

Contents

	Content	Page No
	Chapter 1	1-24
	Introduction	
1	Introduction	
	1.1 The vanadium element	2-3
	1.2 Coordination chemistry of vanadium	4
	1.3 Insulin-mimetic vanadium compounds	4-8
	1.4 Other therapeutic applications of vanadium compounds	8-9
2	Brief Review	9-17
3	Aims and objective	17-18
	References	18-24
	Chapter 2	25-84
	Metal-organic hybrids based on a [VO₂(L)]-tecto- n with cations of imidazole derivatives: Synthesis, characterization and <i>in vitro</i> antidiabetic activity	
1	Introduction	26-27
2	Experimental	27
	2.1 Materials	27
	2.2 Physical Measurements	27-28
	2.3 Synthesis	28-30
	▪ 2.3.1 Synthesis of Schiff base (H ₂ L)	
	▪ 2.3.2 Synthesis of [VO ₂ (L)]ImH 1	
	▪ 2.3.3 Synthesis of [VO ₂ (L)] ₂ -MeImH 2	
	▪ 2.3.4 Synthesis of [VO ₂ (L)]M-ImH 3	
	▪ 2.3.5 Synthesis of [VO ₂ (L)] ₂ -EthImH 4	
	▪ 2.3.6 Synthesis of [VO ₂ (L)]BenzImH 5	
	▪ 2.3.7 Synthesis of [VO ₂ (L)] ₂ -MeBenzImH 6	
	2.4 Antidiabetic activity	31-32
	▪ 2.4.1 Antioxidant activity	
	▪ 2.4.2 α-Glucosidase inhibition activity	
	▪ 2.4.3 α-Amylase inhibition activity	
	▪ 2.4.4 β-Glucosidase inhibition activity	
	2.5 Computational Studies	33
3	Results and discussion	33-36
	3.1 NMR spectral study	37-38
	3.2 Magnetic susceptibility	38
	3.3 Molar conductance	38-39
	3.4 FTIR Spectral studies	39-43
	3.5 Electronic spectral studies	43-45
	3.6 Electrochemistry studies	45-47

Contents

	3.7 Mass spectral analysis	47-50
	3.8 X-ray structures of complexes 1 and 2	50-56
	3.9 Thermal analysis	57-58
	3.10 Antidiabetic activity	59-64
	▪ 3.10.1 Antioxidant activity	
	▪ 3.10.2 α -Glucosidase inhibition activity	
	▪ 3.10.3 α -Amylase inhibition activity	
	▪ 3.10.4 β -Glucosidase inhibition activity	
	▪ 3.10.5 α -Glucosidase inhibition activity	
	▪ 3.10.6 α -Amylase inhibition activity	
	3.11 Hirshfeld Surface Analysis (HSA)	64-66
	3.12 Computational studies of complexes	67-78
	▪ 3.12.1 Mulliken spin population analysis	
	▪ 3.12.2 Geometrical optimization	
	▪ 3.12.3 HOMO-LUMO Analysis	
4	Conclusions	78-79
	References	79-83
	Published paper (front page)	84
	<u>Chapter 3</u>	85-165
	New oxidovanadium(IV/V) complexes with tridentate Schiff base ligands: Synthesis, molecular structure and <i>in vitro</i> antidiabetic activity	
1	Introduction	86-87
2	Experimental	87
	2.1 Material	87
	2.2 Physical Measurements	87-88
	2.3 Synthesis	88-93
	▪ Synthesis of ligand HL ¹	
	▪ 2.3.2 Synthesis of ligand HL ²	
	▪ 2.3.3 Synthesis of ligand HL ³	
	▪ 2.3.4 Synthesis of ligand HL ⁴	
	▪ 2.3.5 Synthesis of [VO(L ¹)(H ₂ O)]NO ₃ 1	
	▪ 2.3.6 Synthesis of [VO(L ²)(H ₂ O)]NO ₃ 2	
	▪ 2.3.7 Synthesis of [VO(L ¹)(ImH) ₂]SO ₄ ·H ₂ O 3	
	▪ 2.3.8 Synthesis of [VO(L ²)(ImH)]NO ₃ 4	
	▪ 2.3.9 Synthesis of [V(O) ₂ L ¹] 5	
	▪ 2.3.10 Synthesis of [V(O) ₂ L ²] 6	
	▪ 2.3.11 Synthetic of [V(O ₂)L ¹]ImH 7	
	2.4 Computational Studies	93
	2.5 Hirshfeld Surface Analysis (HAS)	93-94
	2.6 Docking Studies	94
	2.7 Antidiabetic activity	94-95
	▪ 2.7.1 α -Glucosidase inhibition activity	

Contents

	<ul style="list-style-type: none"> ▪ 2.7.2 α-Amylase inhibition activity 	
3	Results and discussion	95
	3.1 Synthetic Strategy	95-97
	3.2 NMR spectra of Ligands	97-101
	3.3 FTIR Analysis	102-108
	3.4 Electronic spectra	108-110
	3.5 Molecular structure of ligand HL2	110-113
	3.6 Molecular structure of complex 3	113-117
	3.7 Molecular structures of complexes 5-7	117-130
	3.8 Hirshfeld Surface Analysis	130-134
	<ul style="list-style-type: none"> ▪ 3.8.1 Hirshfeld surfaces analysis of complexes 3 ▪ 3.8.2 The Hirshfeld surface analysis of complexes 5 and 6 ▪ 3.8.3 Hirshfeld surface of the complex 7 	
	3.9 Magnetic and EPR spectral study	134-136
	3.10 Cyclic Voltammetry	137-139
	3.11 Theoretical calculations	139-142
	3.12 HOMO-LUMO analysis	142-144
	3.13 Mulliken charge analysis	144-145
	3.14 Global chemical reactivity indices of complexes 1-4	145-146
	3.15 Computational studies of complexes 5-7	147-151
	3.16 Molecular Docking	151-154
	3.17 Antidiabetic activity	154-159
	<ul style="list-style-type: none"> ▪ 3.17.1 α-Glucosidase inhibition activity ▪ 3.17.2 α-Amylase inhibition activity ▪ 3.17.3 α-Glucosidase inhibition activity ▪ 3.17.4 α-Amylase inhibition activity 	
4	Conclusions	159
	References	159-164
	Published paper (front page)	165
	Chapter 4	166-215
	Anionic dioxidovanadium(V) complexes [VO₂(L)]-with (Z)-N'-(2-hydroxy-3-methoxybenzylidene) isonicotinic hydrazide as proligand and cation of imidazole units as ancillary ligands: Synthesis, characterization and <i>in-vitro</i> antidiabetic activity	
1	Introduction	167-169
2	Experimental	169
	2.1 Materials	169
	2.2 Physical Measurements	169-170
	2.3 Computational Studies	170
	2.4 Antidiabetic activity	170-171
	<ul style="list-style-type: none"> ▪ 2.4.1 α-Glucosidase inhibition activity ▪ 2.4.2 β-Glucosidase inhibition activity ▪ 2.4.3 α-Amylase inhibition activity 	

Contents

2.5	Synthesis of Schiff base (H ₂ L)	172
2.6	Synthesis of the dioxidovanadium(V) complexes	172-174
	▪ 2.6.1 Synthesis of [V(O) ₂ (L)]ImH	1
	▪ 2.6.2 Synthesis of [V(O) ₂ (L)]2-MeImH	2
	▪ 2.6.3 Synthesis of [V(O) ₂ (L)]2-EthImH	3
	▪ 2.6.4 Synthesis of [V(O) ₂ (L)]1-MeImH	4
	▪ 2.6.5 Synthesis of [V(O) ₂ (L)]BezImH	5
	▪ 2.6.6 Synthesis of [V(O) ₂ (L)]2-MeBenzImH	6
3	Results and discussion	174-176
	3.1 NMR Spectra of Ligand	176-178
	3.2 Mass spectral studies	178-181
	3.3 Crystal Structure of Ligand (H ₂ L)	182-185
	3.4 Powder X-ray diffraction	185-189
	3.5 Molar conductance	189-190
	3.6 FTIR spectral study	190-194
	3.7 Electronic spectral studies	194-195
	3.8 Electrochemical studies	195-197
	3.9 Hirshfeld Surface Analyses	197-199
	3.10 Molecular modelling	199-202
	3.11 Frontier Molecular Orbital (FMO) analysis	202-205
	3.12 Thermo gravimetric analysis	205-206
	3.13 Antidiabetic activity	206-209
	▪ 3.13.1 α-Glucosidase inhibition activity	
	▪ 3.13.2 β-Glucosidase inhibition activity	
	▪ 3.13.3 α-Amylase inhibition activity	
4	Conclusions	210
	References	210-215
	Published paper (front page)	216
	Chapter 5	217-283
	Syntheses, spectral characterization and antidiabetic activities of vanadium(IV/V) complexes with bi-and tridentate ligands (In situ reaction)	
1	Introduction	218
2	Experimental	219
	2.1 Materials and physical measurements	219
	2.2 Synthesis	219-223
	▪ 2.2.1 Synthesis of [VO(BPA)(OH ₂) ₂] ₂ SO ₄	1
	▪ 2.2.2 Synthesis of [VO(BPA)(bipy)]SO ₄	2
	▪ 2.2.3 Synthesis of [VO(BPA)(phen)]SO ₄	3
	▪ 2.2.4 Synthesis of [VO(L ¹)(Mol)]	4
	▪ 2.2.5 Synthesis of [VO(L ²)(Mol)]	5
	▪ 2.2.6 Synthesis of [VO(L ³)(Mol)]	6
	▪ 2.2.7 Synthesis of [VO(L ⁴)(Mol)]	7

Contents

	▪ 2.2.8 Synthesis of [VO(L ¹)(E-mol)]	8
	▪ 2.2.9 Synthesis of [VO(L ²)(E-mol)]	9
	▪ 2.2.10 Synthesis of [VO(L ³)(E-mol)]	10
	▪ 2.2.11 Synthesis of [VO(L ⁴)(E-mol)]	11
	2.3 Antidiabetic activity	223-224
	▪ 2.3.1 α -Glucosidase inhibition activity	
	▪ 2.3.2 α -Amylase inhibition activity	
3	Results and Discussion	225
	3.1 Synthesis and Spectroscopic Properties	225-228
	3.2 Powder XRD	228-229
	3.3 FTIR Analysis	230-237
	▪ 3.3.1 FTIR spectra of complexes 1-3	
	▪ 3.3.2 FTIR Spectra of complexes 4-11	
	3.4 ESI Mass Analysis	237-243
	3.5 Magnetic and EPR spectral properties	243-245
	3.6 Electronic spectra	245-247
	3.7 Electrochemical Study	247-250
	▪ 3.7.1 Electrochemical Study of complexes 1-3	
	▪ 3.7.2 Electrochemical studies of complexes 4-11	
	3.8 Thermogravimetric Analysis (TGA)	250-251
	3.9 Antidiabetic activity	252-258
	▪ 3.9.1 α -Glucosidase inhibition activity	
	▪ 3.9.2 α -Amylase inhibition activity	
	▪ 3.9.3 α -Glucosidase inhibition activity	
	▪ 3.9.4 α -Amylase inhibition activity	
	▪ 3.9.5 α -Glucosidase inhibition activity	
	▪ 3.9.6 α -Amylase inhibition activity	
	3.10 Computational Study	258-277
	▪ 3.10.1 Optimized structure of complexes	
	▪ 3.10.2 HOMO-LUMO analysis	
	▪ 3.10.3 Global reactivity parameters	
	▪ 3.10.4 Electron density	
4	Conclusions	277-278
	References	278-282
	Published paper (front page)	283
	Published papers	284
	Conferences and workshop	285-286