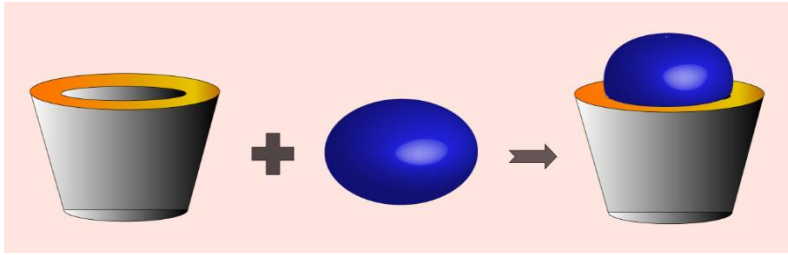
ABSTRACT

Supramolecular assembly as well as various nanocomposites have gained enormous significance these days in drug release due to their excellent bioavailability and remarkable ability to alter various properties of the drug such as its solubility, stability within the body, pharmacokinetics and pharmacodynamics.

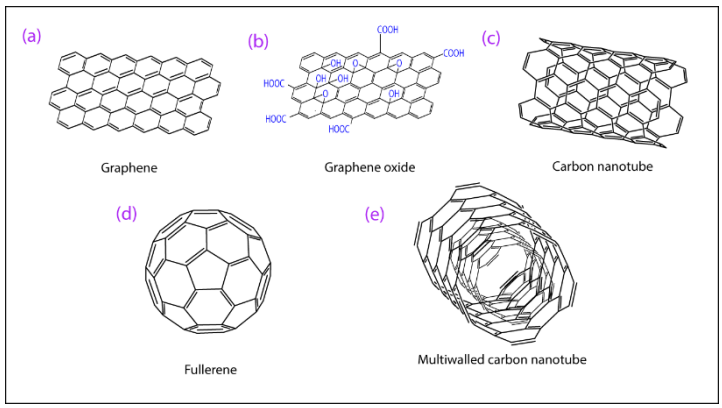


They also exhibit nontoxic properties, better encapsulation and controlled release.

The spectroscopic contribution confirms the inclusion complexation of various drug molecules as well as graphene based nanocomposites and their different photophysical properties in aqueous media. The inclusion phenomena can be satisfactorily expressed by UV-visible, FT-IR, ESI-MS, fluorescence emission spectroscopy and FT-NMR studies. Theoretical molecular modelling studies of the supramolecular system confirm the data obtained from the experimental studies.

In this study, various biologically active molecules such as, Ambroxol hydrochloride, Trigonelline hydrochloride, Rebamipide and Umbelliferone have been investigated. These bio-molecules have potential applications in living systems. Pharmacological activity is often considered to describe beneficial effects of bio molecules.

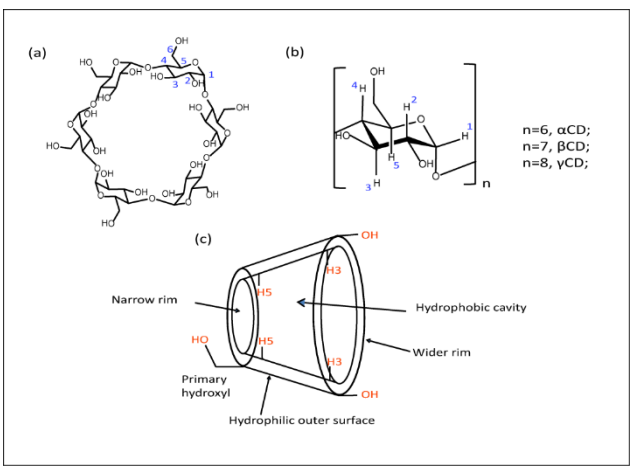
Extensive studies on Nile blue and its derivatives have suggested that it could be potentially useful as fluorescent probes in this regard, because of their unique optical properties, excellent thermo and photo-stability, and low toxicity.



Graphene sheets that are one atom thick and consist of 2D layers of carbon atoms have gained enormous

importance over the past few years because of their unique attributes such as large surface area, better absorbing properties as well as high electric and thermal conductivities.

In host–guest chemistry, the application of macrocyclic hosts in molecular recognition and sensing field has received considerable interest. Incorporation of guest molecules in aqueous environment with the cavity based host molecules, e. g., α-cyclodextrins, β-Cyclodextrins or highly water soluble hydroxypropyl β-cyclodextrin or water soluble calixarene provides the new insight into the molecular recognition (e. g. inclusion or complexation) through non-covalent interactions.



Supramolecular host-guest chemistry gives a broad idea about the formation of inclusion complex between the host and the guest molecules. Hydrophobic cavities of host are capable of binding different guest molecules. In recent ages, the whole supramolecular assemble has been enormously studied in many fields such as drug-delivery and analytical chemistry. Among the various host molecules, cyclodextrins and its derivative seems to be the most promising to form inclusion complexes, especially with various guest molecules with suitable dimension.

Therefore, the primary object of this thesis is to find out the influence of supramolecular recognition and graphene based nanocomposites that are inevitably significant because of their wide range of applications in many fields ranging from pharmaceutical to advanced application in medicine and industrial purpose.

SUMMARY OF THE WORKS:

CHAPTER I

This chapter deals with the **introduction and overview** of the research work. This thesis mainly focuses on biologically potent drugs that are encapsulated in different host as well as graphene functionalized nanocomposites. The selections of different guest and macromolecular host systems as well as graphene based materials have also been discussed. A brief review on different applications, scope and objective the work associated with this thesis have been raised.

CHAPTER II

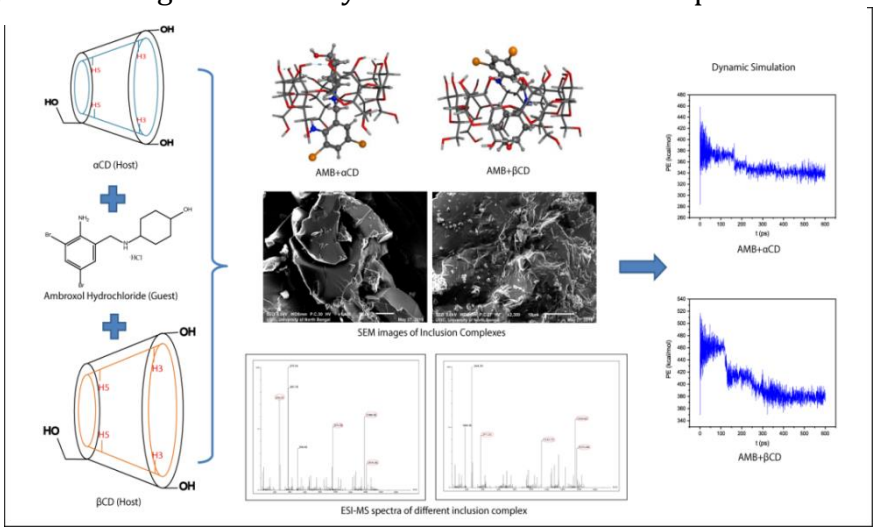
This chapter depicts all the **literature review** of the previous work. The brief discussions on synthesis and different theories of investigation for characterization of supramolecular complexation and various nanocomposites have been presented here.

CHAPTER III

This part of the thesis explains **the experimental sections** consisting of the materials, their structures, purity and their different applications. Various experimental techniques are incorporated such as spectroscopic, spectrometric and microscopic technique for the characterization of the synthesized materials. Various computational models have also been introduced to correlate the experimental data.

CHAPTER IV

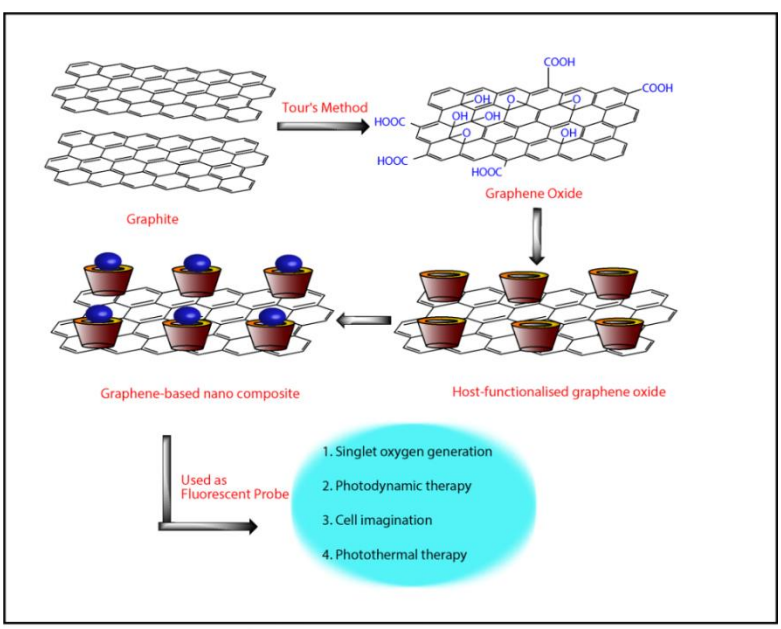
This chapter gives an insight into the synthesis of inclusion complex of AMB in two different cyclodextrins leading to host-guest assemblies. The study has been carried out with Ambroxol hydrochloride (AMB) with α-cyclodextrin (αCD) and β-cyclodextrin (βCD) and the complexation has been



confirmed by experimental (UV-vis titration, FTIR, ESI-MS, ^{1}NMR, 2D-NMR) and computational studies (molecular docking, molecular mechanics calculation). The molecular docking studies help to reveal a better insight into geometry and inclusion mode of AMB inside αCD as well as βCD cavity computationally. Further it was found that formation of inclusion complexes with different cyclodextrins causes some structural changes of guest molecules during the encapsulation process confirmed by bond length, dihedral angle changes and dynamic simulations (This work was published in **Chemical Physical Letters, Elsevier, 2020**).

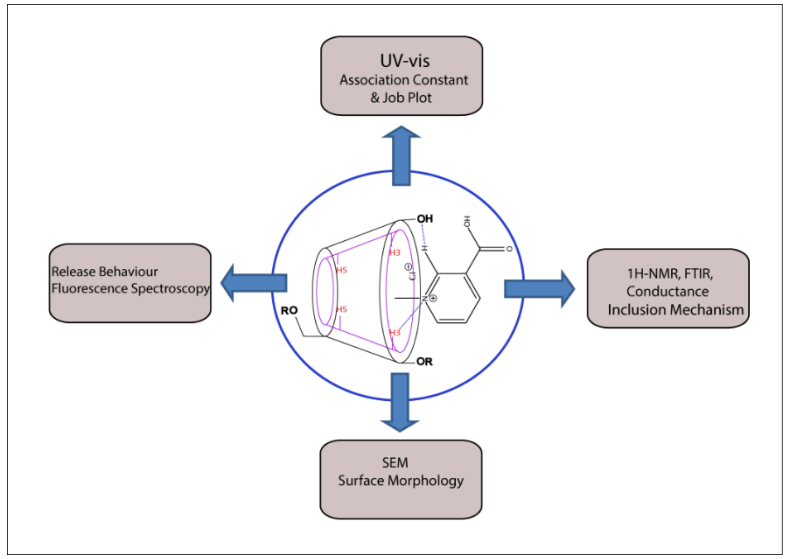
CHAPTER V

Here, we have designed and synthesized β-cyclodextrin grafted Graphene Oxide based fluorescent probe with encapsulated fluorescent dye. The nanocomposites were characterized by several spectroscopic methods such as FTIR, DLS, zeta potential, UV-vis and fluorescence spectroscopy. Thermal gravimetric analysis (TGA) was employed to account for thermal stability of β-CD grafted graphene oxide nanocomposites. Nile blue molecules are well encapsulated into the cyclodextrin cavity and embedded on the surface of Graphene Oxide sheet. Molecular Docking study helps us to understand the feasibility of encapsulation process of fluorescent dye inside our synthesized nanocomposites. Various physicochemical properties like UV-vis and fluorescence spectra of composite in different solvent and photophysical properties like fluorescence quantum yield, molar extinction coefficient, stokes shift have been calculated (Communicated).



CHAPTER VI

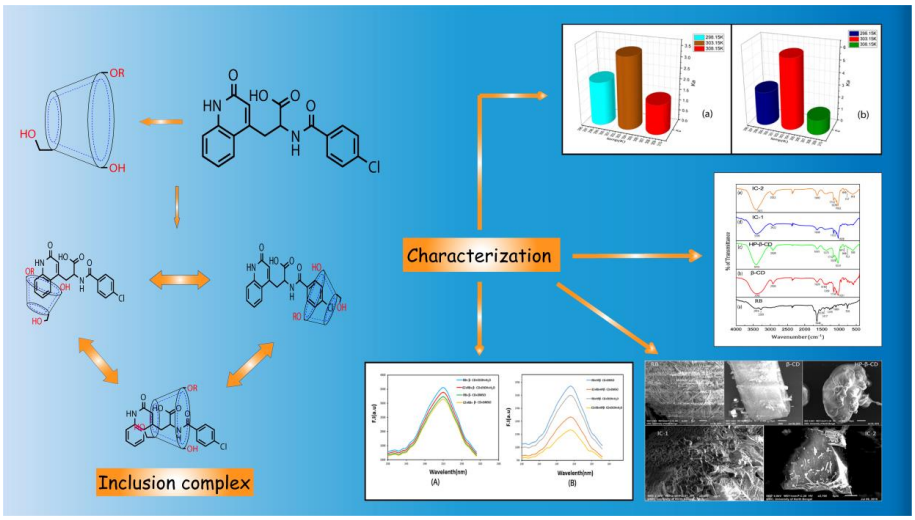
In this chapter, an inclusion complex of a biologically active alkaloid Trigonelline hydrochloride (TgC) and hydroxypropyl-β-cyclodextrin (HP-β-CD) was synthesized and characterized by different physico-chemical and spectroscopic methods. The TgC+HP-β-CD inclusion complex was confirmed by UV-vis Job's plot, fluorescence, conductance and SEM. Here, the inclusion mode is described with regard to structural aspect using ^{1}H NMR, FTIR spectroscopy. ^{1}H NMR has showed that methyl part of the guest molecule has been inserted through wider rim although interaction with H-3 proton was not very strong. Trigonelline hydrochloride (TgC) being an anti diabetic natural product, its inclusion complex was precisely checked for its sustained release by fluorescence spectroscopy (This work was published in Journal of **Molecular Structure, Elsevier, 2019**).



CHAPTER VII

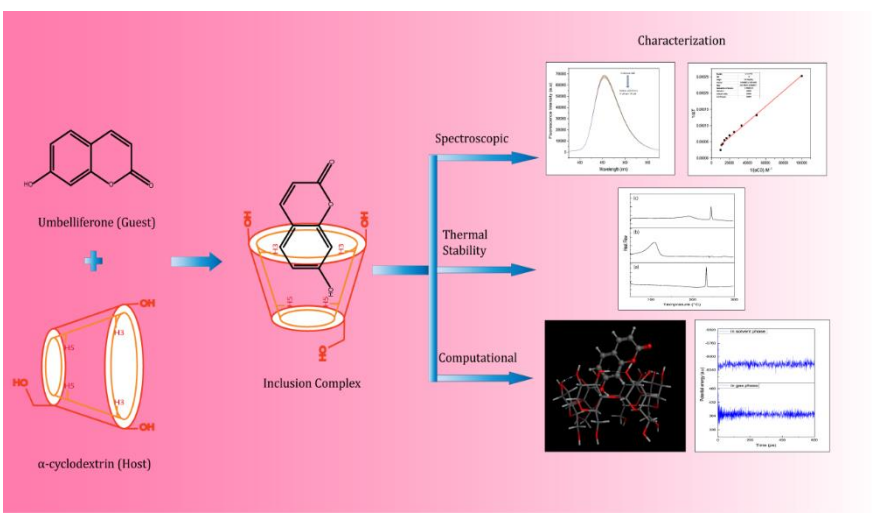
The objective of this study was to synthesize 1:1 solid rebamipide-cyclodextrin based inclusion complexes by freeze-dry method and characterized by FTIR, UV-vis, ^{1}H-NMR, 2D-ROESY, fluorescence spectroscopy, SEM and conductance. The association constant of the inclusion complexes was determined using the VU-vis titration method. Job's plot method was used to obtain the 1:1 ratio whereas, DSC method was used to confirm the thermal stability between guest and host molecule. The enzyme substituted emission spectrum of the two comparative inclusion complexes with β-CD and HP-β-CD had been studied in the diverse solvent systems. Amylase along with the inclusion complexes increased the stability of the inclusion complexation as well as the effectiveness and impact of the inclusion complexes will

have a prolonged effect in the body. (This work was published in **Z Phys Chem, 2020**).

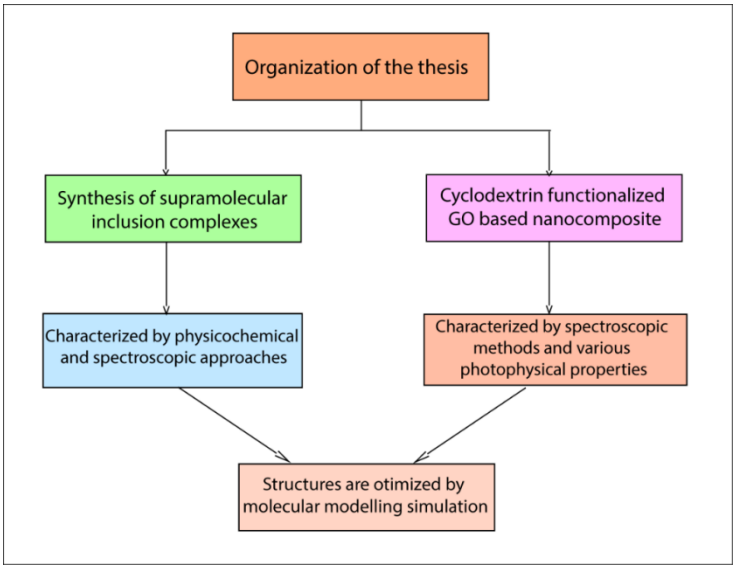


CHAPTER VIII

Umbelliferone and different host molecules have been mixed up through a coprecipitation method to prepare supramolecular complexes with improved photostability. The prepared inclusion complex was characterized by ^{1}H-NMR, FTIR spectroscopy, ESI-MS, DSC, fluorescence spectroscopy. The results of molecular modeling were systematically analyzed to determine the stability of inclusion complexes. In preliminary computational screening, α-cyclodextrin inclusion complexes of umbelliferone were found to be quite stable based on docking score and binding free energies. In addition, results from ^{1}H-NMR study supported the inclusion phenomenon. The results obtained from computational studies were found to be in consistent with experimental data to ascertain the encapsulation of umbelliferone into α-cyclodextrin (***ACS Omega, American Chemical Society, 2020***)



CHAPTER IX



This chapter includes the concluding remarks on the works associated with the thesis. The comprehension of this investigation provides the insight into comparison between experimental observations with theoretical as well as computational data in a very simplified method. This thesis also depicted the scenario of cyclodextrin based supramolecular chemistry with graphene based nanocomposites and helps to correlate these two different fields. This approach can be used to create novel materials with superior properties for predicting different purposes such as sensing, drug discovery, cell imaging, which can help to broader the band of biological applications.

CHAPTER X

Bibliography and references of all the previous chapters has been included in this chapter.