Contents

Title	Content	Pg.No
	Abstract	I
Chapter: 1	Novel quinoline derivatives containing substituted	1
	oxadiazole-5(4H)-one as an anticancer agent	1
	1.1 Introduction	1
	1.1.1 Synthetic methodologies for the substituted quinoline framework and its biological significance	3
	1.2 Result and discussion 1.2.1 Chemistry	11
	1.3 Biological Activity	13
	1.4 Conclusion	18
	1.5 Experimental section	10
	1.5.1 Chemistry	18
	1.5.2 Protocol of biological activity	35
	1.6 Spectral Data	36
Chapter: 2	Novel quinoline derivatives containing substituted	80
	oxadiazole- $5(4H)$ -thione as an anticancer agent	80
	2.1 Introduction	80
	2.1.1 Synthetic methodologies for the substituted quinoline and oxadiazole framework and its biological significance	81
	2.2 Result and Discussion 2.2.1 Chemistry	85
	2.3 Biological Activity	86
	2.4 Conclusion	89
	2.5 Experimental Section	89
	2.5.1. Chemistry	09
	2.6 Spectral data	97
Chapter: 3	Novel quinoline derivatives containing substituted DHPM	
	hybrids, In vitro Antimicrobial Assessment and Corresponding In silico Analysis	120

	3.1 Introduction	120
	3.1.1 Synthetic methodologies for the substituted quinoline-DHPM framework and its biological significance	121
	3.2 Results and Discussion	125
	3.2.1 Chemistry	
	3.3 Biological Activity	127
	3.4 Structure-Activity Relationship (SAR)	129
	3.5 Molecular Docking	130
	3.6 Conclusion	132
	3.7 Experimental section	133
	3.7.1 Chemistry	133
	3.7.2 Experimental protocol of anti-microbial activity	140
	3.7.3 Experiment protocol of molecular docking study	141
	3.8 Spectral data	141
Chapter: 4	Synthesis of Novel Quinoline-Isoxazole Hybrid Molecules, In	155
	vitro Anti-Microbial Evaluation and Their In silico Studies	133
	4.1. Introduction	155
	4.1.1 Synthetic methodologies for the substituted quinoline-isoxazole hybrids and its biological significance	158
	4.2. Results and Discussion	161
	4.2.1 Chemistry	101
	4.3 Biological Activity	162
		102
	4.4 Structure-Activity Relationship (SAR)	164
	4.4 Structure-Activity Relationship (SAR) 4.5 Molecular Docking	
	* * * /	164
	4.5 Molecular Docking	164 165
	4.5 Molecular Docking 4.5.1 Molecular Dynamics Simulation analysis	164 165 168
	4.5 Molecular Docking 4.5.1 Molecular Dynamics Simulation analysis 4.5.2 Root Mean Square Deviation	164 165 168 168
	4.5 Molecular Docking 4.5.1 Molecular Dynamics Simulation analysis 4.5.2 Root Mean Square Deviation 4.5.3 Root Mean Square Fluctuations	164 165 168 168 169 172
	4.5 Molecular Docking 4.5.1 Molecular Dynamics Simulation analysis 4.5.2 Root Mean Square Deviation 4.5.3 Root Mean Square Fluctuations 4.6 Conclusion	164 165 168 168 169
	4.5 Molecular Docking 4.5.1 Molecular Dynamics Simulation analysis 4.5.2 Root Mean Square Deviation 4.5.3 Root Mean Square Fluctuations 4.6 Conclusion 4.7 Experimental Section	164 165 168 168 169 172

	4.7.4 Protocol of molecular dynamic simulation	184
	4.8 Spectral Data	185
Chapter: 5	Synthesis, In-Vitro Anti-Diabatic Activity, ADMET	
	Properties and Molecular Docking Studies of Novel Thiazole	218
	Derivative	
	5.1. Introduction	218
	5.1.1 Synthetic methodologies for the substituted	
	quinoline-isoxazole hybrids and its biological	221
	significance 5.2. Results and Discussion	
	5.2.1 Chemistry	224
	5.3 Biological Activity	226
	5.3.1 <i>In vitro</i> study for anticancer activity	226
	· · · · · · · · · · · · · · · · · · ·	
	5.4 Molecular Docking	236
	5.4.1 ADMET study	239
	5.4.2 Molecular Dynamics Simulation analysis	243
	5.4.3 Molecular mechanics and generalized born surface	244
	area (MM-GBSA) calculations	
	5.4.4 Density functional theory (DFT) studies	245
	5.5 Conclusion	248
	5.6 Experimental Section	249
	5.6.1 Chemistry	∠ 4 7
	5.6.2 Experimental protocol of molecular docking study	256
	5.6.3 <i>In silico</i> ADMET study	256
	5.6.4 Molecular Dynamics Simulation Studies and MM-	256
	GBSA calculations	230
	5.6.5 Density functional theory (DFT) studies	257
	5.7 Spectral data	258
	Bibliography	276
Appendix A	Plagiarism Report	299
Appendix B	Publication	300
Appendix C	List of seminar/conference	304