Supporting Information

Solubility of *D*-Histidine in Aqueous Co-solvent Mixtures of *N*,*N*-Dimethylformamide, Ethanol, Dimethyl Sulfoxide and *N*-Methyl-2-pyrrolidone: Determination, Preferential Solvation and Solvent Effect

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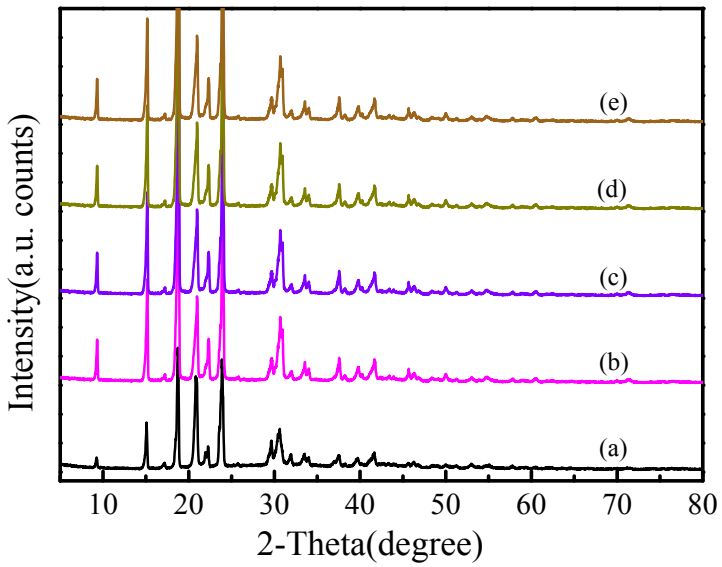

Fig. S1. XRD patterns of *D*-histidine: (a) raw material; (b) equilibrated with DMF (1) + water (2) mixture; (c) equilibrated with DMSO (1) + water (2) mixture; (d) equilibrated with NMP (1) + water (2) mixture; (e) equilibrated with ethanol (1) + water (2) mixture.

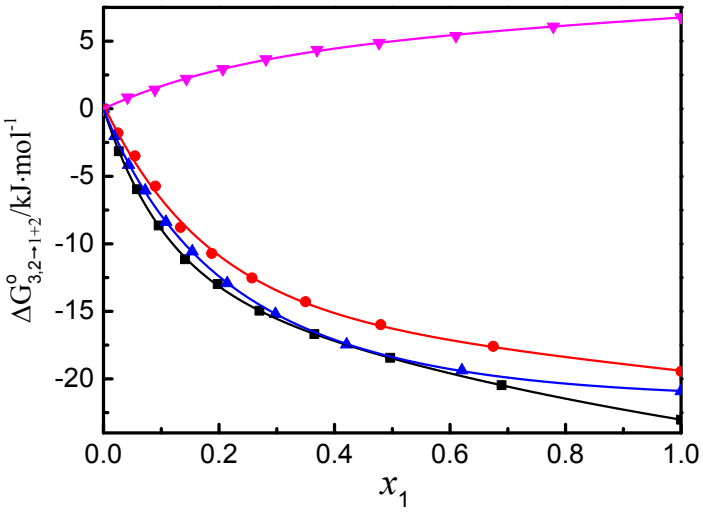

Fig. S2. Gibbs energy of transfer (kJ·mol^{-1}) of *D*-histidine (3) from neat water (2) to DMF (1) + water (2), DMSO (1) + water (2), NMP (1) + water (2) and ethanol (1) + water (2) mixtures at 298.15 K. ■, DMF (1) + water (2); ●, DMSO (1) + water (2); ▲, NMP (1) + water (2); ▼, ethanol (1) + water (2).

Table S1 pH values of the saturated solutions for *D*-histidine dissolved in DMF (*w*) + water (1-*w*), DMSO (*w*) + water (1-*w*), NMP (*w*) + water (1-*w*) and ethanol (*w*) + water (1-*w*) mixtures at 298.15 K under pressure of *p*=101.2 kPa.[a]

System	*w*										
	0	0.1000	0.2000	0.3000	0.4000	0.5000	0.6000	0.7000	0.8000	0.9000	1
DMF (*w*) + water (1-*w*)	8.12	8.08	8.04	7.99	7.90	7.81	7.63	7.58	7.56	7.69	7.99
DMSO (*w*) + water (1-*w*)	8.12	8.00	7.93	7.92	7.93	7.94	7.95	7.96	8.02	8.21	8.63
NMP (*w*) + water (1-*w*)	8.12	8.04	7.97	7.82	7.59	7.58	7.59	7.66	7.85	8.05	8.51
ethanol (*w*) + water (1-*w*)	8.12	7.83	7.59	7.41	7.29	7.18	7.09	6.98	6.90	6.81	6.66

[a] Relative standard uncertainty for initial solvent mixtures, $u_r(w) = 0.0002$. Standard uncertainties u are u (pH) = 0.01 unit; $u(p) = 0.45$ kPa for pressure, $u(T) = 0.02$ K for temperature; *w* denotes the mass fraction composition of DMF/ DMSO/ NMP/ ethanol in the mixture of DMF/ DMSO/ NMP/ ethanol (*w*) + water (1-*w*) absence of *D*-histidine.

Table S2 Kamlet-Taft parameters π^* (dipolarity-polarizability), α (hydrogen bond donor parameter) and β (hydrogen bond donor parameter) and Hildebrand solubility parameter, δ_H, of aqueous solution of DMF, DMSO,NMP and ethanol at 298.15 K.

DMF (1) + water (2)					DMSO (1) + water (2)					NMP (1) + water (2)					ethanol (1) + water (2)				
x_1[a]	π^*[b]	β[b]	α[b]	δ_H[c]	x_1	π^*	β	α	δ_H	x_1	π^*	β	α	δ_H	x_1	π^*	β	α	δ_H
0	1.09	0.47	1.17	47.82	0	1.09	0.47	1.17	47.82	0	1.09	0.47	1.17	47.82	0	1.09	0.47	1.17	47.82
0.02666	1.10	0.50	1.05	45.41	0.02499	1.10	0.49	1.08	45.87	0.01980	1.12	0.56	1.03	45.36	0.04165	1.08	0.52	0.99	45.12
0.05806	1.11	0.52	0.93	43.03	0.05452	1.11	0.51	0.97	43.86	0.04347	1.13	0.62	0.91	42.90	0.08908	1.05	0.57	0.79	42.59
0.09556	1.12	0.55	0.80	40.67	0.08995	1.11	0.54	0.85	41.88	0.07228	1.13	0.65	0.79	40.49	0.1436	0.97	0.62	0.72	40.20
0.1412	1.13	0.56	0.68	38.34	0.1333	1.11	0.57	0.74	39.89	0.1081	1.13	0.66	0.70	38.01	0.2068	0.90	0.66	0.72	37.84
0.1978	1.12	0.58	0.57	36.03	0.1874	1.11	0.59	0.62	37.76	0.1538	1.13	0.67	0.61	35.54	0.2812	0.83	0.70	0.75	35.66
0.2700	1.09	0.60	0.49	33.75	0.2570	1.11	0.61	0.52	35.66	0.2143	1.12	0.68	0.53	33.05	0.3698	0.79	0.71	0.75	33.59
0.3652	1.05	0.62	0.42	31.49	0.3499	1.09	0.63	0.42	33.50	0.2978	1.10	0.69	0.42	30.55	0.4772	0.74	0.72	0.75	31.60
0.4965	1.00	0.65	0.36	29.26	0.4799	1.06	0.66	0.33	31.18	0.4210	1.07	0.71	0.31	28.03	0.6101	0.69	0.74	0.78	29.72
0.6893	0.93	0.68	0.28	27.05	0.6749	1.03	0.69	0.22	29.07	0.6206	1.01	0.74	0.17	25.51	0.7788	0.63	0.75	0.80	27.86
1	0.88	0.69	0.00	24.86	1	1.00	0.76	0.00	26.75	1	0.92	0.77	0.00	22.96	1	0.54	0.75	0.86	26.13

[a] x_1 is the mole fraction of DMF (DMSO, NMP and ethanol) (1) in DMF (DMSO, NMP and ethanol) (1) + water (2) solvent mixtures free of the solute (3).

[b] Kamlet-Taft parameters for DMF (DMSO, NMP and ethanol) are taken from different sources [S1-S3], and then corrected for homogenous presentation by taken the accepted literature data for pure solvents [S4] as the reference points according to method explained previously [S5,S6].

[c] δ_H values for pure solvents are gathered from Ref. [S7], and for binary mixtures are estimated as a function of the volume fraction of solvent, ϕ_1, by $\phi_1\delta_{H1} + \phi_2\delta_{H2}$ in the mixture.

Table S3 Multiple linear regression analysis of KAT-LSER model on solubility of *D*-histidine in DMF (1) + water (2) mixture at 298.15 K.

c_0	c_1	c_2	c_3	c_4	r^{2b}	F^c
6.990(1.632)[a]	-3.003(0.329)	-6.435(1.771)	0.05502(0.16066)	-6.043(0.568)	1.00	6127
-9.440(2.168)	0.06702(0.64803)	11.17(2.60)	-1.087(0.493)		0.99	477.8
6.753(1.382)	-2.945(0.263)	-6.210(1.538)		-5.913(0.395)	1.00	9348
1.089(0.256)	-1.938(0.246)		-0.1617(0.2471)	-4.114(0.335)	1.00	2977
-6.875(2.147)		8.012(2.858)	-0.7009(0.4926)	-1.483(0.971)	0.99	636.6
-13.61(1.28)	0.3576(0.7727)	16.67(0.90)			0.99	481.6
-0.4324(0.9957)	-1.106(1.049)		-3.120(0.250)		0.98	222.0
1.191(0.195)	-2.008(0.213)			-4.327(0.073)	1.00	4809
-9.297(1.561)		11.06(2.21)	-1.098(0.452)		0.99	817.8
-7.411(2.245)		**8.939(2.955)**		**-2.212(0.876)**	**0.99**	**845.6**
-0.8685(0.1846)			-1.016(0.654)	-3.386(0.946)	0.99	512.0
8.372(2.991)	-11.25(2.82)				0.60	15.89
-13.05(0.30)		16.33(0.50)			0.99	1055
-1.475(0.111)			-3.324(0.159)		0.98	437.5
-0.6243(0.1044)				-4.838(0.163)	0.99	882.6

[a] Number in bracket is standard deviation;

[b] Squared correlation coefficient;

[c] *F*-statistic values.

Table S4 Multiple linear regression analysis of KAT-LSER model on solubility of *D*-histidine in DMSO (1) + water (2) mixture at 298.15 K.

c_0	c_1	c_2	c_3	c_4	r^{2b}	F^c
0.06503(0.71251)[a]	-2.371(0.192)	-1.691(0.834)	-0.7961(0.3062)	-1.039(0.222)	1.00	5726
1.811(1.214)	-2.334(0.384)	-4.445(1.182)	-2.095(0.260)		1.00	1910
-1.456(0.549)	-2.233(0.250)	0.3423(0.3889)		-1.560(0.127)	1.00	4188
-1.323(0.239)	-2.166(0.197)		-0.2131(0.1272)	-1.356(0.189)	1.00	5282
-6.417(2.283)		3.692(3.372)	0.2402(1.3985)	-0.9286(1.0519)	0.99	336.3
-7.568(1.013)	-0.07284(0.78387)	5.019(0.332)			0.98	315.9
-2.658(0.406)	-1.208(0.391)		-1.120(0.040)		1.00	1081
-0.9923(0.1492)	-2.409(0.147)			-1.670(0.024)	1.00	6464
-4.765(1.289)		1.152(1.734)	-0.9369(0.4159)		0.99	518.3
-6.043(0.642)		3.130(0.767)		-0.7564(0.2973)	0.99	574.0
-3.923(0.143)			-1.245(0.344)		0.99	491.6
5.637(2.632)	-9.513(2.428)2.428)				0.59	15.35
-7.661(0.113)		**5.044(0.189)**			**0.99**	**710.0**

-3.909(0.026)			-1.212(0.036)		0.99	1105
-3.426(0.065)				-1.947(0.096)	0.98	413.0

[a] Number in bracket is standard deviation;

[b] Squared correlation coefficient;

[c] *F*-statistic values.

Table S5 Multiple linear regression analysis of KAT-LSER model on solubility of *D*-histidine in NMP (1) + water (2) at 298.15 K.

c_0	c_1	c_2	c_3	c_4	r^{2b}	F^c
-0.1382(1.3476)[a]	-0.5369(2.2092)	-1.649(1.605)	-0.7530(2.1319)	-2.891(2.136)	1.00	2636
-1.928(0.272)	2.431(0.280)	-3.740(0.460)	-3.633(0.131)		1.00	3141
0.3259(0.2809)	-1.315(0.168)	-1.095(0.327)		-3.645(0.116)	1.00	4017
1.124(0.555)	-2.755(0.469)		1.384(0.466)	-5.004(0.581)	1.00	3487
-0.4584(0.2629)		-2.030(0.315)	-1.269(0.161)	-2.376(0.238)	1.00	4061
-5.411(2.385)	-3.774(1.661)	8.496(1.314)			0.90	44.38
-3.342(0.633)	0.9073(0.6272)		-2.616(0.114)		0.99	511.8
-0.4430(0.2447)	-1.462(0.245)			-3.282(0.063)	1.00	2641
-1.595(0.866)		-1.058(1.097)	-2.725(0.253)		0.99	452.4
-0.4186(0.7715)		-1.764(0.921)		-4.066(0.299)	0.99	703.3
-2.131(0.095)			-1.158(0.394)	-1.904(0.556)	1.00	1003
6.468(3.577)	-9.576(3.287)				0.43	8.48

-10.57(0.88)	**10.11(1.34)**			**0.86**	**57.15**
-2.429(0.058)		-2.495(0.083)		0.99	910.8
-1.893(0.067)			-3.522(0.107)	0.99	1082

[a] Number in bracket is standard deviation;

[b] Squared correlation coefficient;

[c] *F*-statistic values.

Table S6 Multiple linear regression analysis of KAT-LSER model on solubility of *D*-histidine in ethanol (1) + water (2) at 298.15 K.

c_0	c_1	c_2	c_3	c_4	r^{2b}	F^c
-11.42(0.83)[a]	1.413(0.526)	2.179(0.761)	-0.09698(0.22218)	3.643(0.542)	1.00	3327
-10.90(2.22)	4.427(0.746)	-0.1724(1.8289)	0.6899(0.5110)		0.99	604.0
-11.69(0.50)	1.608(0.259)	2.335(0.631)		3.519(0.433)	1.00	5016
-9.229(0.446)	1.311(0.748)		-0.3965(0.2791)	2.931(0.685)	1.00	2186
-10.45(1.02)		2.041(1.043)	-0.6055(0.1595)	4.882(0.390)	1.00	2350
-8.034(0.684)	3.513(0.330)	-2.503(0.634)			0.99	820.7
-11.11(0.13)	4.496(0.116)		0.7353(0.1580)		1.00	1034
-9.8459(0.113)	2.301(0.287)			2.008(0.232)	1.00	2908
2.130(0.801)		-10.88(0.70)	-2.061(0.494)		0.97	168.3
-13.65(0.94)		5.178(1.041)		5.961(0.437)	1.00	1313
-8.457(0.077)			-0.8528(0.1132)	4.127(0.067)	1.00	2603

-10.70(0.16)	**4.729(0.190)**				**0.98**	**620.9**
-0.9191(0.5491)		-8.821(0.829)			0.92	113.1
-9.492(1.544)			3.382(1.847)		0.19	3.35
-8.978(0.091)				3.821(0.143)	0.99	715.6

[a] Number in bracket is standard deviation;

[b] Squared correlation coefficient;

[c] *F*-statistic values.

Table S7 Values of parameters obtained using the Jouyban-Acree model.

parameter	DMF + water	DMSO + water	NMP + water	ethanol + water
J_0	28.7589	-109.0935	-50.1028	-67.6924
J_1	-13.2324	-36.3357	53.3269	-46.8677
J_2	-168.8247	-63.645	-3.3385	181.5217
RAD·10^2	1.69	1.05	2.35	2.78
RMSD·10^4	27.43	2.74	14.95	1.16

Table S8 Gibbs energy of transfer ($\Delta_{tr}G^{o}_{3,2\rightarrow 1+2}$, kJ·mol^{-1}) of *D*-histidine (3) from neat water (2) to DMF (1) + water (2), DMSO (1) + water (2), NMP (1) + water (2) and ethanol (1) + water (2) mixtures at 298.15 K.

DMF (1) + water (2)		DMSO (1) + water (2)		NMP (1) + water (2)		ethanol (1) + water (2)	
x_1[a]	$\Delta_{tr}G^{0}_{3,2\rightarrow 1+2}$	x_1[a]	$\Delta_{tr}G^{0}_{3,2\rightarrow 1+2}$	x_1[a]	$\Delta_{tr}G^{0}_{3,2\rightarrow 1+2}$	x_1[a]	$\Delta_{tr}G^{0}_{3,2\rightarrow 1+2}$
0	0	0	0	0	0	0	0
0.02666	-0.804	0.02499	-0.255	0.01980	-0.588	0.04165	0.832
0.05806	-1.742	0.05452	-0.500	0.04347	-1.270	0.08908	1.418
0.09556	-2.570	0.08995	-0.808	0.07228	-2.026	0.1436	2.212
0.1412	-3.471	0.1333	-1.098	0.1081	-2.652	0.2068	2.939
0.1978	-4.403	0.1874	-1.406	0.1538	-3.297	0.2812	3.664
0.2700	-5.387	0.2570	-1.747	0.2143	-4.046	0.3698	4.354
0.3652	-6.213	0.3499	-2.124	0.2978	-4.780	0.4772	4.873
0.4965	-7.045	0.4799	-2.546	0.4210	-5.462	0.6101	5.391
0.6893	-7.893	0.6749	-2.909	0.6206	-6.059	0.7788	6.082
1	-8.797	1	-3.398	1	-6.692	1	6.774

[a] x_1 represents the mole fraction of DMF (DMSO, NMP or ethanol) in mixed solvents of DMF (DMSO, NMP or ethanol) (*w*) + water (1-*w*) free of *D*-histidine.

Table S9 Coefficients of Eq. (17) (kJ·mol^{-1}) applied to Gibbs energy of transfer of *D*-histidine (3) from water (2) to DMF (1) + water (2), DMSO (1) + water (2), NMP (1) + water (2) and ethanol (1) + water (2) mixtures at 298.15 K.

	DMF (1) + water (2)	DMSO (1) + water (2)	NMP (1) + water (2)	ethanol (1) + water (2)
A_0	-38256.9	-3.6424	-7.1048	87951.4
A_1	38250.3	1.7996	2.9796	-87947.0
t_1	16784.8	0.40039	0.12182	34978.3
A_2	6.5832	1.7996	4.1342	-4.3225
t_2	0.21372	0.40039	0.43680	0.24986

Table S10 Some properties associated to preferential solvation of *D*-histidine (3) in DMF (1) + water (2) mixtures at 298.15 K.

x_1[a]	D kJ·mol^{-1}	$G_{1,3}$ cm^3·mol^{-1}	$G_{2,3}$ cm^3·mol^{-1}	V_{cor} cm^3·mol^{-1}	100 $\delta x_{1,3}$
0.00	-33.08	-349.7	-107.8	613	0
0.05	-26.66	-280.3	-144.1	651	-1.295
0.10	-21.57	-231.8	-163.6	702	-1.154
0.15	-17.55	-197.9	-173.2	758	-0.543
0.20	-14.36	-174.1	-177.0	812	0.072
0.25	-11.84	-157.2	-177.6	865	0.553
0.30	-9.847	-145.1	-176.7	915	0.888
0.35	-8.268	-136.4	-175.3	964	1.104
0.40	-7.019	-130.0	-174.0	1012	1.234
0.45	-6.030	-125.3	-173.1	1058	1.305
0.50	-5.247	-121.8	-172.8	1104	1.334
0.55	-4.628	-119.1	-173.4	1150	1.336
0.60	-4.138	-117.0	-174.8	1194	1.316
0.65	-3.750	-115.2	-177.0	1238	1.275
0.70	-3.443	-113.8	-180.0	1282	1.210
0.75	-3.200	-112.5	-183.5	1325	1.114
0.80	-3.008	-111.4	-187.1	1368	0.977
0.85	-2.856	-110.3	-190.1	1409	0.791
0.90	-2.736	-109.2	-191.7	1450	0.557
0.95	-2.640	-108.2	-190.9	1491	0.285
1.00	-2.565	-107.3	-187.4	1531	0

[a] x_1 is the mole fraction of DMF (1) in the DMF (1) + water (2) mixtures free of *D*-histidine (3).

Table S11 Some properties associated to preferential solvation of *D*-histidine (3) in DMSO (1) + water (2) mixtures at 298.15 K.

x_1[a]	D kJ·mol^{-1}	$G_{1,3}$ cm^3·mol^{-1}	$G_{2,3}$ cm^3·mol^{-1}	V_{cor} cm^3·mol^{-1}	100 $\delta x_{1,3}$
0.00	-8.989	-173.6	-107.8	613	0
0.05	-7.934	-164.9	-118.8	655	-0.410
0.10	-7.002	-154.6	-127.2	700	-0.433
0.15	-6.180	-144.5	-132.3	746	-0.253
0.20	-5.455	-135.5	-134.5	792	-0.026
0.25	-4.814	-128.4	-134.6	837	0.166
0.30	-4.249	-122.9	-133.5	882	0.296
0.35	-3.750	-118.8	-131.7	925	0.369
0.40	-3.310	-115.8	-129.8	967	0.398
0.45	-2.922	-113.7	-127.9	1010	0.398
0.50	-2.579	-112.1	-126.2	1051	0.378
0.55	-2.276	-110.9	-124.7	1092	0.348
0.60	-2.009	-110.1	-123.4	1133	0.313
0.65	-1.773	-109.5	-122.3	1173	0.276
0.70	-1.565	-109.0	-121.5	1214	0.238
0.75	-1.381	-108.6	-121.0	1253	0.202
0.80	-1.219	-108.4	-120.7	1293	0.168
0.85	-1.076	-108.2	-120.9	1332	0.133
0.90	-0.950	-108.0	-121.8	1371	0.099
0.95	-0.838	-107.8	-123.8	1409	0.058
1.00	-0.740	-107.6	-128.9	1447	0

[a] x_1 is the mole fraction of DMSO (1) in the DMSO (1) + water (2) mixtures free of *D*-histidine.

Table S12 Some properties associated to preferential solvation of *D*-histidine (3) in NMP (1) + water (2) mixtures at 298.15 K.

x_1[a]	D kJ·mol^{-1}	$G_{1,3}$ cm^3·mol^{-1}	$G_{2,3}$ cm^3·mol^{-1}	V_{cor} cm^3·mol^{-1}	100 $\delta x_{1,3}$
0.00	-33.92	-356.1	-107.8	613	0
0.05	-24.67	-295.4	-157.2	663	-1.316
0.10	-18.29	-239.7	-182.1	734	-0.949
0.15	-13.85	-197.4	-189.1	809	-0.170
0.20	-10.72	-168.5	-187.1	879	0.429
0.25	-8.482	-149.7	-182.1	945	0.788
0.30	-6.847	-137.5	-176.8	1008	0.978
0.35	-5.630	-129.5	-172.3	1069	1.068
0.40	-4.705	-124.1	-168.8	1128	1.100
0.45	-3.987	-120.3	-166.3	1186	1.095
0.50	-3.416	-117.5	-164.4	1244	1.064
0.55	-2.955	-115.3	-162.8	1300	1.010
0.60	-2.574	-113.6	-161.2	1356	0.934
0.65	-2.255	-112.2	-159.4	1411	0.836
0.70	-1.984	-111.1	-157.1	1466	0.721
0.75	-1.752	-110.1	-154.3	1519	0.593
0.80	-1.550	-109.4	-151.3	1573	0.461
0.85	-1.375	-108.8	-148.3	1626	0.334
0.90	-1.221	-108.3	-145.8	1678	0.216
0.95	-1.085	-107.9	-144.4	1731	0.107
1.00	-0.966	-107.6	-145.2	1783	0

[a] x_1 is the mole fraction of NMP (1) in the NMP (1) + water (2) mixtures free of *D*-histidine (3).

Table S13 Some properties associated to preferential solvation of *D*-histidine (3) in ethanol (1) + water (2) mixtures at 298.15 K.

x_1[a]	D kJ·mol^{-1}	$G_{1,3}$ cm^3·mol^{-1}	$G_{2,3}$ cm^3·mol^{-1}	V_{cor} cm^3·mol^{-1}	100 $\delta x_{1,3}$
0.00	19.81	36.55	-107.8	611	0
0.05	16.68	21.04	-87.38	651	0.904
0.10	14.11	4.570	-69.87	686	1.074
0.15	12.01	-11.57	-55.71	718	0.841
0.20	10.28	-26.33	-44.67	749	0.414
0.25	8.875	-39.13	-36.05	778	-0.078
0.30	7.721	-49.78	-28.96	808	-0.566
0.35	6.777	-58.39	-22.43	838	-1.019
0.40	6.004	-65.22	-15.58	868	-1.432
0.45	5.371	-70.58	-7.608	898	-1.809
0.50	4.853	-74.80	2.215	928	-2.160
0.55	4.429	-78.21	14.43	958	-2.488
0.60	4.082	-81.18	29.09	989	-2.781
0.65	3.797	-84.12	45.08	1020	-2.998
0.70	3.565	-87.48	59.02	1052	-3.052
0.75	3.374	-91.52	64.92	1085	-2.840
0.80	3.218	-96.00	57.17	1121	-2.321
0.85	3.091	-100.1	36.11	1158	-1.610
0.90	2.986	-103.2	8.680	1196	-0.912
0.95	2.900	-105.1	-17.67	1232	-0.367
1.00	2.830	-106.0	-39.23	1267	0

[a] x_1 is the mole fraction of ethanol (1) in the ethanol (1) + water (2) mixtures free of *D*-histidine (3).

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