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Host-guest inclusion complexes of RNA nucleosides insight into aqueous cyclodextrins explored by physicochemical and spectroscopic contrivances

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Theory:

The physical properties of binary mixtures in different molarity (w_n=0.001, 0.0025, 0.004, where n=1, 2 for α and β-CD respectively) of aqueous α and β-CD solutions at 298.15K have been reported in table S1. The values of density, viscosity, refractive index, and ultrasonic speed of RNA nucleosides (*i.e.*, adenosine, guanosine, uridine and cytidine) in different molarity of aqueous α and β-CD mixture, as a function of concentration (molality) has been listed in tables given below.

Surface tension

The concentrations at which the inclusion occurred (the break point of the surface tension) have been calculated by solving the equation of two straight lines, and represented in table 1. For instance, in case of adenosine in w_2=0.001 molarity of β-cyclodextrin

$$\gamma = 985.61\, c + 71.24$$

$$\gamma = 539.6\, c + 73.92$$

γ = 77.16 mN·m^{-1} and c = 6.00 millimolal

Apparent molar volume

The apparent molar volumes ϕ_V were determined from the solutions densities (Table S8) using the equation

$$\phi_V = M/\rho \; - 1000(\rho - \rho_o)/m\rho\rho_o \qquad (1)$$

where *M* is the molar mass of the nucleosides, *m* is the molality of the solution, ρ and ρ_0 are the density of the solution and aq. α and β-CD mixture respectively. The limiting apparent molar volumes ϕ_V^0 were obtained by a least-square treatment to the plots of ϕ_V versus $\sqrt{m}$ using the Masson equation and shown in table S4.[1]

$$\phi_V = \phi_V^0 + S_V^* \cdot \sqrt{m} \tag{2}$$

Viscosity

The experimental viscosity data for the studied systems are listed in table S8. The relative viscosity (η_r) has been analyzed using the Jones-Dole equation.[2]

$$(\eta/\eta_o - 1)/\sqrt{m} = (\eta_r - 1)/\sqrt{m} = A + B\sqrt{m} \tag{3}$$

where $\eta_r = \eta/\eta_o$, η and η_0 are the relative viscosities, the viscosities of the ternary solutions (nucleoside + aq. CD) and binary aqueous mixture (aq. CD) and *m* is the molality of the nucleosides in ternary solutions. *A* and *B* are empirical constants known as viscosity *A* and *B*-coefficients, which are specific to solute-solute and solute-solvent interactions, respectively, are estimated by least-square method by plotting $(\eta_r - 1)/\sqrt{m}$ against $\sqrt{m}$, and reported in table S9.

Ultrasonic speed

The adiabatic compressibility is defined by the thermodynamic relation:

$$\beta_s = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_S \tag{4}$$

where *V* is volume, *P* is pressure and *S* is entropy, is related to the solution density ρ, and the ultrasonic speed (*u*), by the Newton-Laplace's equation:

$$\beta_s = 1/u^2\rho \tag{5}$$

which provides the relation between thermodynamics and acoustics. The apparent molar adiabatic compressibility (ϕ_K), of the solutions was determined from the following relation,

$$\phi_K = M\beta_s/\rho + 1000\left(\beta_s\rho_o - \beta_o\rho\right)/m\rho\rho_o \tag{6}$$

where β_0, β_s are the adiabatic compressibility of the binary mixture and ternary solution respectively and m is the molality of the ternary solution. Limiting apparent molar adiabatic compressibilities (ϕ_K^0) or apparent molar adiabatic compressibility at infinite dilution and experimental slopes (S_K^*), were obtained by fitting ϕ_K against the square root of concentration ($\sqrt{m}$) using the least squares method.[3]

$$\phi_K = \phi_K^0 + S_K^* \cdot \sqrt{m} \quad (7)$$

The values of ϕ_K^0 are presented in Table S6. The value of ϕ_K^0 is an important parameter that provides information about the extent of solute-solvent interaction. The behavior is useful in characteristic of solvation and electrostriction (the contraction of the solvent around the solute) in solutions.

Refractive index

The molar refraction, R_M can be evaluated from the Lorentz-Lorenz relation.[4]

$$R_M = \{(n_D^2 - 1)/(n_D^2 + 2)\}(M/\rho) \quad (8)$$

where R_M, n_D, M and ρ are the molar refraction, the refractive index, the molar mass and the density of solution respectively. The Limiting molar refraction (R_M^0) estimated from the following euation,[5]

$$R_M = R_M^0 + R_S \sqrt{m} \quad (9)$$

References:

1 D.O. Masson, *Phil Mag.*, 1929, **8**, 218-223.

2 G. Jones and D. Dole, *J. Am. Chem. Soc.,* 1929, **51**, 2950-2964.

3 D. Ekka and M. N. Roy, *Amino Acids*, 2013, **45**, 755-777.

4 V. Minkin, O. Osipov and Y. Zhdanov, *Dipole Moments in Organic Chemistry,* Plenum Press, New York, 1970.

5 M. N. Roy, P. Chakraborti and D. Ekka, *Mol. Phys.,* 2014, **112**, 2215.

Tables

Table S1. Experimental values of density (ρ), viscosity (η), refractive index (n_D), surface tension (γ), pH and ultrasonic sound (u) in deferent molarity of aqueous α and β-cyclodextrin mixtures:

aq. solvent mixture	Temp /K[a]	$\rho \cdot 10^{-3}$ /kg·m^{-3}	η /mP·s	n_D	γ /mN·m^{-1}	pH	u /m·s^{-1}
w_1=0.001[b]	298.15	0.99742	1.300	1.3000	71.78	6.43	1492.5
	303.15	0.99600	1.202	-	-	-	-
	308.15	0.99412	1.098	-	-	-	-
w_1=0.0025[b]	298.15	0.99794	1.308	1.3070	71.71	6.40	1493.5
	303.15	0.99653	1.210	-	-	-	-
	308.15	0.99470	1.105	-	-	-	-
w_1=0.004[b]	298.15	0.99846	1.315	1.3170	71.65	6.35	1494.7
	303.15	0.99708	1.217	-	-	-	-
	308.15	0.99532	1.113	-	-	-	-
w_2=0.001[b]	298.15	0.99758	1.306	1.3040	71.75	6.64	1490.4
	303.15	0.99622	1.207	-	-	-	-
	308.15	0.99442	1.103	-	-	-	-
w_2=0.0025[b]	298.15	0.99809	1.313	1.3110	71.69	6.59	1491.5
	303.15	0.99675	1.213	-	-	-	-
	308.15	0.99500	1.108	-	-	-	-
w_2=0.004[b]	298.15	0.99861	1.322	1.3200	71.62	6.52	1492.6
	303.15	0.99730	1.221	-	-	-	-
	308.15	0.99552	1.115	-	-	-	-

[a] Standard uncertainties in temperature (T) = ±0.01 K.

[b] w_1 and w_2 are the molarity of α and β-CD in aqueous mixture respectively.

Table S2 Data for the Job plot performed by UV-Vis spectroscopy for aqueous uridine-*α*-CD system:

Uridine (mL)	*α*-CD (mL)	Uridine (μM)	*α*-CD (μM)	[U]/([U]+[α-CD])	Absorbance (A)	ΔA	ΔA×[U]/([U]+[*α*-CD])
0.0	1.0	0	100	0.0	0.00	0.96	0.000
0.1	0.9	10	90	0.1	0.08	0.88	0.088
0.2	0.8	20	80	0.2	0.17	0.79	0.158
0.3	0.7	30	70	0.3	0.28	0.68	0.204
0.4	0.6	40	60	0.4	0.37	0.59	0.236
0.5	0.5	50	50	0.5	0.45	0.51	0.255
0.6	0.4	60	40	0.6	0.57	0.39	0.234
0.7	0.3	70	30	0.7	0.68	0.28	0.196
0.8	0.2	80	20	0.8	0.79	0.17	0.136
0.9	0.1	90	10	0.9	0.88	0.08	0.072
1.0	0.0	100	0	1.0	0.96	0.00	0.000

Table S3 Data for the Job plot performed by UV-Vis spectroscopy for aqueous cytidine-*α*-CD system:

Cytidine (mL)	*α*-CD (mL)	Cytidine (μM)	*α*-CD (μM)	[C]/([C]+[α-CD])	Absorbance (A)	ΔA	ΔA×[C]/([C]+[*α*-CD])
0.0	1.0	0	100	0.0	0.00	0.78	0.000
0.1	0.9	10	90	0.1	0.06	0.72	0.072
0.2	0.8	20	80	0.2	0.14	0.64	0.128
0.3	0.7	30	70	0.3	0.21	0.57	0.171
0.4	0.6	40	60	0.4	0.29	0.49	0.196
0.5	0.5	50	50	0.5	0.37	0.41	0.205
0.6	0.4	60	40	0.6	0.45	0.33	0.198
0.7	0.3	70	30	0.7	0.53	0.25	0.175
0.8	0.2	80	20	0.8	0.61	0.17	0.136
0.9	0.1	90	10	0.9	0.69	0.09	0.081
1.0	0.0	100	0	1.0	0.78	0.00	0.000

Table S4 Data for the Job plot performed by UV-Vis spectroscopy for aqueous adenosine-*β*-CD system:

Adenosine (mL)	*β*-CD (mL)	Adenosine (μM)	*β*-CD (μM)	[A]/([A]+[*β*-CD])	Absorbance (A)	ΔA	ΔA×[A]/([A]+[*β*-CD])
0.0	1.0	0	100	0.0	0.00	0.92	0.000
0.1	0.9	10	90	0.1	0.08	0.84	0.084
0.2	0.8	20	80	0.2	0.16	0.76	0.152
0.3	0.7	30	70	0.3	0.25	0.67	0.201
0.4	0.6	40	60	0.4	0.35	0.57	0.228
0.5	0.5	50	50	0.5	0.44	0.48	0.240
0.6	0.4	60	40	0.6	0.54	0.38	0.228
0.7	0.3	70	30	0.7	0.63	0.29	0.203
0.8	0.2	80	20	0.8	0.72	0.20	0.160
0.9	0.1	90	10	0.9	0.81	0.11	0.099
1.0	0.0	100	0	1.0	0.92	0.00	0.000

Table S5 Data for the Job plot performed by UV-Vis spectroscopy for aqueous guanosine-*β*-CD system:

Guanosine (mL)	*β*-CD (mL)	Guanosine (μM)	*β*-CD (μM)	[G]/([G]+[*β*-CD])	Absorbance (A)	ΔA	ΔA×[G]/([G]+[*β*-CD])
0.0	1.0	0	100	0.0	0.00	1.02	0.000
0.1	0.9	10	90	0.1	0.09	0.93	0.093
0.2	0.8	20	80	0.2	0.20	0.82	0.164
0.3	0.7	30	70	0.3	0.29	0.73	0.219
0.4	0.6	40	60	0.4	0.41	0.61	0.244
0.5	0.5	50	50	0.5	0.50	0.52	0.260
0.6	0.4	60	40	0.6	0.62	0.40	0.240
0.7	0.3	70	30	0.7	0.71	0.31	0.217
0.8	0.2	80	20	0.8	0.81	0.21	0.168
0.9	0.1	90	10	0.9	0.91	0.11	0.099
1.0	0.0	100	0	1.0	1.02	0.00	0.000

Table S6 Data for the Job plot performed by UV-Vis spectroscopy for aqueous uridine-*β*-CD system:

Uridine (mL)	*β*-CD (mL)	Uridine (μM)	*β*-CD (μM)	[U]/([U]+[*β*-CD])	Absorbance (A)	ΔA	ΔA×[U]/([U]+[*β*-CD])
0.0	1.0	0	100	0.0	0.00	1.01	0.000
0.1	0.9	10	90	0.1	0.11	0.90	0.090
0.2	0.8	20	80	0.2	0.20	0.81	0.162
0.3	0.7	30	70	0.3	0.31	0.70	0.210
0.4	0.6	40	60	0.4	0.41	0.60	0.240
0.5	0.5	50	50	0.5	0.50	0.51	0.255
0.6	0.4	60	40	0.6	0.61	0.40	0.240
0.7	0.3	70	30	0.7	0.71	0.30	0.210
0.8	0.2	80	20	0.8	0.82	0.19	0.152
0.9	0.1	90	10	0.9	0.90	0.11	0.099
1.0	0.0	100	0	1.0	1.01	0.00	0.000

Table S7 Data for the Job plot performed by UV-Vis spectroscopy for aqueous cytidine-*β*-CD system:

Cytidine (mL)	*β*-CD (mL)	Cytidine (μM)	*β*-CD (μM)	[C]/([C]+[*β*-CD])	Absorbance (A)	ΔA	ΔA×[C]/([C]+[*β*-CD])
0.0	1.0	0	100	0.0	0.00	0.99	0.000
0.1	0.9	10	90	0.1	0.08	0.91	0.091
0.2	0.8	20	80	0.2	0.19	0.80	0.160
0.3	0.7	30	70	0.3	0.28	0.71	0.213
0.4	0.6	40	60	0.4	0.39	0.60	0.240
0.5	0.5	50	50	0.5	0.48	0.51	0.255
0.6	0.4	60	40	0.6	0.60	0.39	0.234
0.7	0.3	70	30	0.7	0.71	0.28	0.196
0.8	0.2	80	20	0.8	0.79	0.20	0.160
0.9	0.1	90	10	0.9	0.90	0.09	0.081
1.0	0.0	100	0	1.0	0.99	0.00	0.000

Table S8. Experimental values of densities (ρ) and viscosities (η) corresponding to concentrations of nucleosides in different molarity of aq. α and β-cyclodextrin at different temperature

Conc (m)	$\rho \cdot 10^{-3}$ /kg·m^{-3}	η /mP·s	Conc (m)	$\rho \cdot 10^{-3}$ /kg·m^{-3}	η /mP·s	Conc (m)	$\rho \cdot 10^{-3}$ /kg·m^{-3}	η /mP·s
	298.15 K[a]			303.15K[a]			308.15K[a]	
				w_1=0.001 [b]				
				Adenosine				
0.0010	0.99748	1.310	0.0010	0.99610	1.211	0.0010	0.99426	1.105
0.0025	0.99761	1.318	0.0025	0.99628	1.217	0.0025	0.99449	1.111
0.0040	0.99775	1.325	0.0040	0.99648	1.223	0.0040	0.99474	1.115
0.0055	0.99791	1.332	0.0055	0.99670	1.229	0.0055	0.99500	1.120
0.0070	0.99809	1.338	0.0070	0.99693	1.234	0.0070	0.99527	1.124
0.0085	0.99827	1.344	0.0085	0.99717	1.239	0.0086	0.99555	1.127
				Guanosine				
0.0010	0.99749	1.310	0.0010	0.99610	1.211	0.0010	0.99426	1.106
0.0025	0.99763	1.319	0.0025	0.99629	1.218	0.0025	0.99450	1.111
0.0040	0.99779	1.327	0.0040	0.99650	1.224	0.0040	0.99476	1.116
0.0055	0.99798	1.334	0.0055	0.99673	1.230	0.0055	0.99503	1.121
0.0070	0.99818	1.342	0.0070	0.99698	1.236	0.0070	0.99531	1.126
0.0085	0.99842	1.348	0.0085	0.99724	1.241	0.0086	0.99560	1.130
				Uridine				
0.0010	0.99744	1.311	0.0010	0.99605	1.211	0.0010	0.99421	1.106
0.0025	0.99749	1.320	0.0025	0.99617	1.219	0.0025	0.99437	1.112
0.0040	0.99758	1.329	0.0040	0.99631	1.226	0.0040	0.99456	1.118
0.0055	0.99769	1.337	0.0055	0.99648	1.232	0.0055	0.99477	1.123
0.0070	0.99783	1.344	0.0070	0.99666	1.238	0.0070	0.99498	1.128
0.0085	0.99798	1.352	0.0085	0.99685	1.244	0.0086	0.99520	1.133
				Cytidine				
0.0010	0.99743	1.311	0.0010	0.99604	1.211	0.0010	0.99420	1.106

0.0025	0.99746	1.321	0.0025	0.99613	1.219	0.0025	0.99435	1.113
0.0040	0.99753	1.330	0.0040	0.99625	1.226	0.0040	0.99453	1.119
0.0055	0.99762	1.339	0.0055	0.99640	1.233	0.0055	0.99472	1.125
0.0070	0.99774	1.348	0.0070	0.99656	1.240	0.0070	0.99492	1.130
0.0085	0.99790	1.356	0.0085	0.99674	1.246	0.0086	0.99514	1.135
w_1=0.0025 [b]								
Adinosine								
0.0010	0.99800	1.318	0.0010	0.99662	1.219	0.0010	0.99483	1.113
0.0025	0.99812	1.327	0.0025	0.99679	1.226	0.0025	0.99505	1.118
0.0040	0.99827	1.335	0.0040	0.99699	1.232	0.0040	0.99530	1.123
0.0055	0.99845	1.342	0.0055	0.99720	1.238	0.0055	0.99555	1.128
0.0070	0.99864	1.349	0.0070	0.99743	1.243	0.0070	0.99581	1.132
0.0085	0.99884	1.356	0.0085	0.99767	1.249	0.0086	0.99609	1.136
Guanosine								
0.0010	0.99801	1.318	0.0010	0.99663	1.219	0.0010	0.99484	1.113
0.0025	0.99814	1.328	0.0025	0.99681	1.226	0.0025	0.99507	1.119
0.0040	0.99831	1.336	0.0040	0.99702	1.233	0.0040	0.99533	1.124
0.0055	0.99850	1.343	0.0055	0.99725	1.239	0.0055	0.99560	1.129
0.0070	0.99871	1.350	0.0070	0.99749	1.245	0.0070	0.99587	1.134
0.0085	0.99895	1.357	0.0085	0.99775	1.251	0.0086	0.99616	1.138
Uridine								
0.0010	0.99796	1.319	0.0010	0.99658	1.219	0.0010	0.99479	1.113
0.0025	0.99802	1.328	0.0025	0.99669	1.227	0.0025	0.99495	1.119
0.0040	0.99812	1.337	0.0040	0.99683	1.234	0.0040	0.99514	1.125
0.0055	0.99824	1.345	0.0055	0.99700	1.240	0.0055	0.99534	1.130
0.0070	0.99840	1.353	0.0070	0.99717	1.247	0.0070	0.99556	1.135
0.0085	0.99857	1.361	0.0085	0.99736	1.253	0.0086	0.99579	1.140
Cytidine								
0.0010	0.99795	1.319	0.0010	0.99657	1.220	0.0010	0.99478	1.113
0.0025	0.99799	1.329	0.0025	0.99667	1.227	0.0025	0.99493	1.120

0.0040	0.99807	1.339	0.0040	0.99680	1.235	0.0040	0.99510	1.126
0.0055	0.99819	1.348	0.0055	0.99696	1.241	0.0055	0.99530	1.132
0.0070	0.99834	1.356	0.0070	0.99713	1.249	0.0070	0.99550	1.137
0.0085	0.99851	1.365	0.0085	0.99732	1.255	0.0086	0.99574	1.143
w_1=0.004 [b]								
Adinosine								
0.0010	0.99851	1.326	0.0010	0.99716	1.226	0.0010	0.99544	1.121
0.0025	0.99863	1.336	0.0025	0.99732	1.234	0.0025	0.99566	1.127
0.0040	0.99878	1.344	0.0040	0.99751	1.241	0.0040	0.99590	1.132
0.0055	0.99895	1.352	0.0055	0.99772	1.247	0.0055	0.99615	1.137
0.0070	0.99914	1.359	0.0070	0.99794	1.253	0.0070	0.99640	1.142
0.0085	0.99933	1.367	0.0085	0.99817	1.259	0.0085	0.99668	1.147
Guanosine								
0.0010	0.99852	1.326	0.0010	0.99717	1.226	0.0010	0.99545	1.121
0.0025	0.99865	1.336	0.0025	0.99735	1.234	0.0025	0.99568	1.127
0.0040	0.99881	1.345	0.0040	0.99755	1.242	0.0040	0.99593	1.133
0.0055	0.99899	1.354	0.0055	0.99777	1.248	0.0055	0.99620	1.139
0.0070	0.99919	1.362	0.0070	0.99801	1.255	0.0070	0.99647	1.144
0.0085	0.99942	1.370	0.0085	0.99826	1.262	0.0085	0.99677	1.149
Uridine								
0.0010	0.99847	1.326	0.0010	0.99712	1.226	0.0010	0.99540	1.121
0.0025	0.99853	1.337	0.0025	0.99723	1.235	0.0025	0.99556	1.128
0.0040	0.99862	1.347	0.0040	0.99737	1.243	0.0040	0.99574	1.134
0.0055	0.99874	1.356	0.0055	0.99753	1.250	0.0055	0.99595	1.140
0.0070	0.99889	1.364	0.0070	0.99770	1.257	0.0070	0.99615	1.146
0.0085	0.99905	1.373	0.0085	0.99789	1.264	0.0085	0.99638	1.151
Cytidine								
0.0010	0.99846	1.326	0.0010	0.99711	1.227	0.0010	0.99539	1.121
0.0025	0.99850	1.338	0.0025	0.99721	1.236	0.0025	0.99553	1.128
0.0040	0.99858	1.348	0.0040	0.99733	1.244	0.0040	0.99570	1.135

0.0055	0.99870	1.358	0.0055	0.99748	1.251	0.0055	0.99590	1.141
0.0070	0.99885	1.367	0.0070	0.99765	1.259	0.0070	0.99610	1.147
0.0085	0.99901	1.376	0.0085	0.99782	1.266	0.0085	0.99631	1.153
w_2=0.001 [b]								
Adenosine								
0.0010	0.99760	1.317	0.0010	0.99627	1.217	0.0010	0.99451	1.111
0.0025	0.99769	1.328	0.0025	0.99639	1.225	0.0025	0.99467	1.118
0.0040	0.99781	1.337	0.0040	0.99655	1.233	0.0040	0.99486	1.124
0.0055	0.99797	1.347	0.0055	0.99673	1.240	0.0055	0.99506	1.130
0.0070	0.99816	1.356	0.0070	0.99694	1.247	0.0070	0.99528	1.136
0.0085	0.99838	1.366	0.0085	0.99717	1.254	0.0086	0.99552	1.142
Guanosine								
0.0010	0.99761	1.317	0.0010	0.99628	1.217	0.0010	0.99451	1.111
0.0025	0.99771	1.328	0.0025	0.99642	1.226	0.0025	0.99469	1.118
0.0040	0.99785	1.339	0.0040	0.99658	1.234	0.0040	0.99489	1.125
0.0055	0.99802	1.349	0.0055	0.99680	1.241	0.0055	0.99512	1.131
0.0070	0.99824	1.359	0.0070	0.99703	1.249	0.0070	0.99536	1.138
0.0085	0.99845	1.369	0.0085	0.99729	1.256	0.0086	0.99562	1.144
Uridine								
0.0010	0.99760	1.317	0.0010	0.99627	1.216	0.0010	0.99450	1.111
0.0025	0.99767	1.326	0.0025	0.99637	1.224	0.0025	0.99465	1.117
0.0040	0.99777	1.335	0.0040	0.99651	1.231	0.0040	0.99482	1.123
0.0055	0.99792	1.343	0.0055	0.99666	1.237	0.0055	0.99501	1.128
0.0070	0.99809	1.351	0.0070	0.99684	1.243	0.0070	0.99521	1.133
0.0085	0.99829	1.359	0.0085	0.99703	1.249	0.0086	0.99542	1.138
Cytidine								
0.0010	0.99759	1.317	0.0010	0.99626	1.216	0.0010	0.99449	1.111
0.0025	0.99765	1.327	0.0025	0.99635	1.224	0.0025	0.99463	1.117
0.0040	0.99774	1.336	0.0040	0.99648	1.232	0.0040	0.99479	1.123
0.0055	0.99787	1.345	0.0055	0.99663	1.239	0.0055	0.99497	1.129

0.0070	0.99805	1.354	0.0070	0.99680	1.245	0.0070	0.99516	1.135
0.0085	0.99825	1.362	0.0085	0.99699	1.252	0.0086	0.99537	1.140
w_2=0.0025 [b]								
Adinosine								
0.0010	0.99810	1.324	0.0010	0.99679	1.223	0.0010	0.99508	1.116
0.0025	0.99818	1.335	0.0025	0.99690	1.231	0.0025	0.99523	1.123
0.0040	0.99829	1.345	0.0040	0.99705	1.239	0.0040	0.99541	1.130
0.0055	0.99844	1.355	0.0055	0.99722	1.247	0.0055	0.99561	1.136
0.0070	0.99862	1.365	0.0070	0.99742	1.255	0.0070	0.99582	1.142
0.0085	0.99882	1.375	0.0085	0.99766	1.262	0.0086	0.99605	1.148
Guanosine								
0.0010	0.99811	1.324	0.0010	0.99680	1.223	0.0010	0.99509	1.116
0.0025	0.99820	1.336	0.0025	0.99692	1.232	0.0025	0.99525	1.124
0.0040	0.99833	1.347	0.0040	0.99708	1.240	0.0040	0.99545	1.130
0.0055	0.99849	1.357	0.0055	0.99728	1.248	0.0055	0.99567	1.137
0.0070	0.99869	1.368	0.0070	0.99749	1.256	0.0070	0.99590	1.144
0.0085	0.99891	1.378	0.0085	0.99775	1.264	0.0086	0.99615	1.150
Uridine								
0.0010	0.99810	1.324	0.0010	0.99679	1.222	0.0010	0.99507	1.116
0.0025	0.99816	1.334	0.0025	0.99689	1.230	0.0025	0.99521	1.122
0.0040	0.99825	1.343	0.0040	0.99702	1.238	0.0040	0.99537	1.128
0.0055	0.99839	1.352	0.0055	0.99718	1.245	0.0055	0.99555	1.134
0.0070	0.99853	1.360	0.0070	0.99735	1.251	0.0070	0.99574	1.139
0.0085	0.99874	1.369	0.0085	0.99755	1.258	0.0086	0.99593	1.145
Cytidine								
0.0010	0.99809	1.324	0.0010	0.99678	1.223	0.0010	0.99506	1.116
0.0025	0.99814	1.334	0.0025	0.99686	1.231	0.0025	0.99519	1.123
0.0040	0.99823	1.344	0.0040	0.99699	1.238	0.0040	0.99534	1.129
0.0055	0.99837	1.353	0.0055	0.99713	1.246	0.0055	0.99551	1.135
0.0070	0.99851	1.362	0.0070	0.99731	1.253	0.0070	0.99569	1.141

0.0085	0.99870	1.371	0.0085	0.99750	1.260	0.0086	0.99589	1.146
w_2=0.004 [b]								
Adinosine								
0.0010	0.99861	1.333	0.0010	0.99733	1.231	0.0010	0.99559	1.123
0.0025	0.99868	1.345	0.0025	0.99743	1.240	0.0025	0.99574	1.131
0.0040	0.99878	1.356	0.0040	0.99757	1.249	0.0040	0.99591	1.137
0.0055	0.99891	1.366	0.0055	0.99774	1.257	0.0055	0.99610	1.144
0.0070	0.99908	1.376	0.0070	0.99794	1.265	0.0070	0.99631	1.151
0.0085	0.99929	1.387	0.0085	0.99816	1.273	0.0085	0.99653	1.157
Guanosine								
0.0010	0.99862	1.334	0.0010	0.99734	1.231	0.0010	0.99560	1.123
0.0025	0.99870	1.346	0.0025	0.99745	1.241	0.0025	0.99576	1.131
0.0040	0.99882	1.357	0.0040	0.99761	1.250	0.0040	0.99595	1.138
0.0055	0.99897	1.368	0.0055	0.99779	1.258	0.0055	0.99617	1.145
0.0070	0.99916	1.379	0.0070	0.99801	1.267	0.0070	0.99640	1.152
0.0085	0.99938	1.390	0.0085	0.99824	1.275	0.0085	0.99664	1.159
Uridine								
0.0010	0.99862	1.333	0.0010	0.99733	1.231	0.0010	0.99558	1.123
0.0025	0.99868	1.343	0.0025	0.99741	1.239	0.0025	0.99572	1.130
0.0040	0.99878	1.353	0.0040	0.99753	1.246	0.0040	0.99587	1.136
0.0055	0.99891	1.362	0.0055	0.99768	1.254	0.0055	0.99605	1.142
0.0070	0.99909	1.372	0.0070	0.99784	1.261	0.0070	0.99623	1.148
0.0085	0.99927	1.381	0.0085	0.99802	1.269	0.0085	0.99642	1.154
Cytidine								
0.0010	0.99861	1.333	0.0010	0.99732	1.231	0.0010	0.99558	1.123
0.0025	0.99865	1.344	0.0025	0.99739	1.239	0.0025	0.99570	1.130
0.0040	0.99874	1.354	0.0040	0.99751	1.247	0.0040	0.99584	1.137
0.0055	0.99886	1.363	0.0055	0.99765	1.255	0.0055	0.99601	1.143
0.0070	0.99901	1.373	0.0070	0.99781	1.263	0.0070	0.99618	1.149
0.0085	0.99918	1.383	0.0085	0.99800	1.271	0.0085	0.99637	1.156

[a] Standard uncertainties in temperature (T) = 0.01 K. [b] w_1 and w_2 are the molarity of α and β-CD in aqueous mixture respectively.

Table S9. Limiting apparent molar volume (ϕ_v^o), experimental slope (S_v^*), viscosity *B* and A-coefficient of different nucleosides in deferent molarity of aqueous α and β-cyclodextrin mixtures:

Temp /K[a]	$\phi_v^o \times 10^6$	S_v^*	*B*	*A*
		w_1=0.001[b]		
		Adenosine		
298.15	223.6	-745.1	2.066	0.175
303.15	187.4	-624.6	1.716	0.171
308.15	143.1	-471.3	1.338	0.164
		Guanosine		
298.15	238.7	-769.8	2.500	0.170
303.15	202.4	-695.4	1.963	0.171
308.15	157.5	-520.7	1.613	0.163
		Uridine		
298.15	256.9	-837.0	2.904	0.165
303.15	215.4	-769.1	2.249	0.169
308.15	175.5	-634.7	1.948	0.161
		Cytidine		
298.15	267	-828.9	3.302	0.159
303.15	230.3	-790.0	2.514	0.164
308.15	184.9	-663.7	2.203	0.162
		w_1=0.0025[b]		
		Adenosine		
298.15	233.3	-776.8	2.410	0.170
303.15	198.8	-711.9	1.896	0.170
308.15	152.4	-522.4	1.477	0.166

		Guanosine		
298.15	245.1	-858.2	2.587	0.170
303.15	209.4	-753.6	2.130	0.166
308.15	163.5	-565.4	1.477	0.161
		Uridine		
298.15	259.0	-948.3	2.973	0.163
303.15	220.3	-800.1	2.333	0.165
308.15	178.1	668.2	2.002	0.159
		Cytidine		
298.15	274.0	-1034	3.365	0.159
303.15	233.9	-907.4	2.569	0.161
308.15	192.0	761.6	2.262	0.159
		w_1=0.004 [b]		
		Adenosine		
298.15	240.6	-830.2	2.824	0.168
303.15	208.2	-755.1	2.258	0.163
308.15	161.5	-587	1.865	0.155
		Guanosine		
298.15	250.9	-863	3.170	0.162
303.15	217.3	-794.6	2.647	0.153
308.15	173.8	-659.9	2.186	0.148
		Uridine		
298.15	265.9	-981.7	3.528	0.154
303.15	229.3	-879.5	2.864	0.152
308.15	186.8	-733.7	2.384	0.149
		Cytidine		
298.15	280.3	-1089	3.921	0.145
303.15	241.1	-936	3.104	0.149
308.15	201	-815.6	2.601	0.144
		w_2=0.001 [b]		

		Adenosine		
298.15	283.5	-1178	3.800	0.141
303.15	250.6	-1021	2.851	0.159
308.15	203.6	-694.2	2.586	0.143
		Guanosine		
298.15	294.4	-1234	4.205	0.132
303.15	259.2	-1084	3.108	0.154
308.15	215	-782.1	2.798	0.139
		Uridine		
298.15	261.5	-1067	3.005	0.159
303.15	224.1	-805.7	2.302	0.165
308.15	184.6	-625.1	1.993	0.155
		Cytidine		
298.15	273	-1141	3.403	0.151
303.15	238	-921.6	2.612	0.159
308.15	195.1	-682.7	2.304	0.148
		$w_2=0.0025$ [b]		
		Adenosine		
298.15	295.7	-1238	4.002	0.135
303.15	262.6	-1091	3.109	0.147
308.15	213.8	-754.2	2.706	0.140
		Guanosine		
298.15	304.2	-1267	4.402	0.126
303.15	270.7	-1115	3.306	0.143
308.15	224.5	-825.9	2.912	0.136
		Uridine		
298.15	272.6	-1109	3.348	0.149
303.15	235.5	-919.7	2.602	0.158
308.15	194.7	-657.8	2.200	0.151
		Cytidine		

298.15	282.3	-1188	3.601	0.145
303.15	250.7	-1033	2.854	0.152
308.15	202.6	-686.8	2.418	0.146
		w_2=0.004 [b]		
		Adenosine		
298.15	302.2	-1224	4.302	0.133
303.15	270.6	-1120	3.401	0.142
308.15	221.7	-795.2	2.936	0.135
		Guanosine		
298.15	314.4	-1311	4.616	0.129
303.15	278.8	-1143	3.708	0.136
308.15	231.4	-868.2	3.207	0.128
		Uridine		
298.15	275.4	-1113	3.600	0.144
303.15	248.4	-965	2.902	0.150
308.15	202.3	-703.6	2.506	0.143
		Cytidine		
298.15	284.6	-1168	3.801	0.144
303.15	260	-1069	3.111	0.147
308.15	209.3	-715.2	2.710	0.139

[a] Standard uncertainties in temperature (T) = 0.01 K. [b] w_1 and w_2 are the molarity of α and β-CD in aqueous mixture respectively.

Table S10. Experimental values of refractive index (n_D) and ultrasonic speed (u) of RNA nucleosides in different molarity of aq. aqueous α and β-cyclodextrin mixtures at 298.15 K[a]

	Adenosine		Guanosine		Uridine		Cytidine	
Conc. (m)	u/m·s^{-1}	n_D	u/m·s^{-1}	n_D	u/m·s^{-1}	n_D	u/m·s^{-1}	n_D
				w_1=0.001[b]				
0.0010	1502.2	1.3001	1505.3	1.3001	1500.1	1.3360	1504.0	1.3480

0.0025	1508.1	1.3120	1511.2	1.3010	1511.1	1.3385	1522.2	1.3493
0.0040	1515.0	1.3250	1519.0	1.3125	1518.0	1.3402	1535.2	1.3502
0.0055	1524.2	1.3355	1527.2	1.3410	1535.1	1.3420	1549.1	1.3512
0.0070	1533.1	1.3460	1536.3	1.3550	1541.3	1.3430	1567.3	1.3521
0.0085	1542.1	1.3550	1545.1	1.3590	1559.3	1.3440	1580.2	1.3530
				$w_1=0.0025$ [b]				
0.0010	1510.2	1.3075	1513.0	1.3075	1499.1	1.3420	1502.0	1.3552
0.0025	1512.2	1.3213	1515.0	1.3110	1510.1	1.3433	1518.1	1.3554
0.0040	1520.3	1.3350	1528.1	1.3300	1522.1	1.3443	1531.1	1.3555
0.0055	1528.3	1.3550	1533.1	1.3620	1565.3	1.3452	1559.2	1.3557
0.0070	1537.3	1.3600	1537.2	1.3700	1570.2	1.3460	1571.2	1.3558
0.0085	1548.2	1.3690	1540.1	1.3790	1582.0	1.3470	1585.3	1.3560
				$w_1=0.004$ [b]				
0.0010	1509.2	1.3171	1520.2	1.3171	1507.0	1.3485	1510.2	1.3640
0.0025	1518.2	1.3257	1521.3	1.3172	1518.0	1.3487	1532.2	1.3642
0.0040	1528.1	1.3390	1525.1	1.3300	1529.1	1.3489	1548.1	1.3644
0.0055	1537.1	1.3700	1531.1	1.3700	1576.1	1.3491	1559.1	1.3646
0.0070	1545.3	1.3780	1535.2	1.3855	1585.2	1.3493	1573.3	1.3648
0.0085	1555.0	1.3782	1541.3	1.3885	1594.3	1.3495	1598.2	1.3650
				$w_2=0.001$ [b]				
0.0010	1520.0	1.3513	1523.2	1.3531	1510.2	1.3278	1512.1	1.3323
0.0025	1530.0	1.3513	1532.3	1.3531	1520.1	1.3279	1519.3	1.3325
0.0040	1541.2	1.3514	1544.1	1.3532	1526.2	1.3280	1521.1	1.3327
0.0055	1552.3	1.3515	1557.4	1.3532	1530.1	1.3281	1524.0	1.3329
0.0070	1563.1	1.3516	1568.2	1.3533	1535.0	1.3282	1527.2	1.3331
0.0085	1575.1	1.3517	1582.0	1.3534	1540.0	1.3283	1530.1	1.3333
				$w_2=0.0025$ [b]				
0.0010	1524.2	1.3582	1526.1	1.3600	1523.0	1.3330	1525.2	1.3405
0.0025	1531.1	1.3590	1536.2	1.3602	1525.2	1.3334	1534.1	1.3407
0.0040	1543.1	1.3596	1547.2	1.3603	1524.1	1.3338	1535.2	1.3409

0.0055	1555.0	1.3600	1559.2	1.3605	1530.3	1.3341	1537.0	1.3411
0.0070	1566.0	1.3604	1572.3	1.3606	1532.2	1.3345	1538.0	1.3413
0.0085	1577.3	1.3608	1586.1	1.3608	1533.2	1.3348	1540.1	1.3415
				w_2=0.004 [b]				
0.0010	1528.2	1.3630	1530.2	1.3670	1527.1	1.3360	1532.2	1.3430
0.0025	1537.3	1.3640	1540.2	1.3679	1534.2	1.3361	1524.3	1.3431
0.0040	1548.3	1.3648	1551.3	1.3686	1536.1	1.3362	1535.2	1.3432
0.0055	1559.2	1.3655	1563.3	1.3691	1542.3	1.3363	1545.3	1.3433
0.0070	1570.3	1.3660	1576.2	1.3695	1545.3	1.3364	1556.2	1.3434
0.0085	1583.2	1.3665	1591.1	1.3700	1550.2	1.3365	1548.2	1.3435

[a] Standard uncertainties in temperature (T) = 0.01 K. [b] w_1 and w_2 are the molarity of α and β-CD in aqueous mixture respectively.

Table S11. Limiting molar refractions (R_M^o) and limiting molar adiabatic compressibilities (ϕ_K^o) of RNA nucleosides in different molarity of aq. α and β-cyclodextrin mixtures at 298.15 K[a]

aq. solvent	R_M^o/m^3·mol^{-1}				ϕ_K^o/ m^3·mol^{-1}·Pa^{-1}			
mixture	Adenosine	Guanosine	Uridine	Cytidine	Adenosine	Guanosine	Uridine	Cytidine
w_1=0.001[b]	45.38	45.79	50.22	51.84	1.02	1.08	1.18	1.23
w_1=0.0025[b]	45.87	46.14	51.22	53.10	1.05	1.09	1.21	1.26
w_1=0.004[b]	46.31	46.79	52.36	54.24	1.08	1.10	1.23	1.27
w_2=0.001[b]	57.83	61.58	49.62	49.99	1.26	1.31	1.16	1.20
w_2=0.0025[b]	58.66	62.60	50.20	51.09	1.308	1.34	1.18	1.22
w_2=0.004[b]	59.26	63.48	50.69	51.44	1.328	1.38	1.19	1.24

[a] Standard uncertainties in temperature (T) = 0.01 K. [b] w_1 and w_2 are the molarity of α and β-CD in aqueous mixture respectively.

Table S12 Data for the Benesi-Hildebrand double reciprocal plot performed by UV-Vis spectroscopy for aqueous uridine-α-CD system:

Temp /K[a]	[U] /μm	[α-CD] /μm	A_o	A	ΔA	1/[α-CD] /m^{-1}	1/ΔA	Intercept	Slope	Ka /m^{-1}
298.15	50	30	0.398	0.431	0.033	33333	30.3	1.221939	0.000875	1396.98
	50	40		0.441	0.043	25000	23.3			
	50	50		0.452	0.054	20000	18.5			
	50	60		0.460	0.062	16667	16.1			
	50	70		0.472	0.074	14286	13.5			
303.15	50	30	0.398	0.430	0.032	33333	31.3	1.114534	0.000917	1215.68
	50	40		0.438	0.040	25000	25.0			
	50	50		0.451	0.053	20000	18.9			
	50	60		0.458	0.060	16667	16.7			
	50	70		0.470	0.072	14286	13.9			
308.15	50	30	0.398	0.429	0.031	33333	32.3	1.000263	0.000952	1050.81
	50	40		0.437	0.039	25000	25.6			
	50	50		0.448	0.050	20000	20.0			
	50	60		0.457	0.059	16667	16.9			
	50	70		0.469	0.071	14286	14.2			

[a] Standard uncertainties in temperature (T) = 0.01 K.

Table S13 Data for the Benesi-Hildebrand double reciprocal plot performed by UV-Vis spectroscopy for aqueous cytidine-α-CD system:

Temp /K[a]	[C] /μm	[α-CD] /μm	Ao	A	ΔA	1/[α-CD] /m^{-1}	1/ΔA	Intercept	Slope	Ka /m^{-1}
298.15	50	30	0.372	0.399	0.027	33333	37.0	1.586949	0.001068	1486.60
	50	40		0.407	0.035	25000	28.6			
	50	50		0.416	0.044	20000	22.7			
	50	60		0.423	0.051	16667	19.6			
	50	70		0.432	0.060	14286	16.7			
303.15	50	30	0.372	0.398	0.026	33333	38.5	1.471382	0.001125	1307.43
	50	40		0.405	0.033	25000	30.3			

	50	50		0.413	0.041	20000	24.4				
	50	60		0.421	0.049	16667	20.3				
	50	70		0.431	0.059	14286	16.9				
	50	30		0.397	0.025	33333	40.0				
	50	40		0.403	0.031	25000	32.3				
308.15	50	50	0.372	0.410	0.038	20000	26.3	1.320772	0.001190	1109.89	
	50	60		0.420	0.048	16667	20.8				
	50	70		0.430	0.058	14286	17.2				

[a] Standard uncertainties in temperature (T) = 0.01 K.

Table S14 Data for the Benesi-Hildebrand double reciprocal plot performed by UV-Vis spectroscopy for aqueous adenosine-*β*-CD system:

Temp /K[a]	[Ad] /μm	[*β*-CD] /μm	Ao	A	ΔA	1/[*β*-CD] /m^{-1}	1/ΔA	Intercept	Slope	Ka /m^{-1}
	50	30		0.426	0.029	33333	34.5			
	50	40		0.435	0.038	25000	26.3			
298.15	50	50	0.397	0.441	0.044	20000	22.7	1.568811	0.000995	1577.33
	50	60		0.454	0.057	16667	17.5			
	50	70		0.462	0.065	14286	16.7			
	50	30		0.424	0.027	33333	37.0			
	50	40		0.432	0.035	25000	28.6			
303.15	50	50	0.397	0.438	0.041	20000	24.4	1.536412	0.001077	1427.23
	50	60		0.450	0.053	16667	18.8			
	50	70		0.458	0.061	14286	16.5			
	50	30		0.422	0.025	33333	40.0			
	50	40		0.429	0.032	25000	31.3			
308.15	50	50	0.397	0.435	0.038	20000	26.3	1.413185	0.001176	1202.20
	50	60		0.446	0.049	16667	20.4			
	50	70		0.454	0.057	14286	17.6			

[a] Standard uncertainties in temperature (T) = 0.01 K.

Table S15 Data for the Benesi-Hildebrand double reciprocal plot performed by UV-Vis spectroscopy for aqueous guanosine-*β*-CD system:

Temp /K[a]	[G] /μm	[*β*-CD] /μm	Ao	A	ΔA	1/[*β*-CD] /m^{-1}	1/ΔA	Intercept	Slope	Ka /m^{-1}
	50	30		0.451	0.019	33333	52.6			
	50	40		0.457	0.025	25000	40.0			
298.15	50	50	0.432	0.462	0.030	20000	33.3	2.557830	0.001506	1697.98
	50	60		0.467	0.035	16667	28.2			
	50	70		0.475	0.043	14286	23.3			
	50	30		0.449	0.017	33333	60.6			
	50	40		0.453	0.021	25000	47.6			
303.15	50	50	0.432	0.458	0.026	20000	38.5	2.600207	0.001765	1473.12
	50	60		0.462	0.030	16667	33.3			
	50	70		0.471	0.039	14286	25.9			
	50	30		0.446	0.014	33333	69.9			
	50	40		0.450	0.018	25000	55.6			
308.15	50	50	0.432	0.454	0.022	20000	45.5	2.664740	0.002058	1295.07
	50	60		0.459	0.027	16667	37.1			
	50	70		0.465	0.033	14286	30.2			

[a] Standard uncertainties in temperature (T) = 0.01 K.

Table S16 Data for the Benesi-Hildebrand double reciprocal plot performed by UV-Vis spectroscopy for aqueous uridine-*β*-CD system:

Temp /K[a]	[U] /μm	[*β*-CD] /μm	Ao	A	ΔA	1/[*β*-CD] /m^{-1}	1/ΔA	Intercept	Slope	Ka /m^{-1}
	50	30		0.421	0.023	33333	42.6			
	50	40		0.428	0.030	25000	33.1			
298.15	50	50	0.398	0.436	0.038	20000	26.1	1.294486	0.001248	1037.50
	50	60		0.443	0.045	16667	22.2			
	50	70		0.451	0.053	14286	18.8			
	50	30		0.419	0.021	33333	47.6			
303.15	50	40	0.398	0.427	0.029	25000	34.2	1.258348	0.001375	915.49
	50	50		0.432	0.034	20000	29.4			

	50	60		0.439	0.041	16667	24.4			
	50	70		0.446	0.048	14286	20.8			
	50	30		0.417	0.019	33333	52.6			
	50	40		0.423	0.025	25000	40.0			
308.15	50	50	0.398	0.429	0.031	20000	32.0	1.218668	0.001544	789.09
	50	60		0.435	0.037	16667	27.0			
	50	70		0.441	0.043	14286	23.2			

[a] Standard uncertainties in temperature (T) = 0.01 K.

Table S17 Data for the Benesi-Hildebrand double reciprocal plot performed by UV-Vis spectroscopy for aqueous cytidine-*β*-CD system:

Temp /K[a]	[C] /μm	[*β*-CD] /μm	Ao	A	ΔA	1/[*β*-CD] /m^{-1}	1/ΔA	Intercept	Slope	Ka /m^{-1}
	50	30		0.389	0.017	33333	60.6			
	50	40		0.394	0.022	25000	45.5			
298.15	50	50	0.372	0.399	0.027	20000	37.2	1.939517	0.001755	1104.95
	50	60		0.404	0.032	16667	31.3			
	50	70		0.409	0.037	14286	27.0			
	50	30		0.386	0.014	33333	71.5			
	50	40		0.391	0.019	25000	52.6			
303.15	50	50	0.372	0.395	0.023	20000	43.5	2.056677	0.002067	994.91
	50	60		0.399	0.027	16667	37.2			
	50	70		0.404	0.032	14286	31.4			
	50	30		0.384	0.012	33333	83.3			
	50	40		0.388	0.016	25000	62.5			
308.15	50	50	0.372	0.392	0.020	20000	50.0	2.061330	0.002426	849.61
	50	60		0.396	0.024	16667	41.7			
	50	70		0.398	0.026	14286	38.0			

[a] Standard uncertainties in temperature (T) = 0.01 K.

Table S18 Data of the van't Hoff equation for the calculation of thermodynamic parameters ΔH^o, ΔS^o and ΔG^o of different nucleoside-cyclodextrin inclusion complexes:

	Temp /K[a]	K_a /M^{-1}	1/T	lnK_a	Intercept	Slope	ΔH^o /kJ mol^{-1}	ΔS^o /J $mol^{-1}K^{-1}$	ΔG^o /kJ mol^{-1}
U + *α*-CD	298.15	1396.98	0.00335	3.14519	-0.664	1,135.94	-9.44	-5.52	-7.80
	303.15	1215.68	0.00330	3.08482					
	308.15	1050.81	0.00325	3.02152					
C + *α*-CD	298.15	1486.60	0.00335	3.17220	-0.7328	1,165.10	-9.69	-6.09	-7.87
	303.15	1307.43	0.00330	3.11642					
	308.15	1109.89	0.00325	3.04528					
A + *β*-CD	298.15	1577.33	0.00335	3.197922	-0.4256	1,081.96	-9.00	-3.54	-7.94
	303.15	1427.23	0.00330	3.154494					
	308.15	1202.20	0.00325	3.079976					
G + *β*-CD	298.15	1697.98	0.00335	3.229931	-0.3963	1,081.00	-8.99	-3.30	-8.01
	303.15	1473.12	0.00330	3.168239					
	308.15	1295.07	0.00325	3.112294					
U + *β*-CD	298.15	1037.50	0.00335	3.015987	-0.6427	1,091.4	-9.07	-5.34	-7.48
	303.15	915.49	0.00330	2.961656					
	308.15	789.09	0.00325	2.897126					
C + *β*-CD	298.15	1104.95	0.00335	3.043342	-0.465	1,047.2	-8.71	-3.87	-7.55
	303.15	994.91	0.00330	2.997784					
	308.15	849.61	0.00325	2.929221					

[a] Standard uncertainties in temperature (T) = 0.01 K.

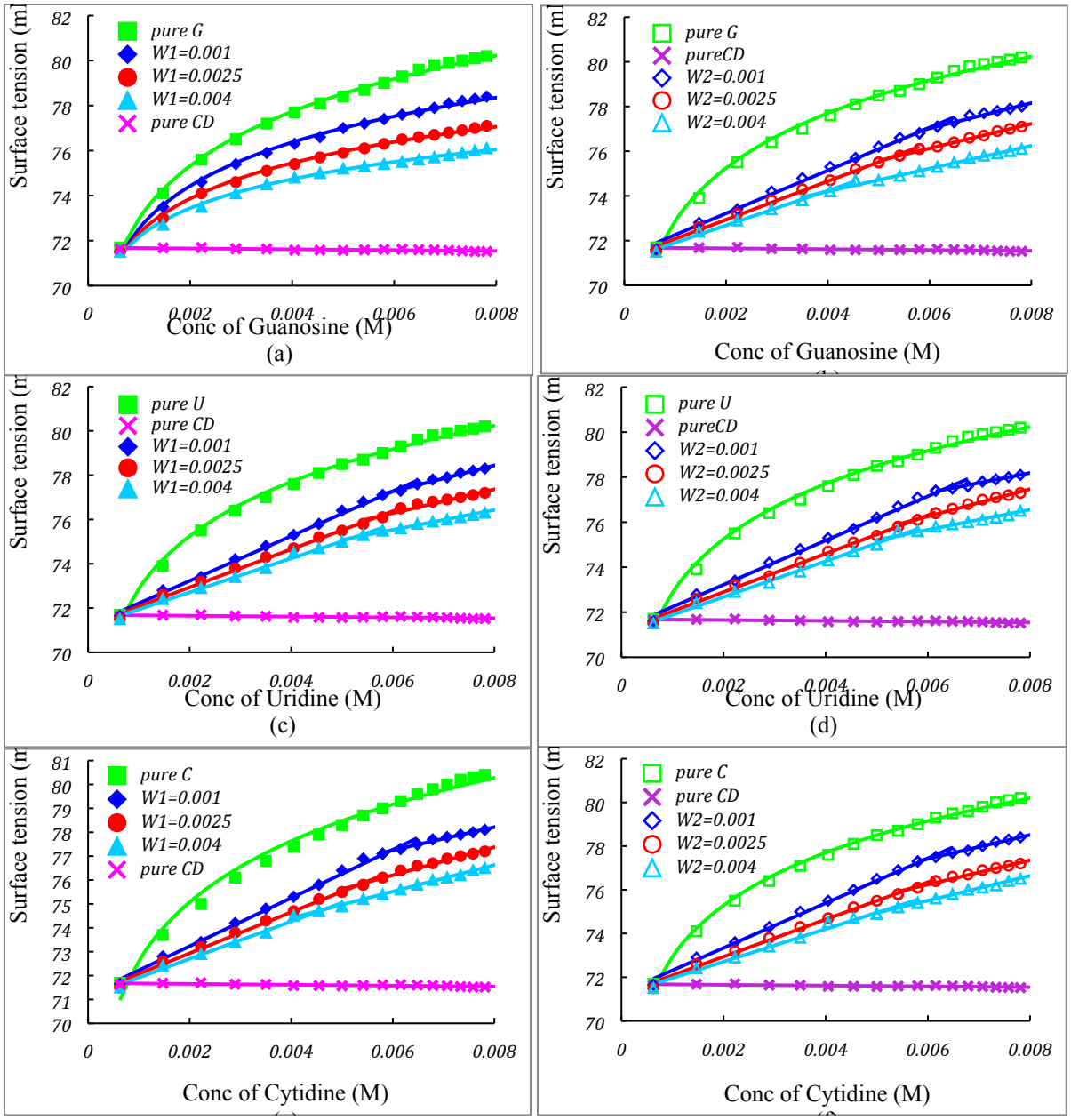


Fig. S1 Plot of surface tension with increasing concentration of nucleosides in different molarity of α-cyclodextrin (w_1) and β-cyclodextrin (w_2) respectively at 298.15 K.

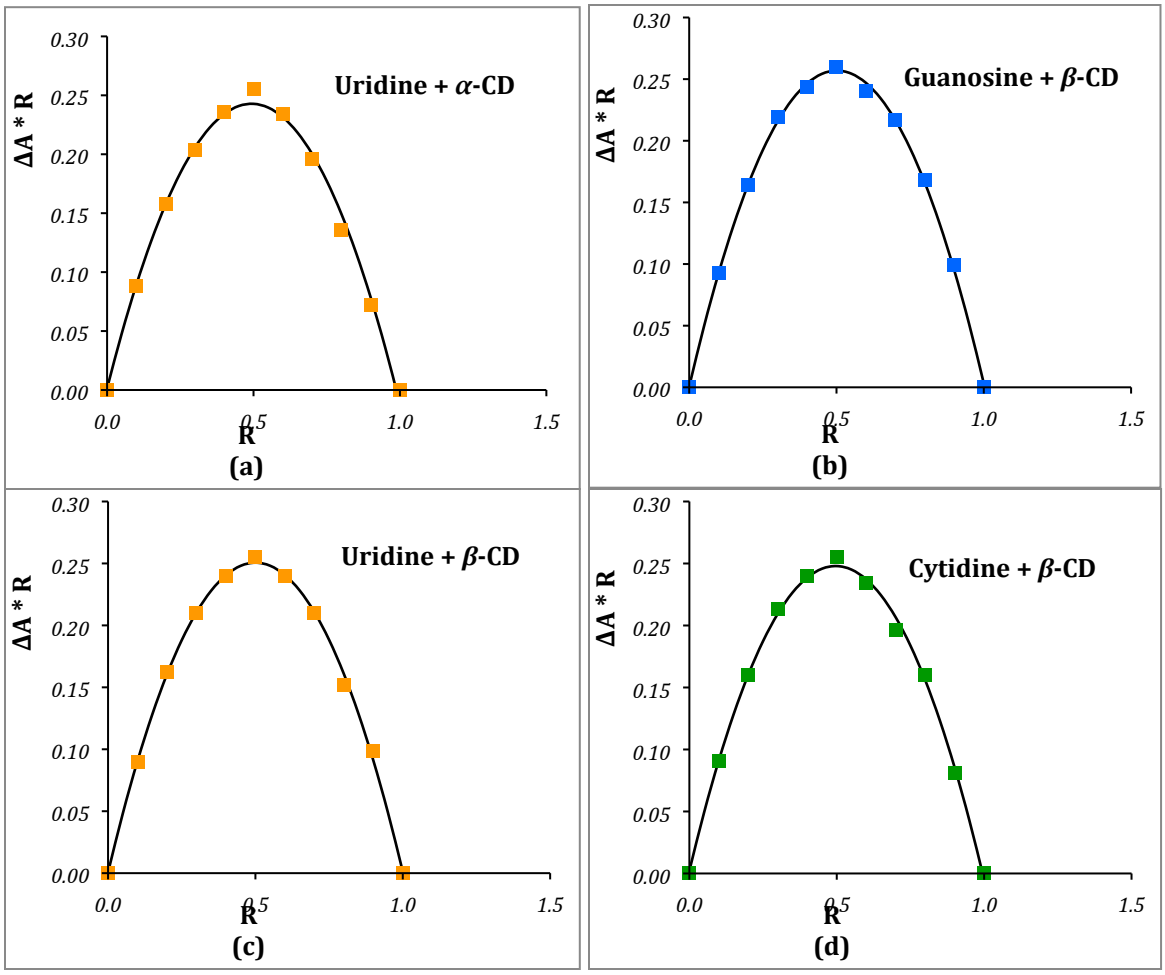


Fig. S2 Job plot of different nucleoside-cyclodextrin systems at λ_{max} (nm) = 261 for uridine, 253 for guanosine and 270 for cytidine at 298.15 K. R = [nucleoside]/([nucleoside] + [CD]), ΔA = absorbance difference of the nucleoside without and with cyclodextrin.

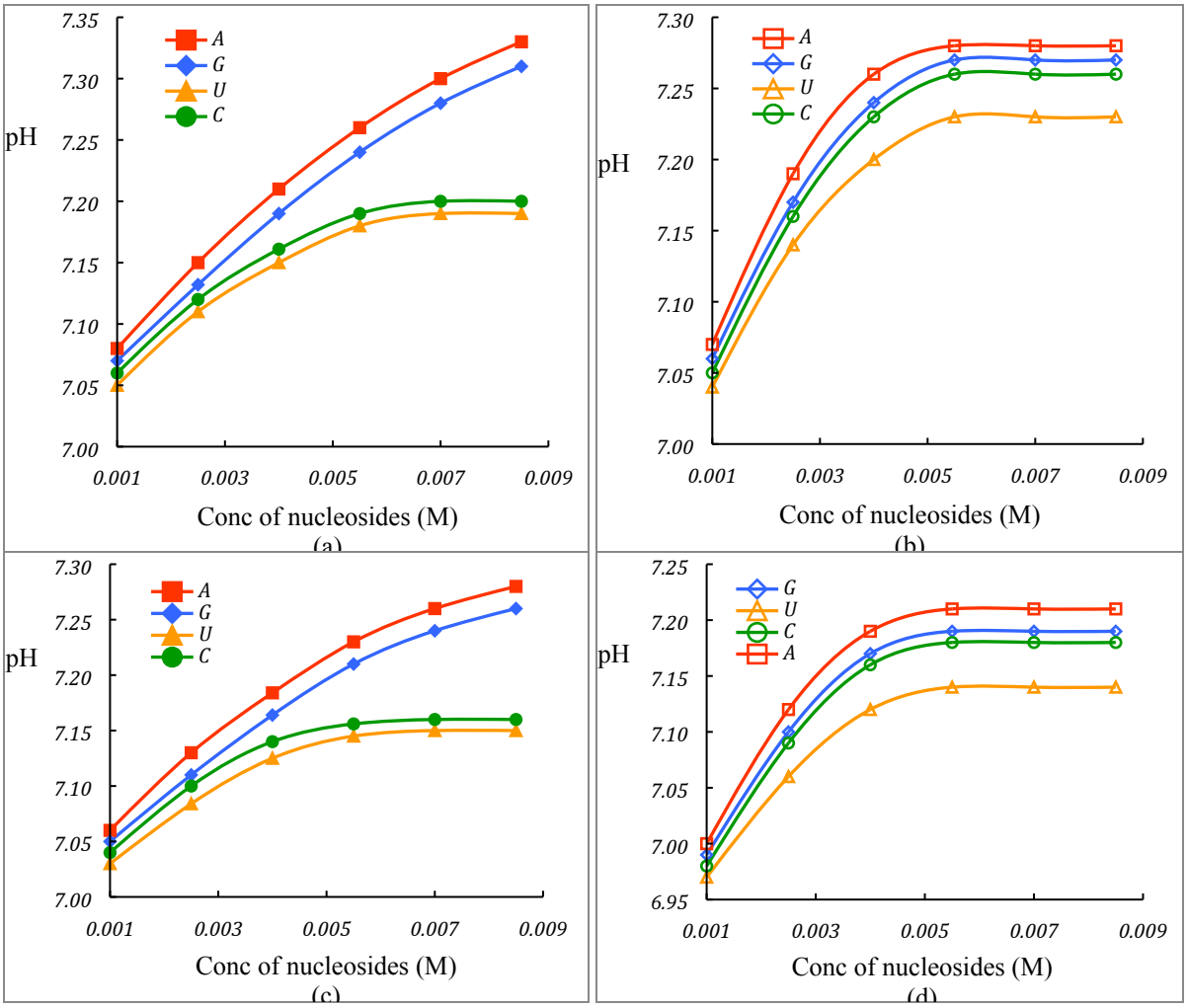


Fig. S3 Plot of pH with increasing concentration of nucleosides. (a) molarity (w_1) of α-cyclodextrine = 0.0025, (b) molarity (w_2) of β-cyclodextrine = 0.0025, (c) molarity (w_1) of α-cyclodextrine = 0.004 and (d) molarity (w_2) of β-cyclodextrine = 0.004 at 298.15 K.

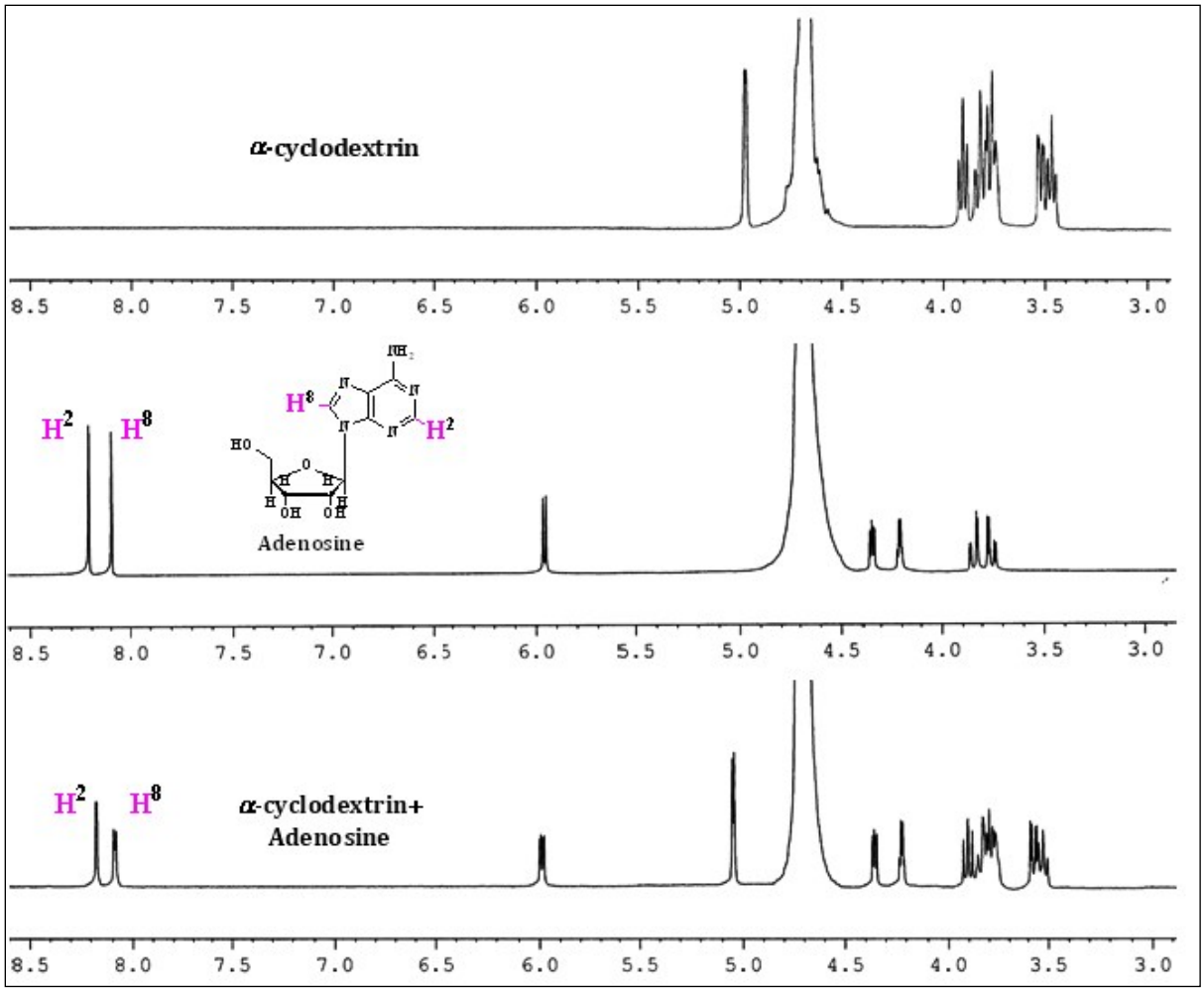


Fig. S4 ^{1}H NMR spectra of α-CD, adenosine and 1:1 molar ratio of α-CD & adenosine in D_2O at 298.15K.

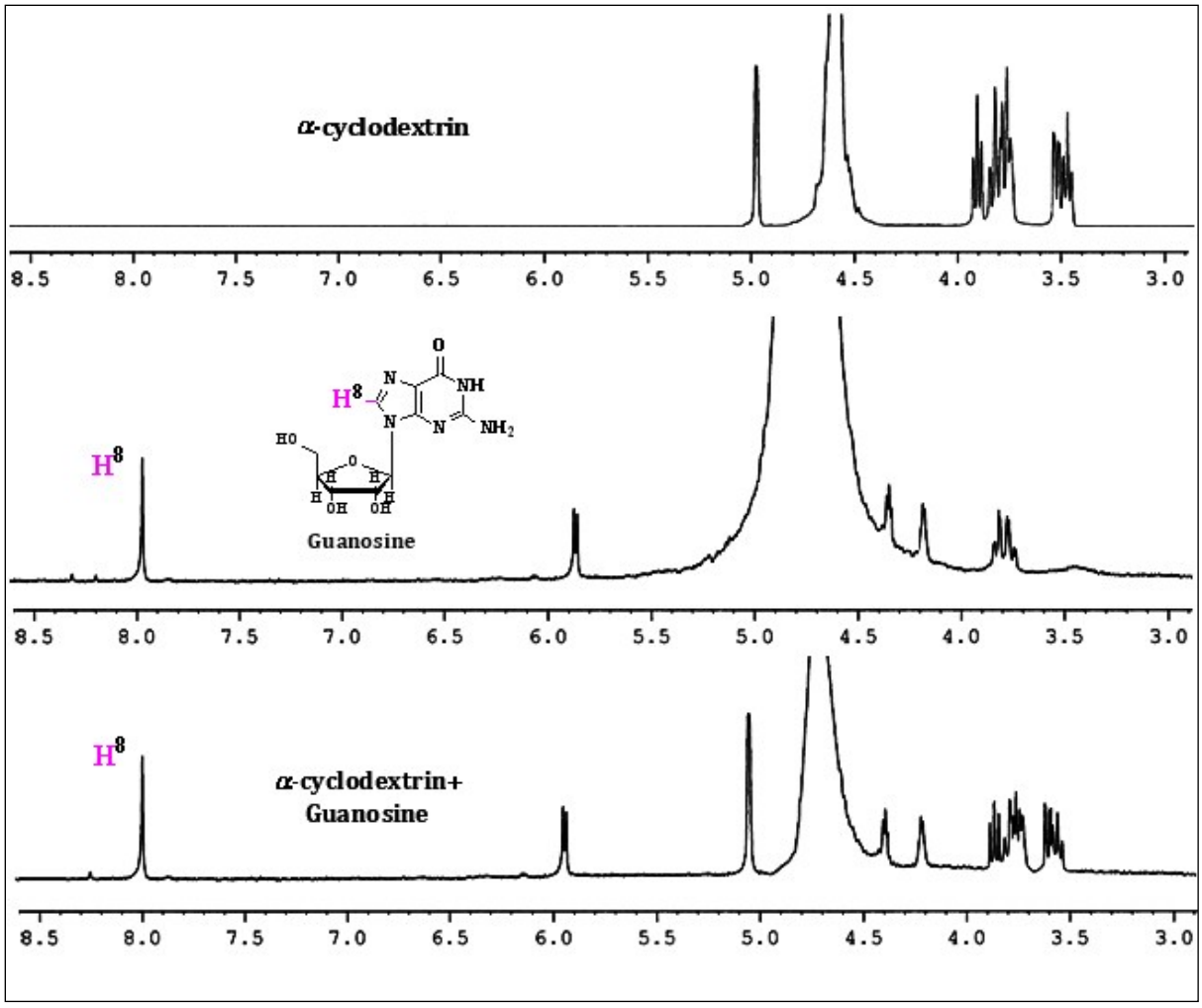


Fig. S5 ^{1}H NMR spectra of α-CD, guanosine and 1:1 molar ratio of α-CD & guanosine in D_2O at 298.15K.

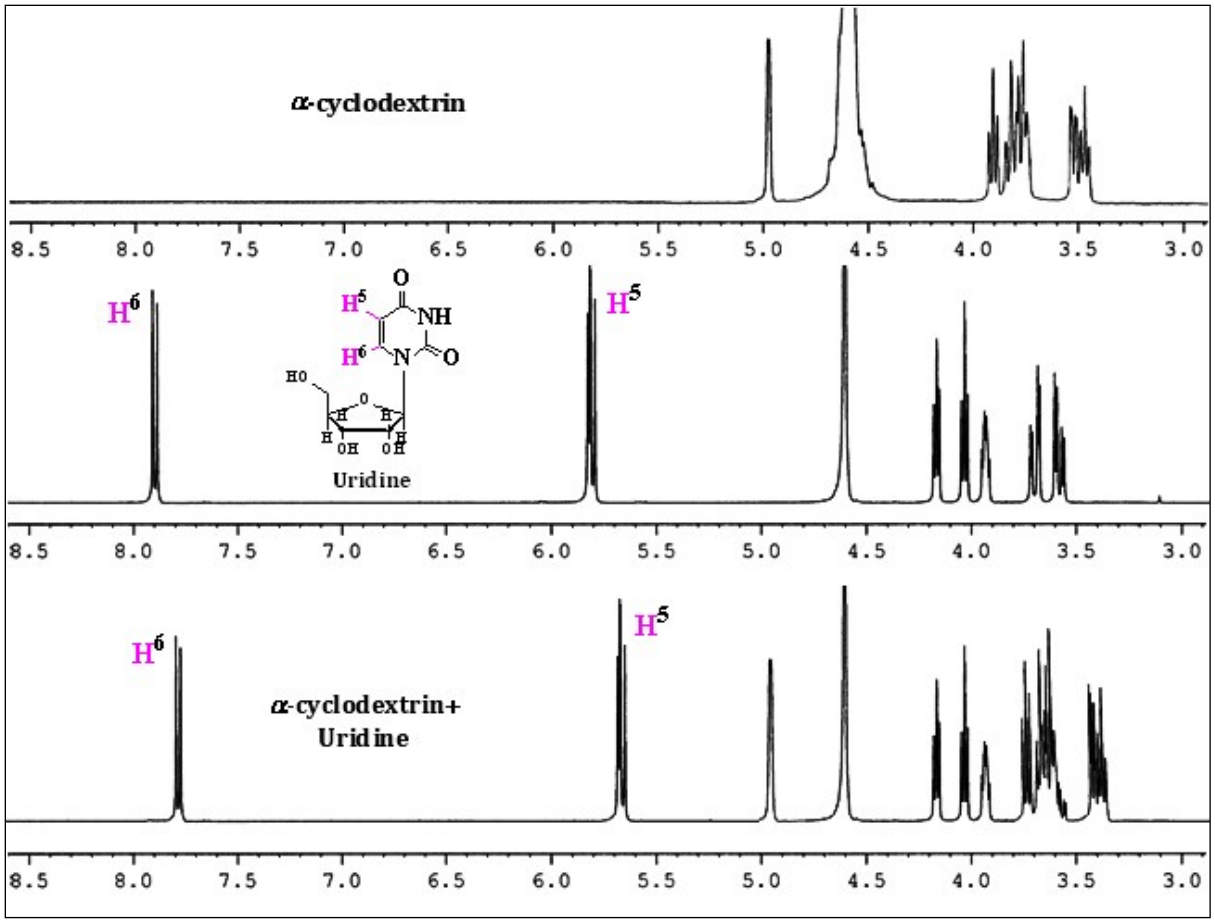


Fig. S6 ^{1}H NMR spectra of α-CD, uridine and 1:1 molar ratio of α-CD & uridine in D_2O at 298.15K.

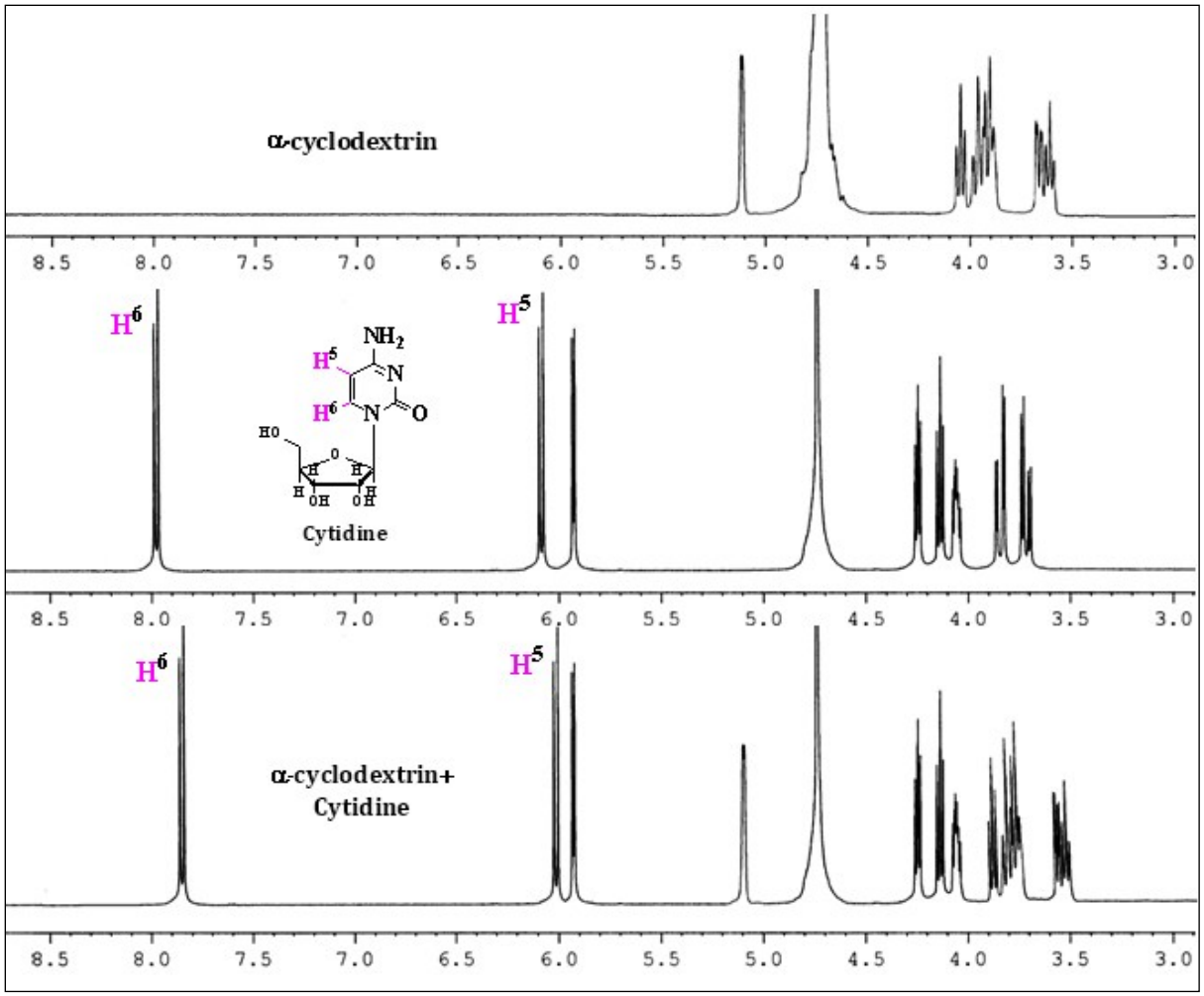


Fig. S7 ^{1}H NMR spectra of α-CD, cytidine and 1:1 molar ratio of α-CD & cytidine in D_2O at 298.15K.

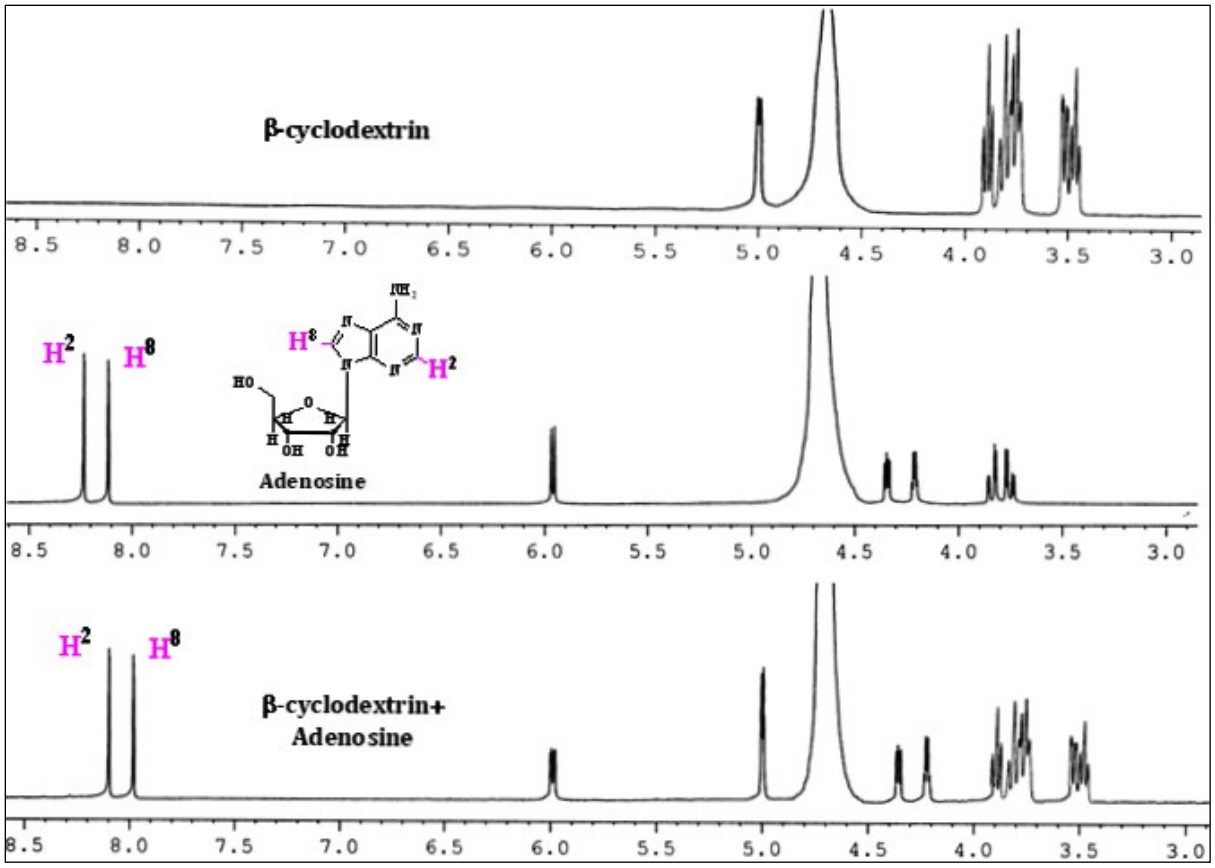


Fig. S8 ^{1}H NMR spectra of *β*-CD, adenosine and 1:1 molar ratio of *β*-CD & adenosine in D_2O at 298.15K.

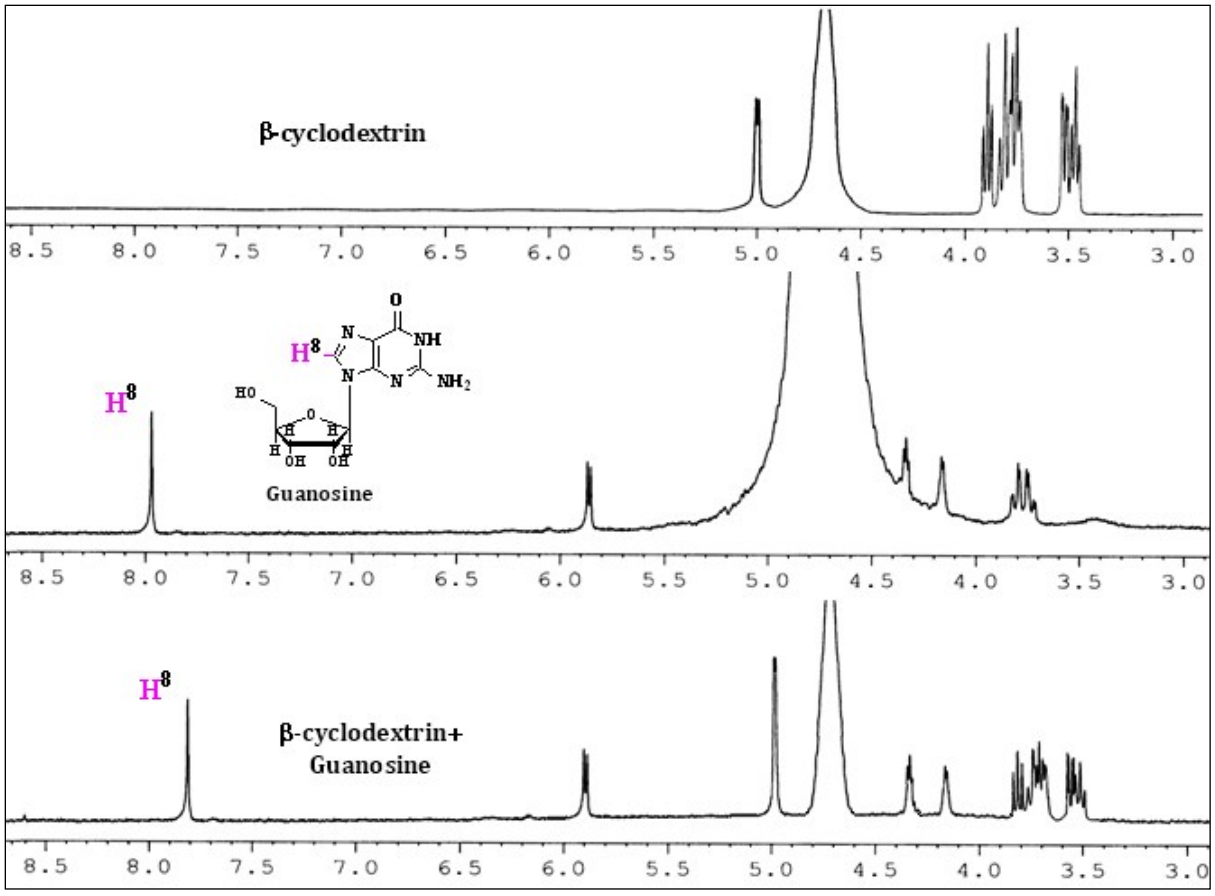


Fig. S9 ^{1}H NMR spectra of β-CD, guanosine and 1:1 molar ratio of β-CD & guanosine in D_2O at 298.15K.

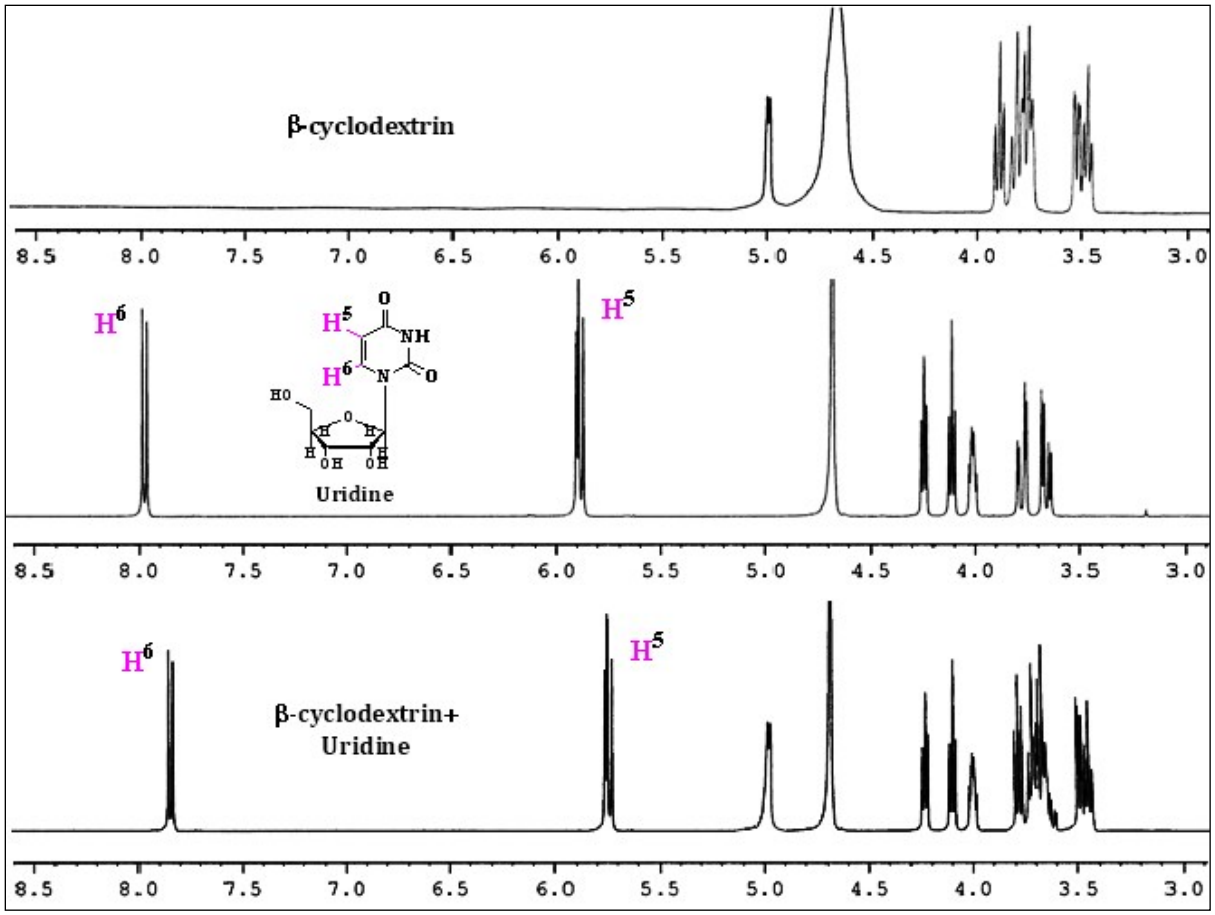


Fig. S10 ^{1}H NMR spectra of β-CD, uridine and 1:1 molar ratio of β-CD & uridine in D_2O at 298.15K.

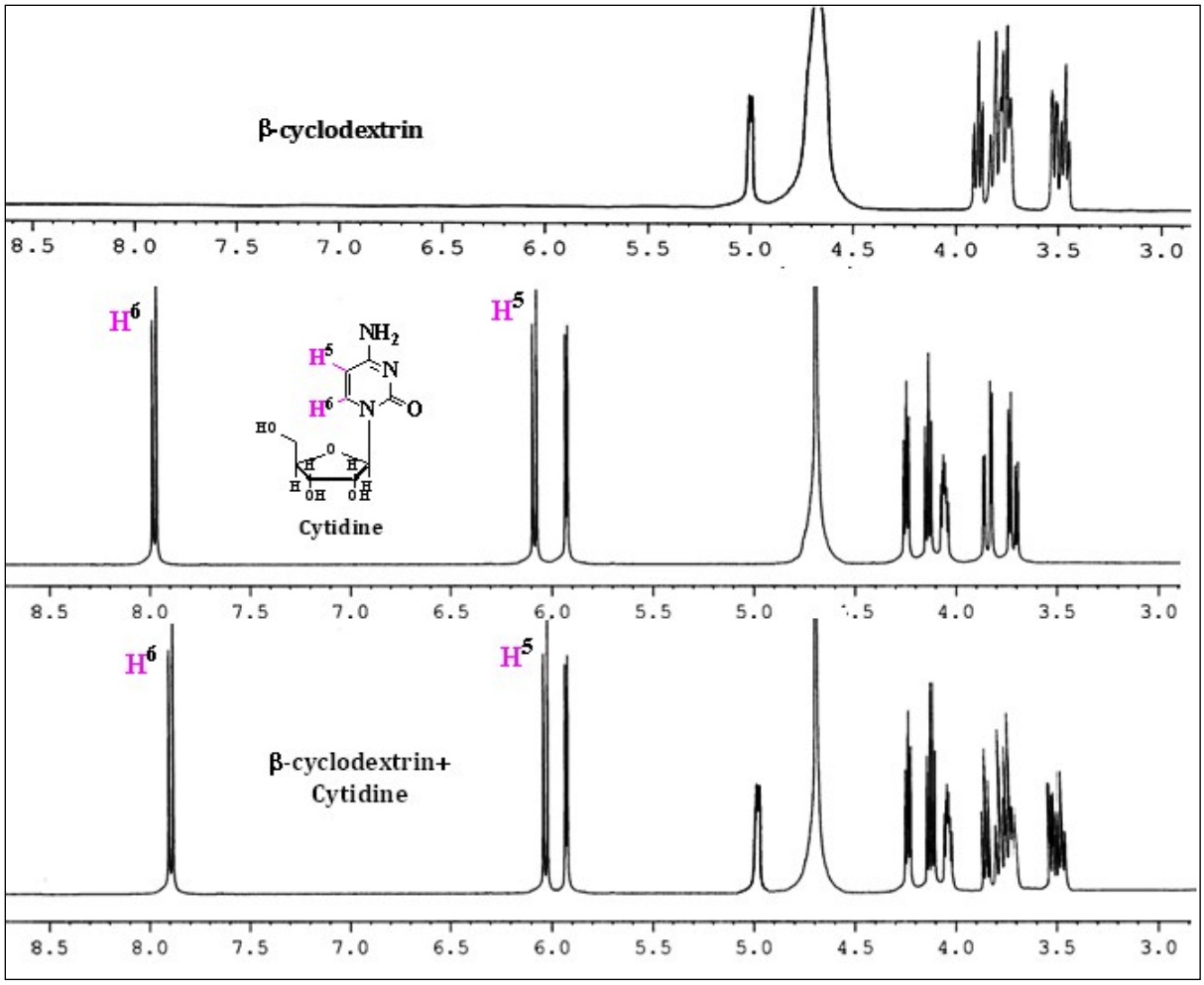
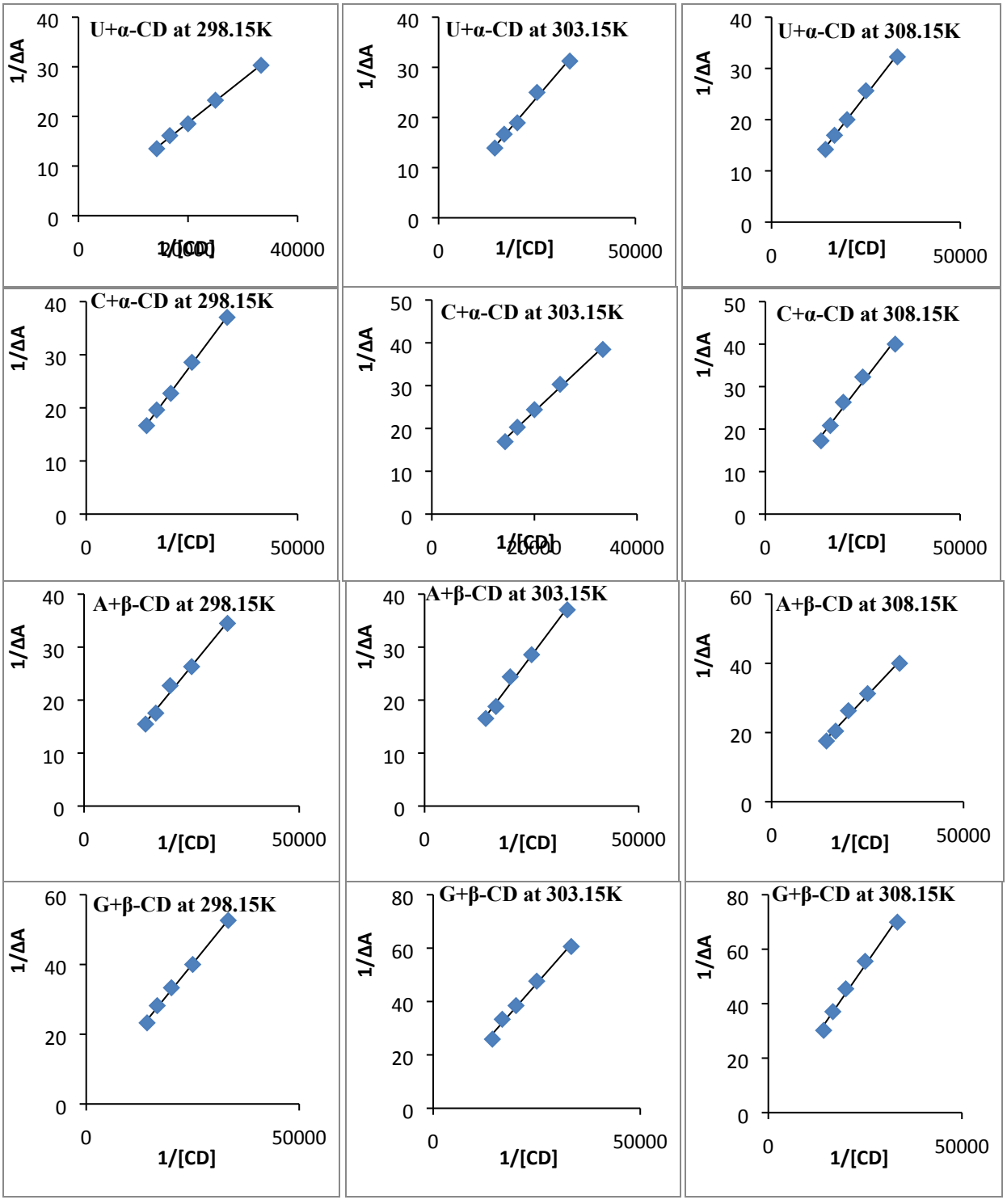


Fig. S11 ^{1}H NMR spectra of β-CD, cytidine and 1:1 molar ratio of β-CD & cytidine in D_2O at 298.15K.


U+α-CD at 298.15K
1/ΔA
1/[CD]
0
10
20
30
40
0
40000
U+α-CD at 303.15K
1/ΔA
1/[CD]
0
10
20
30
40
0
50000
U+α-CD at 308.15K
1/ΔA
1/[CD]
0
10
20
30
40
0
50000
C+α-CD at 298.15K
1/ΔA
1/[CD]
0
10
20
30
40
0
50000
C+α-CD at 303.15K
1/ΔA
1/[CD]
0
10
20
30
40
50
0
40000
C+α-CD at 308.15K
1/ΔA
1/[CD]
0
10
20
30
40
50
0
50000
A+β-CD at 298.15K
1/ΔA
1/[CD]
0
10
20
30
40
0
50000
A+β-CD at 303.15K
1/ΔA
1/[CD]
0
10
20
30
40
0
50000
A+β-CD at 308.15K
1/ΔA
1/[CD]
0
20
40
60
0
50000
G+β-CD at 298.15K
1/ΔA
1/[CD]
0
20
40
60
0
50000
G+β-CD at 303.15K
1/ΔA
1/[CD]
0
20
40
60
80
0
50000
G+β-CD at 308.15K
1/ΔA
1/[CD]
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20
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60
80
0
50000

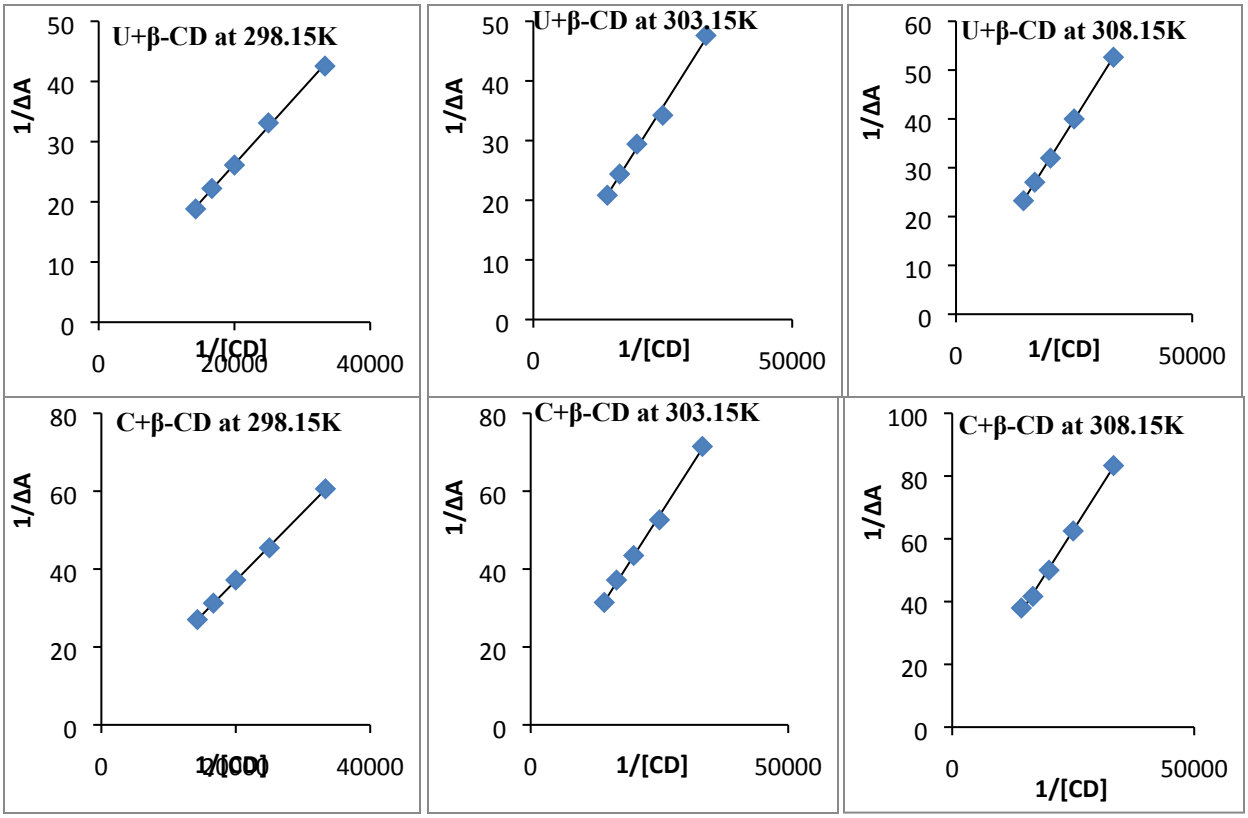

Fig S12 Benesi-Hildebrand double reciprocal plot for the effect of α and β-CD on the absorbance of uridine (261 nm), cytidine (270 nm), adenosine (259 nm) and guanosine (253 nm) at different temperatures.

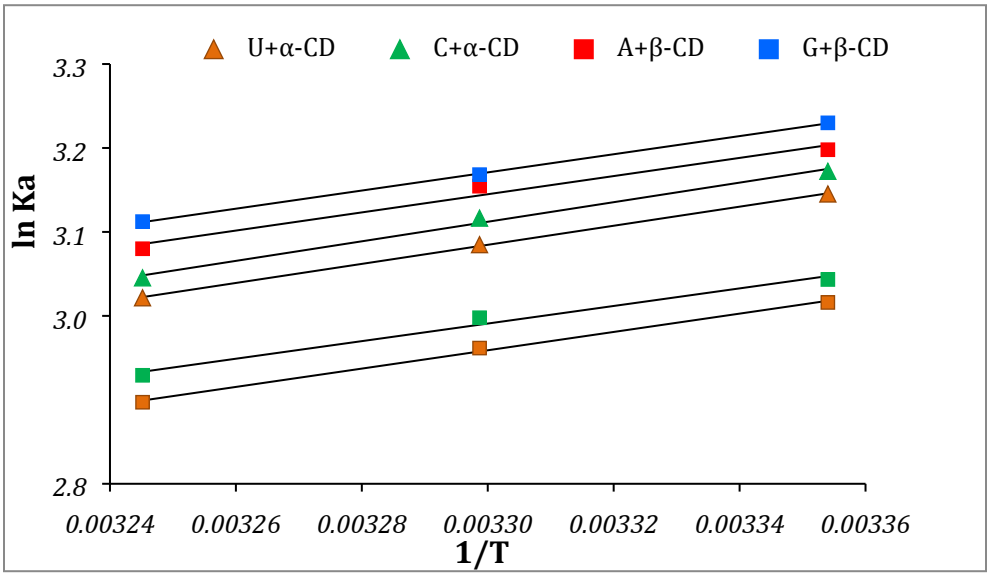

Fig. S13 The linear relationship of $\ln K_a$ vs. 1/T for the interaction of various nucleosides with α and β-CD.