CHAPTER X

Concluding Remarks

In this thesis I investigated the formation of host-guest inclusion complexes of various bio-molecules and ionic liquids with α and *β*-cyclodextrins as host giving emphasis particularly towards there formation, stabilization, carrying and controlled release without chemical modification by different dependable methods like ^{1}H NMR spectroscopy, 2D ROESY, FTIR spectroscopy, UV-visible spectroscopy, high resolution mass spectrometry, surface tension study, conductivity study, pH study, solution density, viscosity, refractive index. These studies primarily focus on the encapsulation of the studied guest molecules i.e. amino acids, drugs and ionic liquids in the hydrophobic cavity of α and *β*-cyclodextrins. The stoichiometry, association constants and thermodynamic parameters for the inclusion complexes have been determined to communicate a quantitative data regarding the encapsulation of the bio-molecules inside into α and *β*-cyclodextrins.

The findings are discussed chapter wise as follows:

Chapter IV deals with the formation of four inclusion complexes of two essential amino acids L-Leucine and L-Isoleucine with α and *β*-cyclodextrins. The four inclusion complexes have 1:1 1:1 stoichiometry which is confirmed by NMR, surface tension and conductivity measurement. The amino acid-CD interactions in the solution have been interpreted by density, viscosity, refractive index and solvation number measurements. Thus the present work adds a dimension in the field of contemporary science of controlled delivery of these two amino acids by using *α* and *β*-CD.

Chapter V investigates the formation of inclusion complexes of the phosphonium based ionic liquid Trihexyltetradecylphosphonium chloride with α and *β*-cyclodextrins in aqueous medium and in solid state. These two IC's can be used for controlled release of this ionic liquid. ^{1}H-NMR study confirms the inclusion

phenomenon whereas surface tension and conductivity study reveal the 1:1 stoichiometry of the complexes. Density ,viscosity and refractive index study show the interaction between the guest and host CD's. FT-IR spectra and mass spectra also supported the formation of IC. The binding constants for the formation of the two IC's have been evaluated from non linear isotherms using conductivity study. It is found to be higher for β-CD. These two IC's have application in various industrial processes to make them greener.

Chapter VI shows that two amino acids L-Asparagine and L-Aspartic Acid form host-guest inclusion complexes with both *α* and *β*-CD. Surface tension and conductivity measurement reveal that the inclusion complex formed with 1:1 stoichiometry. Density and viscosity studies were used to characterize the inclusion complexes through determination of the group contributions toward the limiting apparent molar volume and viscosity *B*-coefficient. The solvation number and hydration number also support the inclusion phenomenon. All the results demonstrate the formation of the inclusion complexes and thus the present work has diverse application in the field of controlled delivery of these two amino acids by using *α* and *β*-CD.

Chapter VII illustrates that the vital drug chloroquine diphosphate form inclusion complex with both α and β-CD in aqueous medium and in solid state. The two IC's can be used for controlled release of this drug. ^{1}H-NMR study confirms the inclusion phenomenon whereas surface tension, conductivity and Job's plot variation suggest the 1:1 stoichiometry of the IC's. FT-IR spectra and mass spectra also supported the formation of IC. The binding constants and thermodynamic parameters have been evaluated from UV-Visible spectroscopy which is higher for β-CD. The overall inclusion process is thermodynamically favorable. These two IC's have potential application in the pharmaceutical industries and biomedical fields.

Chapter VIII highlights about the formation of inclusion complex of probenecid with both α and β-CD in aqueous medium and in solid state. These

two inclusion complexes can be used as regulatory releaser of this drug. 2D ROESY NMR study confirms the inclusion phenomenon and its mechanism. Surface tension, conductance and Job plot from UV-visible spectroscopy determines the 1:1 stoichiometric ratio of the IC. FT-IR spectra and mass spectra also supported the formation of IC. The association constants and thermodynamic parameters have been estimated for both the ICs by reliable techniques and it is higher for β-CD. There is a drop in ΔS^0, which is overcome by higher negative value of ΔH^0, making the overall inclusion process thermodynamically favorable. These two ICs have various applications in the field of modern biochemistry and medical science.

Chapter IX emphasizes that the two ILs, *viz.*, [BMIm]Cl and [BMP]Cl form host-guest ICs with both α and β-CD both in solution and solid state. ^{1}H NMR and 2D ROESY NMR data confirm the inclusion in the apolar cavity of both CD molecules, while surface tension and conductivity measurement suggest 1:1 stoichiometry. Density, viscosity and refractive index data are also in good agreement with the above results and also recommend the IL-CD interactions. Binding constants for the ICs have been determined with the help of conductivity study by using non-linear programme. The solid state characterisations have been done by ESI-MS and FT-IR, confirming their formations also in solid state. The inclusion phenomenon has been found more fascinated in case of α-CD and [BMP]Cl than the other combinations. Thus, the present study has miscellaneous application in the field of nano-sensors, drug delivery tools and recycling extraction agents etc.

In the near future I endeavour to extend our research work with various biologically active molecules as guests and taking modified cyclodextrins as host.