

Contents

Acknowledgements	i
Contents	iii
List of Abbreviations	ix
<i>PREFACE</i>	x
Chapter 1	Introduction: Metal Directed Self-assembly of Dithiocarbamate and their Applications
	Abstract
1	Self-assembly 2
1.1.	Dithiocarbamate Ligands 6
1.1.1	Synthesis and stability of Dithiocarbamates 7
1.1.2	Metal directed Self-assembly of Dithiocarbamates 9
1.1.3	Application of Dithiocarbamates 12
1.2.	Objectives of the present work 19
1.3.	References 20
Chapter 2	Use of dapson (dap) to derive a novel series of diamines and their ensuing metallomacrocyclic complexes: Synthesis, characterization, DFT and cytotoxic study against Hep G2 and C6 cancer cell lines
	Abstract 28
2.1.	Introduction 29
2.2.	Experimental Section 31
2.2.1	Materials and Instrumentations 31
2.2.2	General method of preparation of secondary diamine precursors L ¹ -L ³ 32
2.2.3.	General Synthetic procedure for metallomacrocyclic dithiocarbamate complexes 1a-1c, 2a-2c, 3a-3c 34
2.2.4.	<i>In vitro</i> cytotoxic study 37
2.2.4.1.	Cell line and culture 37
2.2.4.2.	MTT assay for cell viability/ proliferation 38
2.2.4.3.	Statistical Analysis for Determination of IC ₅₀ 38

2.2.4.4.	DNA ladder assay	38
2.3.	Result and Discussion	38
2.3.1.	Syntheses and characterization	38
2.3.2.	NMR, Mass and IR spectral study	40
2.3.3.	UV-visible absorption, magnetic moment and florescence emission study	42
2.3.4.	TGA/DTA study	44
2.3.5.	Geometry Optimization	45
2.3.6.	Electrochemical study	49
2.3.7.	<i>In vitro</i> cytotoxic activity	50
2.4.	Conclusion	55
2.5.	References	56
2.6.	Annexures	59

Chapter 3 Use of 4, 4'-diamino diphenyl methane to derive a novel series of diamines and their ensuing metallomacrocyclic complexes: Synthesis, characterization, DFT and *in vitro* cytotoxic study against Hep G2 cancer cell line

Abstract	80	
3.1.	Introduction	81
3.2.	Experimental Section	83
3.2.1	Materials and Instrumentations	83
3.2.2	General method of preparation of secondary diamine precursors L ¹ -L ³	84
3.2.3.	General Synthetic procedure for metallomacrocyclic dithiocarbamate complexes 1a-1c, 2a-2c, 3a-3c	86
3.2.4.	<i>In vitro</i> cytotoxic study	90
3.2.4.1.	Cell line and Culture	90
3.2.4.2.	MTT assay for cell viability/ proliferation	90
3.2.4.3.	Statistical Analysis for Determination of IC ₅₀	91
2.2.4.4.	Assessment of apoptosis AO/EtBr staining	91
3.3.	Result and Discussion	91

3.3.1.	Syntheses and characterization	91
3.3.2.	NMR, Mass and IR spectral study	93
3.3.3.	UV-visible absorption, magnetic moment and florescence emission study	95
3.3.4.	Thermogravimetric study	98
3.3.5.	Geometry Optimization	98
3.3.6.	<i>In vitro</i> cytotoxic activity	103
3.3.7.	Electrochemical study	107
3.4.	Conclusion	108
3.5.	References	109
3.6.	Annexures	114

Chapter 4 Coordination driven self-assembly of 1,3-bis(2-(alkylamino)acetamido)phenylene, CS₂ and Ni^{II}, Cu^{II} or Zn^{II}:Synthesis, spectroscopic, DFT, crystallographic and cytotoxic study

	Abstract	140
4.1.	Introduction	141
4.2.	Experimental Section	143
4.2.1.	Materials and Instrumentations	143
4.2.2.	Preparation of 1, 3-bis(2-chloroacetamido)phenylene (L')	144
4.2.3.	General method of preparation of secondary diamine precursors 1,3- bis(alkylamino)acetamido)phenylene L ¹ -L ³	144
4.2.4.	General Synthetic procedure for metallomacrocyclic dithiocarbamate complexes 1a-1c, 2a-2c, 3a-3c	146
4.2.5.	<i>In vitro</i> cytotoxic study	149
4.2.5.1.	Cell line and Culture	149
4.2.5.2.	MTT assay for cell viability/ proliferation	149
4.2.5.3.	Statistical Analysis for Determination of IC ₅₀	150
4.2.5.4.	Assessment of apoptosis AO/EtBr staining	150

4.3.	Result and Discussion	151
4.3.1.	Syntheses and characterization	151
4.3.2.	NMR, Mass and IR spectral study	153
4.3.3.	UV-visible absorption, magnetic moment and florescence emission study	155
4.3.4.	Thermogravimetric study	157
4.3.5.	Geometry Optimization	157
4.3.6.	Structural description of L'	160
4.3.7.	<i>In vitro</i> cytotoxic study	165
4.4.	Conclusion	169
4.5.	References	170
4.6.	Annexures	176

Chapter 5 Use of 4,4'-diamino diphenylether to derive a novel series of diamines and their ensuing metallomacrocyclic complexes: Synthesis, characterization, DFT and cytotoxic study against Hep G2 cancer cell line

	Abstract	198
5.1.	Introduction	199
5.2.	Experimental Section	200
5.2.1	Materials and Instrumentations	200
5.2.2	General method of preparation of secondary diamine precursors L ¹ -L ³	201
5.2.3.	General Synthetic procedure for metallomacrocyclic dithiocarbamate complexes 1a-1c, 2a-2c, 3a-3c	203
5.2.4.	<i>In vitro</i> cytotoxic study	206
5.2.4.1.	Cell line and Culture	206
5.2.4.2.	MTT assay for cell viability/ proliferation	207
5.2.4.3.	Statistical Analysis for Determination of IC ₅₀	207
2.2.4.4.	Assessment of apoptosis AO/EtBr staining	207
5.3.	Result and Discussion	208

5.3.1.	Syntheses and characterization	208
5.3.2.	NMR, Mass and IR spectral study	210
5.3.3.	UV-visible absorption, magnetic moment and florescence emission study	213
5.3.4.	Thermogravimetric study	215
5.3.5.	Geometry Optimization	215
5.3.6.	<i>In vitro</i> cytotoxic activity	221
5.4.	Conclusion	226
5.5.	References	227
5.6.	Annexures	231

Chapter 6 Diphenyltin^{IV} dithiocarbamate macrocyclic complexes bearing varied linkers: Synthesis, spectral characterization, density functional theory and *in vitro* cytotoxic study

	Abstract	253
6.1.	Introduction	254
6.2.	Experimental Section	256
6.2.1	Instrumentations	256
6.2.2	Synthesis of binuclear diphenyltin ^{IV} dithiocarbamate macrocyclic complexes (1-5)	256
6.2.3.	<i>In vitro</i> cytotoxic study	259
6.2.3.1.	Cell line and Culture	259
6.2.3.2.	MTT assay for cell viability/ proliferation	259
6.2.3.3.	Statistical Analysis for Determination of IC ₅₀	259
6.2.3.4.	Assessment of apoptosis AO/EtBr staining	260
6.3.	Result and Discussion	260
6.3.1.	Syntheses and characterization	260
6.3.2.	NMR, Mass and IR spectral study	261
6.3.3.	UV-visible absorption, magnetic moment and florescence emission study	263
5.3.4.	Thermogravimetric study	265

5.3.5.	Geometry Optimization	265
6.3.6.	<i>In vitro</i> cytotoxic activity	267
6.4.	Conclusion	272
6.5.	References	273
6.6.	Annexures	277
List of Publications		290
Papers presented in conferences/symposia		293