

CONTENTS

Acknowledgement	i
Abstract	ii
List of Figures	v
List of Tables	xii
List of Abbreviations	xvi
1. INTRODUCTION	1
1.1 Data Mining	2
1.2 Overview of Spinocerebellar Ataxia Disorder	11
1.3 Docking and Binding Affinity	26
1.4 Need for the Proposed Research	35
1.5 Machine Learning and Deep Learning	36
1.5.1 Regression Algorithms	36
1.5.2 Deep Neural Networks	42
1.6 Problem Statement and Objectives of the Research	48
1.7 Organization of the Thesis	49
2 REVIEW OF LITERATURE	51
2.1 Traditional Approaches	51
2.2 Computational Methods	53
3 PROBLEM MODELLING	63
3.1 Overall Framework of Binding Affinity Prediction Model	63
3.2 Development of Corpuses	65
3.3 Design of Features And Datasets	78
3.4 Training And Testing	82
4 BINDING AFFINITY PREDICTION MODEL USING PROTEIN-LIGAND DOCKING AND REGRESSION TECHNIQUES	86
4.1 Protein-Ligand Docking Based Binding Affinity Predictive Models using Supervised Learning	86
4.2 Experiment and Results	97

5	BINDING AFFINITY PREDICTION USING PROTEIN-MUTATED-LIGAND DOCKING AND REGRESSION TECHNIQUES	103
5.1	Protein-Mutated-Ligand Docking Based Binding Affinity Predictive Models using Supervised Learning	103
5.2	Experiment and Results	117
6	BINDING AFFINITY PREDICTION USING PROTEIN-PROTEIN INTERACTIONS AND REGRESSION TECHNIQUES	126
6.1	Protein-Protein Interaction Based Binding Affinity Predictive Models using Supervised Learning	126
6.2	Experiment and Results	134
7	BINDING AFFINITY PREDICTION USING DEEP NEURAL NETWORK ARCHITECTURES	143
7.1	Binding Affinity Prediction Models using Sequential Deep Neural Network	144
7.2	Binding Affinity Prediction Models using Functional Deep Neural Network	162
7.3	Binding Affinity Prediction Models using Deep Neural Network with Customized Layers	178
7.4	Comparative Analysis	195
8.	CONCLUSION	201
	REFERENCES	204
	List of Publications	213
	Appendix	
A.	Datasets	215
B.	Coding	225
C.	Screenshots	233

