## Contents

Preface i  
List of abbreviations vii  
Papers presented in National/International Journals viii  
Papers presented in National/International Seminars/ Symposia ix  
Acknowledgment xii

### Chapter 1

**Introduction** 1  
1.1 Biological macromolecules 1  
1.2 Databases 8  
1.3 Neuraminidases 10  
1.4 Sialyloligosaccharides 20  
1.5 Molecular modeling 25  
1.6 Drug design 35  
1.7 Perspectives of the present study 38

### Chapter 2

**Conformations of terminal sialyloligosaccharide fragments - A molecular dynamics study** 40  
2.1 Introduction 40  
2.2 Materials and Methods 43  
2.3 Results and Discussion 48  
2.4 Conclusions 61
Chapter 3

Molecular modeling of sialyloligosaccharide fragments into the active site of influenza virus N9 neuraminidase

3.1 Introduction 63
3.2 Materials and Methods 66
3.3 Results and Discussion 71
3.4 Conclusions 81

Chapter 4

Interaction of sialyloligosaccharides with *Salmonella typhimurium* LT2 and *Vibrio cholerae* neuraminidases

4.1 Introduction 82
4.2 Materials and Methods 85
4.3 Results and Discussion 88
4.4 Conclusions 104

Chapter 5

Structure-based design of sialic acid analogues as inhibitors to *Vibrio cholerae* neuraminidase

5.1 Introduction 106
5.2 Materials and Methods 109
5.3 Results and Discussion 111
5.4 Conclusions 114

Conclusions

References 120