

LIST OF TABLES

CHAPTERS	TABLES	PAGE NO.
<p>Chapter IV</p>	<p>Table 1. Values of Surface Tension (γ^a) at the Break Point with Corresponding Concentrations of DGs and CDs at 298.15 K^a</p> <p>Table 2. Values of Conductivity (κ) at the Break Point with Corresponding Concentrations of DGs and CDs at 298.15 K^a to 308.15 K^a</p> <p>Table 3. Association Constant obtained from Benesi-Hildebrand method (K_a), Association Constant obtained from the Nonlinear Program (K_a^θ), Association Constant obtained from Program based mathematical calculation of non-linear changes in the conductivity data (K_a^C), Association Constant obtained from Benesi-Hildebrand equation, using the spectrofluorometric data (K_a^F) at 298.15 to 308.15 K^a.</p> <p>Table 4. Thermodynamic parameters (ΔH^0, ΔS^0, ΔG^0) calculated, using the association constants (K_a, K_a^θ, K_a^C) obtained from Benesi-Hildebrand method, nonlinear Program, program based mathematical calculation of non-linear changes in the conductivity data respectively.</p> <p>Table S5. Data for surface tension of aqueous (SNP+α-CD) and (SNP+β-CD) systems at 298.15 K^a.</p> <p>Table S6. Data for surface tension of aqueous (PEH+α-CD) and (PEH+β-CD) systems at 298.15 K^a</p>	<p>106-121</p>

<p>Table S7. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (SNP+α-CD) system at 298.15 to 308.15 K^a.</p> <p>Table S8. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (SNP+β-CD) systems at 298.15 to 308.15 K^a.</p> <p>Table S9. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (PEH+α-CD) system at 298.15 to 308.15 K^a.</p> <p>Table S10. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (PEH+β-CD) systems at 298.15 to 308.15 K^a.</p> <p>Table S11. Spectro-fluorimetric data for the Benesi-Hildebrand double reciprocal plot of (SNP+α-CD) system at 298.15 K^a.</p> <p>Table S12. Spectro-fluorimetric data for the Benesi-Hildebrand double reciprocal plot of (SNP+β-CD) system at 298.15 K^a.</p> <p>Table S13. Spectro-fluorimetric data for the Benesi-Hildebrand double reciprocal plot of (PEH+α-CD) system at 298.15 K^a.</p> <p>Table S14. Spectro-fluorimetric data for the Benesi-Hildebrand double reciprocal plot of (PEH+β-CD) system at 298.15 K^a.</p> <p>Table S15. Data of the van't Hoff equation for calculation of thermodynamic parameters ΔH°, ΔS° and ΔG° of different (SNP+α-CD) and (SNP+β-CD) inclusion complexes.</p>	
---	--

	<p>Table S16. Data of the van't Hoff equation for calculation of thermodynamic parameters ΔH°, ΔS° and ΔG° of different (PEH+α-CD) and (PEH+β-CD) inclusion complexes.</p> <p>Table S17. Data of the van't Hoff equation for calculation of thermodynamic parameters $\Delta H^{\theta 0}$, $\Delta S^{\theta 0}$ and $\Delta G^{\theta 0}$ of different (SNP+α-CD) and (SNP+β-CD) inclusion complexes.</p> <p>Table S18. Data of the van't Hoff equation for calculation of thermodynamic parameters $\Delta H^{\theta 0}$, $\Delta S^{\theta 0}$ and $\Delta G^{\theta 0}$ of different (PEH+α-CD) and (PEH+β-CD) inclusion complexes.</p> <p>Table S19. Data of the van't Hoff equation for calculation of thermodynamic parameters ΔH^{C0}, ΔS^{C0} and ΔG^{C0} of different (SNP+α-CD) and (SNP+β-CD) inclusion complexes.</p> <p>Table S20. Data of the van't Hoff equation for calculation of thermodynamic parameters ΔH^{C0}, ΔS^{C0} and ΔG^{C0} of different (PEH+α-CD) and (PEH+β-CD) inclusion complexes.</p> <p>Table S21. ^1H NMR data of the pure α-Cyclodextrin, β-Cyclodextrin and the solid inclusion complexes.</p> <p>Table S22. The observed peaks at different m/z with corresponding ions for the solid inclusion complexes.</p> <p>Table S23. Frequencies at FTIR spectra of α-CD, β-CD, SNP, PEH and solid inclusion complexes.</p>	
Chapter V	Table 1: Association Constants derived from Benesi-Hildebrand method (K_a) and also from the Nonlinear Program (K_a^{τ}) using UV-Visible spectroscopic data at 236 to 263 nm in the temperature range 298.15 to 308 K.	150-164

<p>Table 2: Thermodynamic parameters (ΔH^0, ΔS^0, ΔG^0) and ($\Delta H^{0\tau}$, $\Delta S^{0\tau}$, $\Delta G^{0\tau}$) calculated, using the association constants (K_a, K_a^τ) obtained from Benesi-Hildebrand method, Nonlinear Program for λ_{\max}=236 nm and 263 nm.</p> <p>Table 3. Association constants (K_a^Φ) and standard free energy changes for (HSA +THC), (HSA+THC+α-CD) and (HSA+THC+β-CD) systems at 298.15 K.</p> <p>Table S1. UV-Vis spectroscopic data for the generation of Job plots of aqueous THC+α-CD system at 298.15 K^a and 236 nm.</p> <p>Table S2. UV-Vis spectroscopic data for the generation of Job plots of aqueous THC+α-CD system at 298.15 K^a and 263 nm.</p> <p>Table S3. UV-Vis spectroscopic data for the generation of Job plots of aqueous THC+β-CD system at 298.15 K^a and 236 nm.</p> <p>Table S4. UV-Vis spectroscopic data for the generation of Job plots of aqueous THC+β-CD system at 298.15 K^a and 263 nm.</p> <p>Table S5. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (THC+α-CD) system at 298.15 to 308.15 K^a and 236 nm.</p> <p>Table S6. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (THC+α-CD) system at 298.15 to 308.15 K^a and 263 nm.</p>	
--	--

	<p>Table S7. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (THC+β-CD) system at 298.15 to 308.15 K^a and 236 nm.</p> <p>Table S8. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (THC+β-CD) system at 298.15 to 308.15 K^a and 263 nm.</p> <p>Table S9. Data of the van't Hoff equation for calculation of thermodynamic parameters ΔH°, ΔS° and ΔG° of different (THC+α-CD) inclusion complexes at $\lambda_{\max} = 236$ and 263 nm.</p> <p>Table S10. Data of the van't Hoff equation for calculation of thermodynamic parameters ΔH°, ΔS° and ΔG° of different (THC+β-CD) inclusion complexes at $\lambda_{\max} = 236$ and 263 nm.</p> <p>Table S11. Data of the van't Hoff equation for calculation of thermodynamic parameters $\Delta H^{r^{\circ}}$, $\Delta S^{r^{\circ}}$ and $\Delta G^{r^{\circ}}$ of different (THC+α-CD) inclusion complexes at $\lambda_{\max} = 236$ and 263 nm.</p> <p>Table S12. Data of the van't Hoff equation for calculation of thermodynamic parameters $\Delta H^{r^{\circ}}$, $\Delta S^{r^{\circ}}$ and $\Delta G^{r^{\circ}}$ of different (THC+β-CD) inclusion complexes at $\lambda_{\max} = 236$ and 263 nm.</p> <p>Table S13. ¹H NMR data of the pure thiamine hydrochloride, pure α-Cyclodextrin, β-Cyclodextrin and the respective inclusion complexes.</p> <p>Table S14. Frequencies of FTIR spectra of α-CD, β-CD, THC and two solid inclusion complexes.</p>	
--	---	--

	<p>Table S15. Spectro-fluorimetric data for the Benesi-Hildebrand double reciprocal plot of (HSA+THC) system at 298.15 K^a.</p> <p>Table S16. Spectro-fluorimetric data for the Benesi-Hildebrand double reciprocal plot of (HSA+THC) system in presence of fixed amount of α-CD at 298.15 K^a.</p> <p>Table S17. Spectro-fluorimetric data for the Benesi-Hildebrand double reciprocal plot of (HSA+THC) system in presence of fixed amount of β-CD at 298.15 K^a.</p>	
Chapter VI	<p>Table 1. FTIR frequency of some significant groups of β-CD, HP β-CD, HBCDD observed at free and complexed state showing corresponding shift</p> <p>Table 2. Exact mass and the observed m/z values of the two inclusion complexes</p> <p>Table 3. Melting points of HBCDD, IC-1 and IC-2</p> <p>Table 4. Aqueous solubility of HBCDD, IC-1 and IC-2 at 298 K</p> <p>Table S1. Frequencies of FTIR spectra of β-CD, HP-β-CD, HBCDD and two solid inclusion complexes</p>	183-186
Chapter VII	<p>Table 1: The association constant (K_a) and complexation efficiency of the inclusion complexes at 298.15 K.</p> <p>Table 2: The solubility of ALVC (moles/litre) in the aqueous solution of cyclodextrins of concentration ranging from 0.002 to 0.01 (M).</p> <p>Table 3. Association Constant obtained from Benesi-Hildebrand method (K_a) using the UV-vis spectroscopic</p>	211-218

	<p>data at 293.15 to 303.15 K and the thermodynamic parameters calculated using Van't Hoff equation.</p> <p>Table 4: HSA-ALVC binding constant and number of binding site.</p> <p>Table S1. UV-Vis spectroscopic data for the generation of Job plots of aqueous ALVC+α-CD system at 298.15 K^a.</p> <p>Table S2. UV-Vis spectroscopic data for the generation of Job plots of aqueous ALVC+β-CD system at 298.15 K^a.</p> <p>Table S3. Mass spectrometric data showing the molecular ion peak corresponding to the 2:1 Host –Guest inclusion complexes.</p> <p>Table S4. ¹H NMR data of the pure α-Cyclodextrin, β-Cyclodextrin, alverine citrate and the solid inclusion complexes.</p> <p>Table S5. Frequencies at FTIR spectra of α-CD, β-CD, 18-Crown-6, ALVC and solid inclusion complexes.</p> <p>Table S6. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (ALVC+α-CD) system at 293.15 to 303.15 K^a.</p> <p>Table S7. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (ALVC+β-CD) system at 293.15 to 303.15 K^a.</p> <p>Table S8. Data of the van't Hoff equation for calculation of thermodynamic parameters ΔH°, ΔS° and ΔG° of different (ALVC+α-CD) and (ALVC+β-CD) inclusion complexes.</p>	
--	--	--

<p>Chapter VIII</p>	<p>Table 1. Apparent molar volume (Φ_V^0), Molar Refraction (R_M^0) and viscosity A and viscosity B co-efficient of (BTEACl+SBz+H₂O), (BTEACl+SCyt+H₂O) systems in solution of BTEACl of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15K, 303.15K, 308.15K, 313.15K and 318.15 K.</p> <p>Table 2. Apparent molar volume (Φ_V^0), Molar Refraction (R_M^0) and viscosity A and viscosity B co-efficient of (BTMACl+SBz+H₂O), (BTMACl+SCyt+H₂O) systems in solution of BTMACl of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15K, 303.15K, 308.15K, 313.15K and 318.15 K.</p> <p>Table 3: Values of empirical coefficients (a_0, a_1, and a_2) of Eq. 5 for aqueous (BTEACl+SBz), (BTEACl+SCyt), (BTMACl+SBz), (BTMACl+SCyt) systems in different mass fraction of aqueous BTEACl/BTMACl solution at 298.15 to 318.15 K.</p> <p>Table 4. Values of limiting apparent molar expansibilities (Φ_E^0) of aqueous (BTEACl+SBz), (BTEACl+SCyt), (BTMACl+SBz), (BTMACl+SCyt) systems in different mass fraction of aqueous BTEACl/BTMACl solution at 298.15 to 318.15 K.</p> <p>Table 5. Values of dB/dT for aqueous (BTEACl+SBz), (BTEACl+SCyt), (BTMACl+SBz), (BTMACl+SCyt) systems in different mass fraction of aqueous BTEACl/BTMACl solution at 298.15 to 318.15 K.</p>	<p>240-264</p>
----------------------------	--	-----------------------

Table 6. Association constant and Gibb's free energy of (BTEACl+SBz), (BTEACl+SCyt), (BTMACl+SBz) and (BTMACl+SCyt) systems at 298.15 K.

Table 7. Optimisation energies of pure BTEACl, BTMACl, SBz, SCyt and (BTEACl+SBz), (BTEACl+SCyt), (BTMACl+SBz), (BTMACl+SCyt) systems using UB3LYP methodology and 6-31G(d) basis set.

Table S1. Density (ρ), Refractive index (n_D), Viscosity (η) of aqueous pure BTEACl and BTMACl solutions of mass fractions $W = 0.001, 0.003, 0.005$ at temperatures 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.

Table S2. Density (ρ), Refractive Index (n_D) and Viscosity (η) of (BTEACl+SBz+H₂O) and (BTEACl+SCyt+H₂O), systems in aqueous BTEACl solutions of mass fractions $W_1=0.001, W_2=0.003, W_3=0.005$, at 298.15K, 303.15K, 308.15K, 313.15K and 318.15 K.

Table S3. Density (ρ), Refractive Index (n_D) and Viscosity (η) of (BTEACl+SBz+H₂O) and (BTEACl+SCyt+H₂O), systems in aqueous BTEACl solutions of mass fractions $W_1=0.001, W_2=0.003, W_3=0.005$, at 298.15K, 303.15K, 308.15K, 313.15K and 318.15 K.

Table S4. Density (ρ), Refractive Index (n_D) and Viscosity (η) of (BTEACl+SBz+H₂O) and (BTEACl+SCyt+H₂O), systems in aqueous BTEACl solutions of mass fractions $W_1=0.001, W_2=0.003, W_3=0.005$, at 298.15K, 303.15K, 308.15K, 313.15K and 318.15 K.

Table S5. Density (ρ), Refractive Index (n_D) and Viscosity (η) of (BTMACl+SBz+H₂O) and (BTMACl+SCyt+H₂O) systems in aqueous BTMACl solutions of mass fractions $W_1=0.001,$

	<p>$W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K</p> <p>Table S6. Density (ρ), Refractive Index (n_D) and Viscosity (η) of (BTMACl+SBz+H₂O) and (BTMACl+SCyt+H₂O) systems in aqueous BTMACl solutions of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K</p> <p>Table S7. Density (ρ), Refractive Index (n_D) and Viscosity (η) of (BTMACl+SBz+H₂O) and (BTMACl+SCyt+H₂O) systems in aqueous BTMACl solutions of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K</p> <p>Table S8. Apparent molar volume (φ_V), Molar Refraction (R_M) and $(n_r-1)/\sqrt{c}$ of (BTEACl+SBz+H₂O) and (BTEACl+SCyt+H₂O) systems in aqueous BTEACl solutions of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.</p> <p>Table S9. Apparent molar volume (φ_V), Molar Refraction (R_M) and $(n_r-1)/\sqrt{c}$ of (BTEACl+SBz+H₂O) and (BTEACl+SCyt+H₂O) systems in aqueous BTEACl solutions of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.</p> <p>Table S10. Apparent molar volume (φ_V), Molar Refraction (R_M) and $(n_r-1)/\sqrt{c}$ of (BTEACl+SBz+H₂O) and (BTEACl+SCyt+H₂O) systems in aqueous BTEACl solutions of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.</p> <p>Table S11. Apparent molar volume (φ_V), Molar Refraction (R_M) and $(n_r-1)/\sqrt{c}$ of (BTMACl+SBz+H₂O),</p>	
--	---	--

	<p>(BTMACl+SCyt+H₂O) systems in aqueous BTMACl solutions of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.</p> <p>Table S12. Apparent molar volume (φ_V), Molar Refraction (R_M) and $(\eta_r-1)/\sqrt{c}$ of (BTMACl+SBz+H₂O), (BTMACl+SCyt+H₂O) systems in aqueous BTMACl solutions of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.</p> <p>Table S13. Apparent molar volume (φ_V), Molar Refraction (R_M) and $(\eta_r-1)/\sqrt{c}$ of (BTMACl+SBz+H₂O), (BTMACl+SCyt+H₂O) systems in aqueous BTMACl solutions of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.</p> <p>Table S14. Molar conductivities of (BTEAcl+SBz+H₂O) and (BTEAcl+SCyt+H₂O) systems in aqueous BTEAcl solutions of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.</p> <p>Table S15. Molar conductivities of (BTEAcl+SBz+H₂O) and (BTEAcl+SCyt+H₂O) systems in aqueous BTEAcl solutions of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.</p> <p>Table S16. Molar conductivities of (BTMAcl+SBz+H₂O) and (BTMAcl+SCyt+H₂O) systems in aqueous BTMAcl solution of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.</p> <p>Table S17. Molar conductivities of (BTMAcl+SBz+H₂O) and (BTMAcl+SCyt+H₂O) systems in aqueous BTMAcl solution of mass fractions $W_1=0.001$, $W_2=0.003$, $W_3=0.005$, at 298.15 K, 303.15 K, 308.15 K, 313.15 K and 318.15 K.</p>	
--	---	--

	<p>Table S18. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (BTEACl+SBz) system at 298.15 K^b.</p> <p>Table S19. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (BTEACl+Scyt) system at 298.15 K^b.</p> <p>Table S20. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (BTMACl+SBz) system at 298.15 K^b.</p> <p>Table S21. UV-vis spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (BTMACl+Scyt) system at 298.15 K^b.</p>	
--	---	--