

## Supporting Information

### **Theory:**

The physical properties of binary mixtures in different mass fractions ( $w_n=0.001, 0.003, 0.005$ , where  $n=1, 2$  for  $\alpha$ - and  $\beta$ -CD respectively) of aqueous  $\alpha$ - and  $\beta$ -CD solutions at 298.15K has been reported in Table S1. The experimental measured values of density, viscosity, refractive index of chosen three  $\alpha$ -amino acids (i.e., L-Lys, L-Phe, L-Glu) in different mass fractions of aqueous  $\alpha$ - and  $\beta$ -CD mixture, as a function of concentration (molarity) has been listed in Table S2.

### **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 lysine in  $w_1=0.001$  mass fraction of  $\alpha$ -cyclodextrin

$$\gamma = -307.8 c + 74.06$$

$$\gamma = -134.0 c + 67.72$$

$\gamma = 62.84$  and  $c = 0.0364$ .

### **Apparent molar volume**

The apparent molar volumes  $\phi_V$  were determined from the solutions densities using the equation and given in Table S3.

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

where  $M$  is the molar mass of the amino acids,  $m$  is the molality of the solution,  $\rho$  and  $\rho_o$  are the density of the solution and aq.  $\alpha$ - and  $\beta$ -CD mixture respectively.

The limiting apparent molar volumes  $\phi_V^0$  were obtained by a least-square treatment to the plots of  $\phi_V$  versus  $\sqrt{m}$  using the Masson equation<sup>1</sup> and shown in Table S4.

$$\phi_V = \phi_V^0 + S_V^* \cdot \sqrt{m} \quad (2)$$

The standard deviations ( $\sigma$ ) were determined using the following equation:

$$\sigma = \sqrt{\sum (Y_{\text{exp}} - Y_{\text{obs}})^2 / (N - 1)} \quad (3)$$

where  $N$  is the number of data points.

### **Contributions of the zwitterionic end group, CH<sub>2</sub> groups and other alkyl chains of the amino acids to $\phi_V^0$**

The  $\phi_V^0$  value of zwitterionic end group and methylene group, and other alkyl chain of the amino acids were estimated from

$$\phi_V^0 = \phi_V^0(\text{NH}_3^+, \text{COO}^-) + n_c \phi_V^0(\text{CH}_2) \quad (4)$$

$$\phi_V^0(R) = \phi_V^0 - \phi_V^0(\text{NH}_3^+, \text{COO}^-) - \phi_V^0(\text{CH}) \quad (5)$$

$$\phi_V^0(R) = \phi_V^0 - \phi_V^0(\text{NH}_3^+, \text{COO}^-) - \phi_V^0(\text{CH}) - \phi_V^0(\text{CH}_2) \quad (6)$$

### **Hydration Number estimated from apparent molar volume**

The number of water molecules ( $n_H$ ) hydrated to amino acids can be estimated from the value of measured standard partial molar volume. The values of  $\phi_V^0$  of studied amino acids can be expressed as<sup>2</sup>

$$\phi_V^0(\text{amino acid}) = \phi_V^0(\text{int}) + \phi_V^0(\text{elect}) \quad (7)$$

here  $\phi_V^0(\text{int})$  is intrinsic partial molar volumes of amino acids and  $\phi_V^0(\text{elect})$  is electrostriction partial molar volume as a result of hydration of amino acids. The  $\phi_V^0(\text{int})$  consists of two terms: van der Waals volume and volume due to packing effects. The values of  $\phi_V^0(\text{int})$  for the amino acids were calculated from their crystal molar volume by<sup>2</sup> using the following relationship,

$$\phi_V^0(\text{int}) = (0.7 / 0.634) \phi_V^0(\text{cryst}) \quad (8)$$

where, 0.7 is the packing density in an organic crystal and 0.634 is the packing density of randomly packed spheres. The molar volume of crystals  $\phi_V^0(\text{cryst})$  was calculated using the crystal densities of the amino acids represented by Berlin and Pallansch.<sup>3</sup> The hydration numbers is estimated using the relation

$$n_H = \phi_V^0(\text{elect}) / (V_e^0 - V_b^0) \quad (9)$$

where  $V_e^0$  is the molar volume of the electrostricted water and  $V_b^0$  is the molar volume of bulk water. This model implies that for every water molecules taken from the bulk phase to the surroundings of amino acid, the volume is decreased by  $(V_e^0 - V_b^0)$ . The value of  $(V_e^0 - V_b^0)$  is calculated<sup>2</sup> to be -3.0 or -3.3, at 298.15K respectively. The obtained  $n_H$  values are listed in Table S6.

## Viscosity

The experimental viscosity data for the studied systems are listed in Table S2. The relative viscosity ( $\eta_r$ ) has been analyzed using the Jones-Dole equation<sup>4</sup>

$$(\eta/\eta_0 - 1)/\sqrt{m} = (\eta_r - 1)/\sqrt{m} = A + B\sqrt{m} \quad (10)$$

where  $\eta_r = \eta/\eta_0$ ,  $\eta$  and  $\eta_0$  are the relative viscosities, the viscosities of the ternary solutions (amino acid + aq.  $\beta$ -CD) and binary aqueous mixture (aq.  $\beta$ -CD) and  $m$  is the molality of the amino acids 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 S4.

The  $B$ -coefficients of zwitterionic group  $B(\text{NH}_3^+, \text{COO}^-)$ , the methylene group  $B(\text{CH}_2)$ , and other alkyl group have been resolved as follows

$$B = B(\text{NH}_3^+, \text{COO}^-) + n_c B(\text{CH}_2) \quad (11)$$

$$B(R) = B(\text{NH}_3^+, \text{COO}^-) - B(\text{CH}) \quad (12)$$

$$B(R) = B(\text{NH}_3^+, \text{COO}^-) + B(\text{CH}) - B(\text{CH}_2) \quad (13)$$

## Refractive index

The molar refraction,  $R_M$  can be evaluated from the Lorentz-Lorenz relation<sup>5</sup>

$$R_M = \left\{ \frac{(n_D^2 - 1)}{(n_D^2 + 2)} \right\} (M/\rho) \quad (14)$$

where  $R_M$ ,  $n_D$ ,  $M$  and  $\rho$  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,<sup>6</sup>

$$R_M = R_M^0 + R_S \sqrt{m} \quad (15)$$

## References:

1. D. O. Masson, *Phil Mag.*, 1929, **8**, 218–226.
2. F. J. Millero, A. L. Surdo and C. Shin, *J. Phys. Chem.*, 1978, **82**, 784-792.
3. E. Berlin and M. J. Pallansch, *J. Phys. Chem.*, 1968, **72**, 1887-1889.
4. G. Jones and D. Dole, *J. Am. Chem. Soc.*, 1929, **51**, 2950-2964.
5. V. Minkin, O. Osipov and Y. Zhdanov, *Dipole Moments in Organic Chemistry*. New York, Plenum Press, 1970.
6. M. N. Roy, P. Chakraborti and D. Ekka, *Mol. Phys.*, 2014, In Press, <http://dx.doi.org/10.1080/00268976.2013.880002>.

**Tables:**

**Table S1: Experimental values of density( $\rho$ ), viscosity ( $\eta$ ), refractive index ( $n_D$ ), surface tension ( $\gamma$ ), pH in deferent mass fraction of aqueous  $\alpha$ - and  $\beta$ -cyclodextrin mixtures at 298.15 K<sup>a</sup>**

Aq. solvent mixture	$\rho \times 10^{-3}$ /kg·m <sup>-3</sup>	$\eta$ /mP·s	$n_D$	$\gamma$ /mN·m <sup>-1</sup>	pH
aq. $\alpha$ -CD					
$w_1 = 0.001$	0.99732	1.300	1.3328	71.62	6.44
$w_1 = 0.003$	0.99792	1.310	1.3331	71.49	6.39
$w_1 = 0.005$	0.99859	1.321	1.3334	71.45	6.32
aq. $\beta$ -CD					
$w_2 = 0.001$	0.99747	1.304	1.3329	71.71	6.65
$w_2 = 0.003$	0.99815	1.313	1.3332	71.61	6.10
$w_2 = 0.005$	0.99890	1.323	1.3336	71.57	5.57

<sup>a</sup> Standard uncertainties  $u$  are:  $u(\rho) = 5 \times 10^{-5}$  g·cm<sup>-3</sup>,  $u(\eta) = 0.003$  mP·s,  $u(n_D) = 0.0002$ ,  $u(\gamma) = 0.03$  mN·m<sup>-1</sup>,  $u(\text{pH}) = 0.01$ , and  $u(T) = 0.01$ K

**Table S2: Experimental values of density ( $\rho$ ), viscosity ( $\eta$ ), refractive index ( $n_D$ ), and pH of selected amino acids in deferent mass fraction of aqueous  $\alpha$ - and  $\beta$ -cyclodextrin mixtures at 298.15 K<sup>a</sup>**

molality /mol·kg <sup>-1</sup>	$\rho \times 10^{-3}$ /kg·m <sup>-3</sup>	$\eta$ /mP·s	$n_D$	pH	molality /mol·kg <sup>-1</sup>	$\rho \times 10^{-3}$ /kg·m <sup>-3</sup>	$\eta$ /mP·s	$n_D$	pH
Glycine					L-Lysine				
$w_1 = 0.001^b$					$w_1 = 0.001^b$				
0.0100	0.99766	1.309	-	-	0.0100	0.99773	1.338	1.3330	9.76
0.0251	0.99819	1.316	-	-	0.0251	0.99841	1.363	1.3334	9.81
0.0402	0.99873	1.322	-	-	0.0403	0.99913	1.384	1.3337	9.89
0.0553	0.99928	1.327	-	-	0.0555	0.99989	1.403	1.3341	9.94
0.0704	0.99984	1.332	-	-	0.0707	1.00068	1.421	1.3345	9.97
0.0855	1.00040	1.336	-	-	0.0859	1.00148	1.437	1.3350	9.99
$w_1 = 0.003^b$					$w_1 = 0.003^b$				
0.0100	0.99826	1.322	-	-	0.0100	0.99828	1.349	1.3333	9.79
0.0251	0.99879	1.331	-	-	0.0251	0.99889	1.377	1.3337	9.84

0.0401	0.99934	1.338	-	-	0.0403	0.99956	1.400	1.3340	9.92
0.0552	0.99990	1.345	-	-	0.0554	1.00027	1.422	1.3344	9.98
0.0703	1.00047	1.350	-	-	0.0707	1.00101	1.442	1.3347	10.01
0.0855	1.00105	1.355	-	-	0.0859	1.00180	1.460	1.3351	10.05
	$w_1 = 0.005^b$					$w_1 = 0.005^b$			
0.0100	0.99893	1.337	-	-	0.0100	0.99890	1.362	1.3336	9.82
0.0251	0.99947	1.348	-	-	0.0251	0.99945	1.393	1.3339	9.89
0.0401	1.00003	1.357	-	-	0.0402	1.00007	1.419	1.3342	9.96
0.0552	1.00060	1.364	-	-	0.0554	1.00074	1.443	1.3345	10.01
0.0703	1.00119	1.372	-	-	0.0706	1.00147	1.466	1.3348	10.07
0.0854	1.00179	1.378	-	-	0.0859	1.00222	1.487	1.3352	10.12
	L-Phenylalanine					L-Glutamic acid			
	$w_1 = 0.001^b$					$w_1 = 0.001^b$			
0.0100	0.99777	1.347	1.3330	6.26	0.0100	0.99795	1.328	1.3330	3.35
0.0251	0.99847	1.381	1.3335	6.12	0.0251	0.99898	1.346	1.3334	3.28
0.0403	0.99919	1.409	1.3339	6.01	0.0402	1.00007	1.361	1.3337	3.24
0.0555	0.99992	1.435	1.3343	5.91	0.0554	1.00121	1.375	1.3341	3.23
0.0708	1.00066	1.459	1.3347	5.82	0.0706	1.00239	1.388	1.3345	3.22
0.0861	1.00142	1.482	1.3351	5.74	0.0858	1.00362	1.400	1.3349	3.21
	$w_1 = 0.003^b$					$w_1 = 0.003^b$			
0.0100	0.99831	1.358	1.3333	6.21	0.0100	0.99850	1.339	1.3334	3.34
0.0251	0.99894	1.395	1.3337	6.08	0.0251	0.99946	1.359	1.3337	3.28
0.0403	0.99961	1.426	1.3341	5.95	0.0402	1.00051	1.376	1.3340	3.25
0.0555	1.00031	1.454	1.3344	5.84	0.0554	1.00162	1.392	1.3343	3.23
0.0707	1.00103	1.481	1.3348	5.76	0.0705	1.00277	1.406	1.3346	3.22
0.0861	1.00178	1.506	1.3352	5.70	0.0857	1.00398	1.419	1.3349	3.21
	$w_1 = 0.005^b$					$w_1 = 0.005^b$			
0.0100	0.99891	1.372	1.3337	6.10	0.0100	0.99912	1.351	1.3336	3.32
0.0251	0.99947	1.412	1.3341	5.95	0.0251	1.00002	1.373	1.3339	3.27
0.0403	1.00008	1.447	1.3345	5.83	0.0402	1.00102	1.392	1.3342	3.25
0.0555	1.00074	1.479	1.3348	5.73	0.0553	1.00207	1.409	1.3345	3.23
0.0707	1.00146	1.509	1.3351	5.68	0.0705	1.00319	1.425	1.3348	3.22
0.0860	1.00219	1.538	1.3354	5.64	0.0857	1.00438	1.441	1.3351	3.21
	Glycine					L-Lysine			

	$w_2 = 0.001^b$					$w_2 = 0.001^b$			
0.0100	0.99781	1.315	-	-	0.0100	0.99786	1.322	1.3331	9.81
0.0251	0.99834	1.323	-	-	0.0251	0.99851	1.338	1.3334	9.88
0.0402	0.99889	1.330	-	-	0.0403	0.99920	1.352	1.3338	9.93
0.0553	0.99944	1.336	-	-	0.0555	0.99992	1.364	1.3342	9.97
0.0704	1.00001	1.341	-	-	0.0707	1.00067	1.375	1.3346	9.99
0.0855	1.00058	1.346	-	-	0.0859	1.00143	1.386	1.3350	10.01
	$w_2 = 0.003^b$					$w_2 = 0.003^b$			
0.0100	0.99849	1.328	-	-	0.0100	0.99848	1.319	1.3334	9.84
0.0251	0.99902	1.338	-	-	0.0251	0.99906	1.334	1.3337	9.91
0.0401	0.99957	1.347	-	-	0.0402	0.99970	1.351	1.3341	9.95
0.0552	1.00014	1.354	-	-	0.0554	1.00039	1.368	1.3345	9.99
0.0703	1.00072	1.360	-	-	0.0706	1.00111	1.385	1.3349	10.02
0.0854	1.00131	1.367	-	-	0.0859	1.00186	1.403	1.3353	10.04
	$w_2 = 0.005^b$					$w_2 = 0.005^b$			
0.0100	0.99924	1.340	-	-	0.0100	0.99918	1.327	1.3339	9.87
0.0251	0.99978	1.352	-	-	0.0251	0.99969	1.348	1.3342	9.94
0.0401	1.00034	1.361	-	-	0.0402	1.00028	1.372	1.3345	9.99
0.0552	1.00092	1.369	-	-	0.0554	1.00093	1.396	1.3349	10.02
0.0703	1.00152	1.376	-	-	0.0706	1.00163	1.424	1.3352	10.05
0.0854	1.00213	1.384	-	-	0.0859	1.00238	1.453	1.3356	10.08
	L-Phenylalanine					L-Glutamic acid			
	$w_2 = 0.001^b$					$w_2 = 0.001^b$			
0.0100	0.99788	1.318	1.3326	6.36	0.0100	0.99808	1.323	1.3332	3.40
0.0251	0.99854	1.333	1.3330	6.18	0.0251	0.99908	1.339	1.3336	3.32
0.0403	0.99924	1.345	1.3333	6.02	0.0402	1.00016	1.352	1.3339	3.26
0.0555	0.99996	1.357	1.3335	5.88	0.0554	1.00129	1.364	1.3343	3.23
0.0708	1.00070	1.368	1.3338	5.76	0.0706	1.00248	1.375	1.3346	3.21
0.0861	1.00146	1.379	1.3341	5.67	0.0858	1.00371	1.386	1.3349	3.20
	$w_2 = 0.003^b$					$w_2 = 0.003^b$			
0.0100	0.99849	1.321	1.3334	6.01	0.0100	0.99870	1.325	1.3335	3.32
0.0251	0.99907	1.339	1.3338	5.90	0.0251	0.99963	1.343	1.3338	3.25
0.0403	0.99969	1.358	1.3342	5.82	0.0402	1.00064	1.360	1.3341	3.21
0.0555	1.00036	1.378	1.3347	5.73	0.0554	1.00173	1.376	1.3344	3.20

0.0707	1.00106	1.398	1.3352	5.65	0.0705	1.00286	1.393	1.3347	3.18
0.0861	1.00178	1.420	1.3357	5.61	0.0857	1.00407	1.410	1.3350	3.17
	$w_2 = 0.005^b$					$w_2 = 0.005^b$			
0.0100	0.99916	1.328	1.3338	5.49	0.0100	0.99939	1.329	1.3338	3.30
0.0251	0.99965	1.355	1.3342	5.40	0.0251	1.00024	1.349	1.3341	3.24
0.0403	1.00020	1.384	1.3346	5.31	0.0402	1.00119	1.370	1.3344	3.21
0.0555	1.00083	1.413	1.3350	5.23	0.0553	1.00223	1.392	1.3347	3.19
0.0707	1.00149	1.443	1.3354	5.15	0.0705	1.00337	1.415	1.3350	3.18
0.0860	1.00222	1.474	1.3359	5.10	0.0857	1.00454	1.439	1.3352	3.16

<sup>a</sup> Standard uncertainties  $u$  are:  $u(\rho) = 5 \times 10^{-5} \text{ kg}\cdot\text{m}^{-3}$ ,  $u(\eta) = 0.003 \text{ mP}\cdot\text{s}$ ,  $u(n_D) = 0.0002$ ,  $u(\text{pH}) = 0.01$ , and  $u(T) = 0.01\text{K}$

<sup>b</sup>  $w_1$  and  $w_2$  are mass fractions of  $\alpha$ - and  $\beta$ -cyclodextrin in aqueous mixture respectively

**Table S3: Apparent molar volume ( $\phi_V$ ),  $(\eta_r - 1)/\sqrt{m}$ , and molar refraction ( $R_M$ ) of selected amino acids in different mass fraction of aqueous  $\alpha$ - and  $\beta$ -cyclodextrin mixtures at 298.15 K<sup>a</sup>**

Aq. solvent mixture	$\phi_V \times 10^{-6}$ /m <sup>3</sup> mol <sup>-1</sup>	$(\eta_r - 1)/\sqrt{m}$ /kg <sup>1/2</sup> mol <sup>-1/2</sup>	$R_M$ /m <sup>3</sup> mol <sup>-1</sup>	Aq. solvent mixture	$\phi_V \times 10^{-6}$ /m <sup>3</sup> mol <sup>-1</sup>	$(\eta_r - 1)/\sqrt{m}$ /kg <sup>1/2</sup> mol <sup>-1/2</sup>	$R_M$ /m <sup>3</sup> mol <sup>-1</sup>
Glycine				L-Lysine			
$w_1 = 0.001^b$				$w_1 = 0.001^b$			
0.0100	41.18	0.069	-	0.0100	105.47	0.223	30.1369
0.0251	40.38	0.078	-	0.0251	102.87	0.243	30.1580
0.0402	39.93	0.084	-	0.0403	101.21	0.261	30.1763
0.0553	39.54	0.088	-	0.0555	99.73	0.274	30.1909
0.0704	39.17	0.093	-	0.0707	98.45	0.289	30.2047
0.0855	38.94	0.095	-	0.0859	97.51	0.299	30.2163
$w_1 = 0.003^b$				$w_1 = 0.003^b$			
0.0100	41.16	0.092	-	0.0100	110.42	0.236	30.1522
0.0251	40.35	0.101	-	0.0251	107.61	0.260	30.1639
0.0401	39.65	0.107	-	0.0403	105.41	0.282	30.1710
0.0552	39.15	0.114	-	0.0554	103.68	0.298	30.1766
0.0703	38.72	0.115	-	0.0707	102.26	0.316	30.1827
0.0855	38.33	0.117	-	0.0859	100.75	0.331	30.1871
$w_1 = 0.005^b$				$w_1 = 0.005^b$			
0.0100	41.13	0.121	-	0.0100	115.35	0.242	30.1364

0.0251	39.93	0.129	-	0.0251	111.95	0.277	30.1546
0.0401	39.13	0.136	-	0.0402	109.34	0.298	30.1662
0.0552	38.58	0.139	-	0.0554	107.25	0.319	30.1757
0.0703	37.98	0.146	-	0.0706	105.20	0.339	30.1849
0.0854	37.48	0.148	-	0.0859	103.63	0.359	30.1947
L-Phenylalanine				L-Glutamic acid			
$w_1 = 0.001^b$				$w_1 = 0.001^b$			
0.0100	120.51	0.299	34.0527	0.0100	84.36	0.169	30.3277
0.0251	119.51	0.335	34.0763	0.0251	80.95	0.189	30.3340
0.0403	118.76	0.356	34.0922	0.0402	78.59	0.199	30.3390
0.0555	118.23	0.385	34.1060	0.0554	76.61	0.209	30.3435
0.0708	117.79	0.399	34.1208	0.0706	74.90	0.220	30.3476
0.0861	117.27	0.419	34.1322	0.0858	73.21	0.229	30.3508
$w_1 = 0.003^b$				$w_1 = 0.003^b$			
0.0100	126.45	0.320	34.0659	0.0100	89.32	0.175	30.3401
0.0251	124.65	0.366	34.0846	0.0251	85.71	0.202	30.3354
0.0403	123.20	0.392	34.0988	0.0402	82.55	0.217	30.3319
0.0555	121.99	0.421	34.1098	0.0554	80.02	0.227	30.3287
0.0707	121.01	0.442	34.1209	0.0705	78.01	0.239	30.3261
0.0861	120.03	0.463	34.1330	0.0857	75.99	0.245	30.3232
$w_1 = 0.005^b$				$w_1 = 0.005^b$			
0.0100	133.38	0.340	34.0791	0.0100	94.26	0.189	30.3350
0.0251	130.17	0.392	34.0943	0.0251	90.06	0.215	30.3424
0.0403	128.12	0.426	34.1064	0.0402	86.50	0.230	30.3468
0.0555	126.28	0.456	34.1158	0.0553	83.98	0.245	30.3512
0.0707	124.37	0.481	34.1237	0.0705	81.53	0.259	30.3547
0.0860	123.01	0.509	34.1300	0.0857	79.12	0.269	30.3588
Glycine				L-Lysine			
$w_2 = 0.001^b$				$w_2 = 0.001^b$			
0.0100	41.17	0.084	-	0.0100	107.46	0.260	30.1270
0.0251	40.37	0.092	-	0.0251	104.86	0.285	30.1510
0.0402	39.67	0.099	-	0.0403	103.20	0.306	30.1694
0.0553	39.35	0.104	-	0.0555	101.90	0.322	30.1852
0.0704	38.88	0.107	-	0.0707	100.73	0.338	30.2002
0.0855	38.58	0.110	-	0.0859	99.85	0.348	30.2148
$w_2 = 0.003^b$				$w_2 = 0.003^b$			
0.0100	41.15	0.114	-	0.0100	113.40	0.274	30.1275



0.0251	40.34	0.120	-	0.0251	109.99	0.308	30.1536
0.0401	39.64	0.129	-	0.0402	107.64	0.330	30.1713
0.0552	38.96	0.133	-	0.0554	105.66	0.353	30.1866
0.0703	38.43	0.135	-	0.0706	104.09	0.370	30.2015
0.0854	37.96	0.141	-	0.0859	102.73	0.382	30.2137
$w_2 = 0.005^b$				$w_2 = 0.005^b$			
0.0100	41.12	0.128	-	0.0100	118.32	0.294	30.1594
0.0251	39.91	0.138	-	0.0251	114.72	0.334	30.1765
0.0401	39.11	0.143	-	0.0402	111.81	0.362	30.1884
0.0552	38.38	0.148	-	0.0554	109.40	0.385	30.1997
0.0703	37.68	0.151	-	0.0706	107.31	0.407	30.2091
0.0854	37.11	0.158	-	0.0859	105.36	0.423	30.2171
L-Phenylalanine				L-Glutamic acid			
$w_2 = 0.001^b$				$w_2 = 0.001^b$			
0.0100	124.51	0.329	34.0132	0.0100	86.35	0.184	30.3372
0.0251	122.70	0.372	34.0265	0.0251	82.94	0.203	30.3432
0.0403	121.25	0.401	34.0373	0.0402	80.08	0.218	30.3473
0.0555	120.22	0.426	34.0448	0.0554	77.87	0.231	30.3508
0.0708	119.35	0.447	34.0519	0.0706	75.75	0.243	30.3537
0.0861	118.55	0.465	34.0588	0.0858	73.91	0.251	30.3566
$w_2 = 0.003^b$				$w_2 = 0.003^b$			
0.0100	131.43	0.342	34.0499	0.0100	92.30	0.198	30.3413
0.0251	128.63	0.394	34.0802	0.0251	88.09	0.221	30.3406
0.0403	126.92	0.429	34.1019	0.0402	85.04	0.239	30.3401
0.0555	125.24	0.456	34.1215	0.0554	82.19	0.256	30.3397
0.0707	123.85	0.481	34.1377	0.0705	79.99	0.267	30.3394
0.0861	122.71	0.501	34.1535	0.0857	77.63	0.276	30.3390
$w_2 = 0.005^b$				$w_2 = 0.005^b$			
0.0100	139.34	0.370	34.0696	0.0100	98.24	0.211	30.3476
0.0251	135.34	0.424	34.0930	0.0251	93.63	0.239	30.3495
0.0403	132.84	0.467	34.1106	0.0402	89.98	0.260	30.3509
0.0555	130.24	0.501	34.1247	0.0553	86.68	0.276	30.3522
0.0707	128.33	0.529	34.1381	0.0705	83.36	0.290	30.3533
0.0860	126.27	0.554	34.1498	0.0857	80.87	0.304	30.3541

<sup>a</sup> Standard uncertainties  $u$  are:  $u(T) = 0.01\text{K}$

<sup>b</sup>  $w_1$  and  $w_2$  are mass fractions of  $\alpha$ - and  $\beta$ -cyclodextrin in aqueous mixture respectively

**Table S4: Limiting apparent molar volume ( $\phi_V^0$ ), experimental slope ( $S_V^*$ ), viscosity  $A$ - and  $B$ -coefficient, and limiting molar refraction ( $R_M^0$ ) of selected amino acids in different mass fraction of aqueous  $\alpha$ - and  $\beta$ -cyclodextrin mixtures at 298.15 K<sup>a</sup>**

sol. mix	$\phi_V^0$ /m <sup>3</sup> mol <sup>-1</sup>	$S_V^*$ /m <sup>3</sup> ·mol <sup>-3/2</sup> ·kg <sup>1/2</sup>	$B$ /kg <sup>1/2</sup> ·mol <sup>-1/2</sup>	$A$ /kg·mol <sup>-1</sup>	$R_M^0$ /m <sup>3</sup> mol <sup>-1</sup>	sol. mix	$\phi_V^0$ /m <sup>3</sup> mol <sup>-1</sup>	$S_V^*$ /m <sup>3</sup> ·mol <sup>-3/2</sup> ·kg <sup>1/2</sup>	$B$ /kg <sup>1/2</sup> ·mol <sup>-1/2</sup>	$A$ /kg·mol <sup>-1</sup>	$R_M^0$ /m <sup>3</sup> mol <sup>-1</sup>
L-Lysine											
$w_1 = 0.001^b$	109.53	-41.41	0.403	0.180	30.09	$w_2 = 0.001^b$	111.23	-39.40	0.462	0.213	30.08
$w_1 = 0.003^b$	115.46	-49.99	0.493	0.184	30.13	$w_2 = 0.003^b$	118.84	-55.45	0.568	0.217	30.08
$w_1 = 0.005^b$	121.56	-61.16	0.599	0.181	30.10	$w_2 = 0.005^b$	125.24	-67.44	0.671	0.227	30.12
L-Phenylalanine											
$w_1 = 0.001^b$	122.15	-16.59	0.619	0.236	34.01	$w_2 = 0.001^b$	127.57	-30.98	0.703	0.259	33.98
$w_1 = 0.003^b$	129.86	-33.35	0.737	0.247	34.03	$w_2 = 0.003^b$	135.89	-45.12	0.822	0.262	33.99
$w_1 = 0.005^b$	138.77	-53.66	0.862	0.254	34.05	$w_2 = 0.005^b$	146.09	-67.14	0.960	0.274	34.02
L-Glutamic acid											
$w_1 = 0.001^b$	90.10	-57.46	0.303	0.139	30.31	$w_2 = 0.001^b$	93.04	-64.91	0.355	0.148	30.32
$w_1 = 0.003^b$	96.49	-69.70	0.359	0.143	30.34	$w_2 = 0.003^b$	100.06	-75.91	0.412	0.157	30.34
$w_1 = 0.005^b$	102.28	-78.44	0.415	0.148	30.32	$w_2 = 0.005^b$	107.79	-90.99	0.482	0.163	30.34

<sup>a</sup> Standard uncertainties  $u$  are:  $u(T) = 0.01\text{K}$

<sup>b</sup>  $w_1$  and  $w_2$  are mass fractions of  $\alpha$ - and  $\beta$ -cyclodextrin in aqueous mixture respectively