

Supporting Information:

Details concerning the chemicals used in the study, the mole fraction solubility of cAMPNa (in pure water, water+ethanol, water+methanol, and water+acetone) at various initial mole fraction composition of binary solvent within 293.15–313.15 K, and fitted parameters of (CNIBS)/Redlich-Kister model and modified Apelblat equation for cAMPNa in water+ethanol, water+methanol, and water+acetone mixtures are given as follows.

Table 1. The substance used in the experiment.

Substance	Purity	Source
cAMPNa·2H ₂ O	≥ 99% (HPLC, mass fraction)	Prepared in laboratory
Methanol	Analytical grade	Tianjin Kewei Chemical Reagent (China)
Ethanol	Analytical grade	Tianjin Kewei Chemical Reagent (China)
Acetone	Analytical grade	Tianjin Kewei Chemical Reagent (China)
Water	Deionized water	Prepared in laboratory

Table 2. The mole fraction solubility of cAMPNa (x_3) in pure water, water (1) + ethanol (2), water (1) + methanol (2) and water (1)+ acetone (2), at various initial mole fraction composition of binary solvent from 293.15 K to 313.15 K.

x_2 (mole fraction)	$10^3 x_3^{\text{exp}}$ (mole fraction)	$10^2 (x_3^{\text{exp}} - x_3^{\text{cal}}) / x_3^{\text{exp}}$ (CNIBS)	$10^2 (x_3^{\text{exp}} - x_3^{\text{cal}}) / x_3^{\text{exp}}$ (Apelblat)
Pure water			
From 293.15 K to 303.15 K			
0.000	39.44 ± 0.02	0.1429	0.0748
0.000	42.23 ± 0.04	0.0560	0.2775
0.000	45.19 ± 0.08	0.1649	-1.3558
0.000	51.43 ± 0.09	0.1429	1.5254
0.000	56.55 ± 0.06	0.6032	-0.5564
Water(1)+ethanol(2)			
T=293.15 K $\pm$ 0.05 K			
0.100	21.84 ± 0.01	0.1868	-1.6887
0.200	12.74 ± 0.03	-0.3275	-0.9937
0.300	7.37 ± 0.02	0.2909	-0.2036
0.400	4.46 ± 0.04	-0.1320	0.0134
0.500	2.34 ± 0.06	0.0235	-2.4525

T=298.15 K $\pm$ 0.05 K			
0.100	31.01 $\pm$ 0.05	-0.2804	4.4620
0.200	19.24 $\pm$ 0.02	0.5581	3.1565
0.300	10.63 $\pm$ 0.06	-0.5609	0.8709
0.400	5.81 $\pm$ 0.03	0.2792	-0.2397
0.500	3.21 $\pm$ 0.04	-0.0558	5.5796
T=303.15 K $\pm$ 0.05 K			
0.100	35.37 $\pm$ 0.04	-0.8291	-4.1363
0.200	23.88 $\pm$ 0.05	1.6370	-3.7038
0.300	13.36 $\pm$ 0.06	-1.6654	-3.7038
0.400	7.21 $\pm$ 0.07	0.8218	-1.4584
0.500	3.49 $\pm$ 0.03	-0.1651	0.0614
T=308.15 K $\pm$ 0.05 K			
0.100	43.34 $\pm$ 0.04	0.1868	0.5613
0.200	30.86 $\pm$ 0.07	-0.3275	1.5920
0.300	15.99 $\pm$ 0.06	0.2909	1.0492
0.400	8.28 $\pm$ 0.05	-0.1320	-0.6013
0.500	3.88 $\pm$ 0.03	0.0235	-2.7394
T=313.15 K $\pm$ 0.05 K			
0.100	47.74 $\pm$ 0.07	-3.0692	0.4209
0.200	34.47 $\pm$ 0.08	5.8688	-0.1886
0.300	16.37 $\pm$ 0.05	-6.2388	-0.2894
0.400	9.21 $\pm$ 0.04	2.9789	-0.1942
0.500	4.28 $\pm$ 0.03	-0.6068	1.7832
Water(1)+methanol(2)			
T=293.15 K $\pm$ 0.05 K			
0.100	24.13 $\pm$ 0.02	-2.1382	-0.8442
0.200	13.11 $\pm$ 0.06	4.1428	2.1117
0.300	6.42 $\pm$ 0.04	-4.3226	-1.3000
0.400	4.36 $\pm$ 0.03	2.0931	0.4776
0.500	3.34 $\pm$ 0.01	-0.4241	0.4636
T=298.15 K $\pm$ 0.05 K			
0.100	30.65 $\pm$ 0.01	-3.3674	2.1117
0.200	19.10 $\pm$ 0.02	6.4093	4.3604
0.300	9.42 $\pm$ 0.03	-6.8487	4.1700
0.400	6.59 $\pm$ 0.04	3.2574	6.8712
0.500	4.28 $\pm$ 0.03	-0.6653	-1.7798
T=303.15 K $\pm$ 0.05 K			
0.100	35.25 $\pm$ 0.04	-1.6990	-1.3000
0.200	23.30 $\pm$ 0.03	3.3129	-6.4298
0.300	11.77 $\pm$ 0.05	-3.4270	-5.7493
0.400	7.74 $\pm$ 0.06	1.6700	-5.1653
0.500	5.92 $\pm$ 0.02	-0.3376	4.7679
T=308.15 K $\pm$ 0.05 K			

0.100	40.87 ± 0.02	-0.3180	-0.4776
0.200	30.34 ± 0.08	2.5851	3.7658
0.300	17.54 ± 0.05	-2.6536	3.1275
0.400	10.42 ± 0.09	1.3006	-0.5789
0.500	6.89 ± 0.07	-0.2621	-4.9328
T=313.15 K $\pm$ 0.05 K			
0.100	45.98 ± 0.09	0.9575	0.4636
0.200	33.85 ± 0.07	-1.9444	-0.8776
0.300	22.84 ± 0.08	1.9061	-0.6476
0.400	13.26 ± 0.05	-0.9673	1.1644
0.500	9.35 ± 0.06	0.1919	1.5962
Water(1)+acetone(2)			
T=293.15 K $\pm$ 0.05 K			
0.100	23.89 ± 0.03	-0.5181	0.1388
0.200	13.08 ± 0.05	1.0284	2.6234
0.300	6.02 ± 0.02	-1.0395	1.5709
0.400	2.79 ± 0.06	0.5148	0.1224
0.500	1.55 ± 0.04	-0.1033	1.7074
T=298.15 K $\pm$ 0.05 K			
0.100	28.81 ± 0.04	0.6101	0.4935
0.200	14.90 ± 0.05	-1.2333	-7.2163
0.300	7.27 ± 0.03	1.2180	-3.6063
0.400	3.40 ± 0.02	-0.6146	-0.6830
0.500	1.71 ± 0.04	0.1219	-4.5482
T=303.15 K $\pm$ 0.05 K			
0.100	33.51 ± 0.06	-0.9720	-2.3918
0.200	21.06 ± 0.04	1.9165	4.5708
0.300	9.86 ± 0.07	-1.9532	0.9499
0.400	4.43 ± 0.05	0.9625	1.3221
0.500	2.21 ± 0.04	-0.1931	2.7955
T=308.15 K $\pm$ 0.05 K			
0.100	42.04 ± 0.06	0.7626	2.6750
0.200	25.55 ± 0.07	-1.5431	0.8957
0.300	13.19 ± 0.05	1.5189	2.3799
0.400	5.74 ± 0.06	-0.7685	-1.1043
0.500	2.67 ± 0.04	0.1532	0.7798
T=313.15 K $\pm$ 0.05 K			
0.100	48.14 ± 0.07	-0.0978	-0.9742
0.200	31.56 ± 0.03	0.1977	-1.2846
0.300	17.02 ± 0.06	-0.1971	-1.4035
0.400	8.01 ± 0.05	0.0994	0.3315
0.500	3.30 ± 0.04	-0.0194	-0.8983

Table 3. Fitted Parameters of CNIBS/Redlich-Kister model for cAMPNa(3) in water(1)+ ethanol(2) , water(1)+methanol(2) and water(1)+acetone(2) mixture.

Model parameters	T=293.15 K	T=298.15 K	T=303.15 K	T=308.15 K	T=313.15 K
Water+ethanol					
B ₀	-3.23 (-0.02)	-3.17 (-0.01)	-3.10 (-0.03)	-2.97 (-0.06)	-2.88 (-0.10)
B ₁	-5.71 (-0.83)	-1.83 (-0.33)	-1.23 (-0.96)	-0.21 (-2.04)	0.49 (-3.53)
B ₂	-2.79 (-7.97)	-13.96 (-3.12)	-12.42 (-9.21)	-13.20 (-19.49)	-20.32 (-33.75)
B ₃	19.21 (-25.16)	18.09 (-9.85)	12.49 (-29.08)	1.20 (-61.50)	22.59 (-106.50)
B ₄	-26.71 (-25.01)	-6.92 (-9.79)	-6.37 (-28.89)	10.81 (-61.11)	-8.87 (-105.83)
RMSD	0.0020	0.0009	0.0027	0.0060	0.0107
Water+methanol					
B ₀	-3.24 (-0.07)	-3.17 (-0.10)	-3.10 (-0.05)	-2.97 (-0.04)	-2.87 (-0.03)
B ₁	-2.51 (-2.47)	0.05 (-3.87)	-0.04 (-1.97)	-1.97 (-1.53)	-2.62 (-1.12)
B ₂	-28.05 (-23.62)	-37.01 (-36.97)	-27.11 (-18.80)	1.62 (-14.62)	9.43 (-10.74)
B ₃	69.84 (-74.52)	91.41 (-116.65)	48.55 (-59.34)	-38.58 (-46.12)	-57.39 (-33.91)
B ₄	-46.83 (-74.05)	-71.63 (-115.92)	-20.79 (-58.97)	54.39 (-45.83)	69.19 (-33.69)
RMSD	0.0060	0.0102	0.0054	0.0045	0.0035
Water+acetone					
B ₀	-3.23 (-0.02)	-3.16 (-0.02)	-3.10 (-0.03)	-2.97 (-0.02)	-2.87 (0.00)
B ₁	-4.69 (-0.60)	-2.02 (-0.72)	-2.26 (-1.13)	-0.76 (-0.89)	0.06 (-0.12)
B ₂	0.26 (-5.77)	-22.27 (-6.84)	-2.94 (-10.80)	-13.15 (-8.54)	-18.50 (-1.10)
B ₃	-33.31 (-18.21)	37.20 (-21.58)	-38.01 (-34.07)	-5.28 (-26.96)	20.46 (-3.47)
B ₄	51.44 (-18.09)	-20.46 (-21.45)	57.66 (-33.86)	21.88 (-26.79)	-12.87 (-3.45)
RMSD	0.0015	0.0018	0.00301	0.0025	0.00034

Table 4. Fitted Parameters of modified Apelblat equation for cAMPNa(3) in water(1)+ethanol(2), water(1)+methanol(2) and water(1)+acetone(2) mixture.

Model parameters	$x_2=0.100$	$x_2=0.200$	$x_2=0.300$	$x_2=0.400$	$x_2=0.500$
Water+ethanol					
a	1398.60 (-606.47)	1796.23 (-485.25)	2233.92 (-189.74)	1243.15 (-85.15)	1370.57 (-692.91)
b	-66230.70 (-27363.65)	-85074.49 (-21894.44)	-104224.85 (-8560.88)	-59141.02 (-3841.99)	-64287.06 (-31263.93)
c	-207.10 (-90.33)	-265.88 (-72.28)	-331.53 (-28.26)	-184.28 (-12.68)	-203.73 (-103.21)
RMSD	0.0085	0.0061	0.0021	0.0008	0.0058
Water+methanol					
a	710.27 (-253.12)	1160.14 (-810.53)	-17.08 (-729.95)	544.44 (-858.98)	17.14 (-677.11)
b	-34666.51 (-11420.75)	-56209.12 (-36570.60)	-4367.77 (-32934.97)	-28977.49 (-38757.06)	-4970.98 (-30550.79)
c	-104.87 (-37.70)	-171.23 (-120.73)	4.74 (-108.73)	-79.39 (-127.94)	-1.04 (-100.85)
RMSD	0.0035	0.0103	0.0079	0.0083	0.0064
Water+acetone					
a	-45.44 (-350.56)	-231.42 (-833.52)	-643.01 (-453.97)	-1153.05 (-176.08)	-734.09 (-528.93)
b	-881.59 (-15817.33)	6671.67 (-37608.17)	24630.57 (-20483.03)	47677.39 (-7944.61)	29803.82 (-23865.27)
c	7.87 (-52.22)	35.96 (-124.15)	97.50 (-67.62)	173.31 (-26.23)	110.19 (-78.78)
RMSD	0.0052	0.0098	0.0047	0.0016	0.0040