CHAPTER-X

CONCLUDING REMARKS

The perception of Host-Guest chemistry has paved the way to the formation of kinetically and thermodynamically stable supramolecular complexes with enhanced physicochemical properties and better bioavailability compared to the guest molecule. Host−guest chemistry can modify the selectivity of biomolecule−ligand association to a considerable extent depending upon recognition-directed interactions. In other words, it can be said that the morphological features and the influence of supramolecular clusters in molecular systems can be regulated precisely through various host−guest chemistry. These particular, strong yet dynamic non-covalent interactions can be accomplished as an alternative methodology for applications in the field of medicines and pharmaceuticals by the means of reversible binding between complementary components. The principal feature of Host-Guest inclusion chemistry is its ability to identify and exchange molecules until the correct combination of building units is achieved from a collection of different molecular components.

This chemistry aims at allowing reorganization and selection in self-organisation to attain adaptation at the molecular as well as supramolecular level. In general, host−guest chemistry can offer new vision into the development of traditional subjects and acts as a precursor to the development of programmable and controllable engineering of new biomaterials and medicines. The aim of my research topic was to study the host-guest inclusion complexes and their nature of interaction with the help of physicochemical methodologies.

The volumetric, viscometric, conductometric and refractive index studies helped us to figure out the extent of molecular interaction in an aqueous solution qualitatively whereas the spectroscopic measurements gave a detailed understanding into the type of molecular interaction occurring in the systems considered. We came to know about several types of interaction such as ion-ion interaction, ionic-hydrophilic interaction, dipole–dipole interaction and hydrogen bonding interaction which play key factors in most of the cases.

CHAPTER-I consists of the object, scope and application of research work , **CHAPTER-II** contains General Introduction and **CHAPTER-III** describes the experimental Section.

Chapter-IV discusses about the nature of interaction between a neurotransmitter Dopamine Hydrochloride and non-essential amino acids (Aspartic Acid and Glutamic Acid) in aqueous medium with the help of some thermodynamic parameters obtained from density, viscosity, conductance and refractive index measurements. The values of limiting apparent molar volume suggest the existence of

stronger ion-ion interactions in case of L-Glutamic acid with Dopamine. The existence of such interactions was also verified by the UV-Visible absorption data and 1H NMR Spectroscopic data. The higher value of association constant suggests greater extent of interaction in Glu-DH system. The Raman spectra sensitively captured partial structure changes of the molecule. This work precisely points out the type of interactions between Dopamine and amino acids in aqueous medium, which is proved to be informative for catecholamine recognition tool in solution phase.

In **Chapter-V,** the results obtained from FTIR spectroscopic study shows that the less polar part of the guest molecule that is the aromatic ring was included inside the hollow cavity of β-CD and the rest part of the the molecule remained outside. The 1:1 stoichiometry was verified by both Job plot method (UV-Visible Spectroscopy) and fluorescence spectroscopy. The upfield chemical shifts experienced by H3 and H5 protons (of β-CD molecule) and H1, H2, H3, H4 protons (of AC molecule) further supports the fact. The cross peaks obtained in 2D ROESY confirms the inclusion phenomena. Such inclusion phenomena led to an improved dye strength and deepen the shades of dyes.T his can also enhance possibility of dyeing at lower temperatures.

In **Chapter-VI,** it has been revealed from the analysis of thermodynamic data that the association process for [bmp]Cl is higher in case of D(+)galactose than in D(-)fructose solution and is endothermic and controlled by entropy at all temperatures. Density and viscosity studies interpret limiting apparent molar volume, ϕ_V^0 and viscosity *B*-coefficient which describes that ion-solvent interaction is increased with increasing the conc. of D(-)fructose and D(+)galactose and decreased with increasing temperature. NMR study analysis reveals that no specific and stronger interactions occur between IL and carbohydrates. However the study confirms that interaction of IL with carbohydrates is higher in D(-)fructose than that of D(+)galactose.

Chapter-VII concludes that Azelaic acid forms more stable. inclusion with β-CD than α-CD.The data obtained from conductivity primarily indicates that the AA molecule successfully enters in the hollow cavity of β-CD molecule. From the Absorption pattern obtained in UV-Vis spectroscopic measurement and the values of association constants, it has been observed that the extent of host-guest interaction is more extensive in case of the AA.β-CD complex than the other one, which is further supported by DFT study. The morphological analysis also provides successful inclusion of Azelaic acid into the cavity of β-CD molecule.

Chapter-VIII describes the the synthesis of inclusion complex between NBTU and cyclodextrin molecules. The Job's plot method and Steady state fluorescence study both confirms the 1:1 stoichiometry for the inclusion complex formed. From the spectral pattern obtained in UV-visible spectroscopic study and Steady state measurement, it has been observed that NBTU molecule successfully enters in the hollow cavity of the β-CD molecule, which is in good agreement with HRMS study. The morphological analysis also supports that the inclusion has taken place successfully. Although great diagnostic and therapeutic advances in antifungal Research has been observed so far but aspergillosis still exists as a question mark for morbidity and mortality. We took strategy to fight against this problem by developing a cost effective and enviroment friendly cyclodextrin based inclusion complex, which will also exhibit less toxicity. We applied the IC in model organisms such as *B. subtilis* (gram positive), *E. coli* (gram negative), *Aspergillus niger* (fungal pathogen) and it has been found that no zone of inhibition is found for *Aspergillus niger*, which indicates on addition of the inclusion complex in cell culture medium pathogen growth of *Aspergillus niger* is diminished to a considerable extent.

In **Chapter–IX**, The complexation of sulphanilamide with crown ethers has been studied in acetonitrile medium by the means of physicochemical and spectroscopic studies. From Job plot method, it has been found that Sulphanilamide binds with Dicyclohexano-18-crown-6 (DC18C6) more efficiently than other crown ethers at 1:1 stoichiometric ratio. This fact is further supported by 1H NMR, other thermodynamic parameters obtained through conductance, density and viscosity study are also in good alignment with the result obtained from NMR Spectroscopy. All the experimental results lead to the CONCLUSION that the extent of inclusion is the highest in case of Dicyclohexano-18-crown-6 among three crown ethers.

From the above discussion a conclusion might be drawn about the modification of physicochemical properties of guest molecule i.e phase solubility, better bio availability, drug delivery, reversible adsorption and resistance of peptides, catalytic activity during the inclusion phenomena. Such method of incorporating guest molecule of desired shape and size inside the cavity of cyclodextrin molecules furnishes a procedure to overcome physicochemical difficulties inherent in some chemical entities. The future looks likely to magnify the scopes and opportunities for host-guest chemistry, which will lead towards an expanding role in everyday lives.