1	Host-Guest Binding Study	12
	1.2.2.2	Heavy metal ion sensing study	16
	1.3	Objective of the present work	18
	1.4	References	18
Chapter 2	**Synthesis and characterization of novel diamino ligand precursors bearing diversified functionalized linker frameworks**		
	Abstract		27
	2.1	Introduction	28
	2.2	Experimental Section	30
	2.2.1	Materials and Instrumentation	30
	2.2.2	General procedure for the synthesis of bisimine and diamine precursors holding diphenylmethane linker	31
	2.2.2.1	Synthesis of bisimines BI-1 and BI-2	31
	2.2.2.2	Synthesis of diamines H_2L^1 and H_2L^2	31
	2.2.3	General procedure for the synthesis of bisimine and diamine precursors holding thiophene linker	31
	2.2.3.1	Synthesis of bisimines BI-3 and BI-4	31
	2.2.3.2	Synthesis of diamines H_2L^3 and H_2L^4	31
	2.2.4	General procedure for the synthesis of bisimine and diamine precursors holding piperazine linker	32
	2.2.4.1	Synthesis of bisimines BI-5 and BI-6	32
	2.2.4.2	Synthesis of diamines H_2L^5 and H_2L^6	32
	2.2.5	Molecular docking study	36
	2.2.5.1	Ligand preparation	36
	2.2.5.2	Protein preparation and Grid Parameters	36
	2.2.5.3	Validation of Docking	36
	2.3	Result and Discussion	36
	2.3.1	Bisimines BI-1, BI-2 and diamines H_2L^1, H_2L^2	36
	2.3.1.1	Synthesis and characterization	36
	2.3.1.2	X-ray Crystallographic Study	37
	2.3.1.3	Density Functional Theory Calculations	40
	2.3.2	Chiral bisimines BI-3, BI-4 and diamines H_2L^3, H_2L^4	42

2.3.2.1	Synthesis and characterization	42
2.3.2.2	Electronic absorption spectral study	44
2.3.2.3	X-ray Crystallographic Study	45
2.3.2.4	Hirshfeld surface analysis	48
2.3.2.5	In-silico study	51
2.3.2.5.1	Density Functional Theory Calculations	51
2.3.2.5.2	Ligand-protein interactions	53
2.3.3	Bisimines BI-5, BI-6 and diamines H_2L^5, H_2L^6	55
2.3.3.1	Synthesis and characterization	55
2.3.3.2	Density Functional Theory Calculations	56
2.4	Conclusions	58
2.5	References	58
2.6	Annexures	62

Chapter 3	**Diphenylmethane Based Metallomacrocyclic Dithiocarbamate Complexes: Synthesis, Characterization and Their Binding Study Towards Environmentally Hazardous Organic Dyes**	
	Abstract	79
3.1	Introduction	80
3.2	Experimental Section	82
3.2.1	Materials and Instrumentations	82
3.2.2	Synthesis of homobimetallic dithiocarbamate macrocyclic complexes [M(II)$_2$-μ^2-bis-{κ^2S^S-$S_2CN(R)CH_2C_6H_3(OH)\}_2CH_2$] (R = 2-thiophenylethyl; Ni(II) **1**, Cu(II) **2**, Zn(II) **3**; R = cyclohexyl; Ni(II) **4**, Cu(II) **5**, Zn(II) **6**)	83
3.3	Result and Discussion	86
3.3.1	Synthesis and Characterization	86
3.3.2	UV-Visible absorption spectral study	88
3.3.3	Thermogravimetric Analysis	89
3.3.4	X-ray crystallographic study	90
3.3.5	Density functional theory calculations	93
3.4	Host-Guest Binding Study	97
3.5	Conclusions	102
3.6	References	103
3.7	Annexures	107

Chapter 4	**Thiophene Based Metallomacrocyclic Dithiocarbamate Complexes: Synthesis, Characterization and Their Involvement in Heavy Metal Ion Sensing Study**	
	Abstract	116
4.1	Introduction	117
4.2	Experimental Section	118
4.2.1	Materials and Instrumentations	118
4.2.2	Synthesis of Binuclear metallomacrocyclic dithiocarbamate complexes M(II)$_2$-μ^2-bis-{(κ^2S,S-$S_2CN(CH(S\text{-}CH_3)Ph)CH_2)_2$thiophene}]; M = Ni(II) **7**, Cu(II) **8**, Zn(II) **9** and [M(II)$_2$-μ^2-bis-{(κ^2S,S-	119

		$S_2CN(CH(R\text{-}CH_3)Ph)CH_2)_2$thiophene}]; M = Ni(II) **10**, Cu(II) **11**, Zn(II) **12**	
	4.3	Result and Discussion	122
	4.3.1	Synthesis and Characterization	122
	4.3.2	UV-Visible absorption spectral study	123
	4.3.3	X-ray Crystallographic Study	124
	4.3.4	Thermogravimetric Analysis	127
	4.3.5	Density functional theory calculations	129
	4.4	Heavy metal ions sensing study	132
	4.5	Conclusions	134
	4.6	References	135
	4.7	Annexures	137
Chapter 5	**Piperazine Based Metallomacrocyclic Dithiocarbamate Complexes: Synthesis, Characterization and Their Photophysical Properties**		
	Abstarct		145
	5.1	Introduction	146
	5.2	Experimental Section	148
	5.2.1	Materials and Instrumentations	148
	5.2.2	Synthesis of Binuclear metallomacrocyclic dithiocarbamate complexes $[M(II)_2\text{-}\mu^2\text{-bis-}\{(\kappa^2S,S\text{-}S_2CN(R)C_3H_6)_2$piperazine}] wherein R = *p*-methoxy benzyl, M = Ni(II) **13**, Cu(II) **14**, Zn(II) **15**; R = *p*-chlorobenzyl, M = Ni(II) **16**, Cu(II) **17**, Zn(II) **18**	149
	5.3	Result and Discussion	152
	5.3.1	Synthesis and Characterization	152
	5.3.2	UV-Visible absorption and fluorescence spectral study	154
	5.3.3	Thermogravimetric Analysis	155
	5.3.4	Density functional theory calculations	156
	5.4	Heavy metal ions sensing study	161
	5.5	Conclusions	164
	5.6	References	165
	5.7	Annexures	168

List of Papers Published

Papers presented in Conferences