

TABLE OF CONTENTS

Antiplagiarism Report.....	iii
Certificate.....	iv
Declaration.....	v
Acknowledgement.....	vi-vii
Preface.....	viii
Abstract.....	ix-xv
Table of Contents.....	xvi-xx
List of Tables.....	xxi-xxiv
List of Figures.....	xxv-xxxii
List of Schemes.....	xxxiii
Abbreviations.....	xxxiv-xxxv
List of Appendices:	
Appendix-A: List of Publications/Communications.....	xxxvi-xxxviii
Appendix-B: List of Seminars/Symposiums/Conferences Attended.....	xxxix

CHAPTER I..... 1-12

INTRODUCTION

- 1.1 Supramolecular chemistry and graphene nanocomposites: a historical overview:
- 1.2 Macromolecular systems and nanomaterials:
 - 1.2.1 Macrocyclic hosts:
 - 1.2.2 Biologically active guest molecules:
 - 1.2.3 Graphene and graphene based materials:
- 1.3 A brief review on different applications:
- 1.4 Scopes and objectives of the thesis:

CHAPTER II..... 13-24

LITERATURE REVIEW:

- 2.1 Host-guest chemistry:

TABLE OF CONTENTS

2.2 Graphene based nanocomposites:

2.3 Theory of investigation:

2.3.1 Stoichiometry:

2.3.2 Binding constant:

2.3.3 Thermodynamic stability and different thermodynamic parameters:

2.3.4 Host-guest inclusion complex in spectroscopic and spectrometric methods:

2.3.5 Thermal stability:

2.3.6 Theoretical calculations:

2.4 Type of supramolecular interactions:

2.4.1 Ionic and dipolar interactions:

2.4.2 Hydrogen bonding:

2.4.3 π -interactions:

2.4.4 van der Waals interactions:

2.4.5 Hydrophobic effect:

2.5 Summary:

CHAPTER III..... 25-48

MATERIALS AND METHODS:

3.1 Materials:

3.2 Synthesis methods:

3.2.1 Synthesis of inclusion complex:

3.2.2 Graphene oxide (GO) synthesis:

3.2.3 Synthesis of GO- β CD nanocomposites:

3.3 Characterization techniques:

3.3.1 Spectroscopic techniques:

3.3.1.1 Fluorescence spectroscopy:

3.3.1.2 Ultraviolet-visible (UV-vis) absorption spectroscopy:

3.3.1.3 Fourier Transform Infrared spectroscopy:

3.3.1.4 Nuclear magnetic resonance spectroscopy ($^1\text{H-NMR}$):

- 3.3.1.5 2D-NMR spectroscopy:
- 3.3.2 Spectrometric techniques:
 - 3.3.2.1 ESI-MS spectrometric analysis:
- 3.3.3 Thermogravimetric techniques:
 - 3.3.3.1 Thermogravimetric (TGA) analysis:
 - 3.3.3.2 Differential scanning calorimetric (DSC) techniques:
- 3.3.4 Dynamic Light Scattering (DLS) measurements:
 - 3.3.4.4 Hydrodynamic diameter and zeta potential analysis
- 3.3.5 Microscopic measurement:
 - 3.3.5.1 Scanning electron microscopy (SEM)
- 3.3.6 Conductivity measurement:
- 3.4 Theoretical analysis Techniques:
 - 3.4.1 Molecular docking:
 - 3.4.2 Dynamic simulations:
 - 3.4.3 Potential energy calculations:

CHAPTER IV 49-86
PROBING HOST-GUEST INCLUSION COMPLEXES OF AMBROXOL HYDROCHLORIDE WITH α - & β -CYCLODEXTRINS BY PHYSICOCHEMICAL CONTRIVANCE SUBSEQUENTLY OPTIMIZED BY MOLECULAR MODELING SIMULATIONS

- 4.1 Introduction
- 4.2 Experimental section
- 4.3 Results and discussion
- 4.4 Conclusion

Tables

Figures

Published in [Chemical Physics Letters, 2020](#) (*Elsevier*)

CHAPTER V 87-106
EXPLORING β -CD GRAFTED GO NANOCOMPOSITES WITH AN ENCAPSULATED FLUORESCENT DYE DULY OPYIMIZED BY MOLECULAR DOCKING FOR INNOVATIVE APPLICATION

TABLE OF CONTENTS

- 5.1 Introduction
- 5.2 Experimental section
- 5.3 Results and discussion
- 5.4 Conclusion

Tables

Figures

Schemes

Published in [Journal of Molecular Liquids, 2021](#) (*Elsevier*)

CHAPTER VI..... 107-131

STUDY TO SYNTHESIZE AND CHARACTERIZE HOST-GUEST ENCAPSULATION OF ANTIDIABETIC DRUG (TGC) AND HYDROXY PROPYL- β -CYCLODEXTRIN AUGMENTING THE ANTIDIABETIC APPLICABILITY IN BIOLOGICAL SYSTEM

- 6.1 Introduction
- 6.2 Experimental section
- 6.3 Results and discussion
- 6.4 Conclusion

Tables

Figures

Schemes

Published in [Journal of Molecular Structure, 2018](#) (*Elsevier*)

CHAPTER VII 132-164

EXPLORING INCLUSION COMPLEXES OF CYCLODEXTRINS WITH QUINOLINONE BASED GASTRO PROTECTIVE DRUG FOR ENHANCING BIOAVAILABILITY AND SUSTAINED DISCHARGEMENT

- 7.1 Introduction
- 7.2 Experimental section
- 7.3 Results and discussion
- 7.4 Conclusion

Tables

Figures

Schemes

Published in **Z Phys Chem, 2020**

CHAPTER VIII165-186

EXPLORING THE INCLUSION COMPLEX OF A DRUG (UMBELLIFERONE) WITH α -CYCLODEXTRIN OPTIMIZED BY MOLECULAR DOCKING AND INCREASING BIO-AVAILABILITY WITH MINIMIZING THE DOSES IN HUMAN BODY

- 8.1 Introduction
- 8.2 Experimental section
- 8.3 Results and discussion
- 8.4 Conclusion

Tables

Figures

Schemes

Published in **ACS Omega, 2020** (*American Chemical Society*)

CHAPTER IX187-189

- Concluding remarks
- 1. Significant contribution of the work
 - 2. Scope for future work
 - 3. Closures

CHAPTER X190-232

Bibliography