

# Electronic Supplementary Material

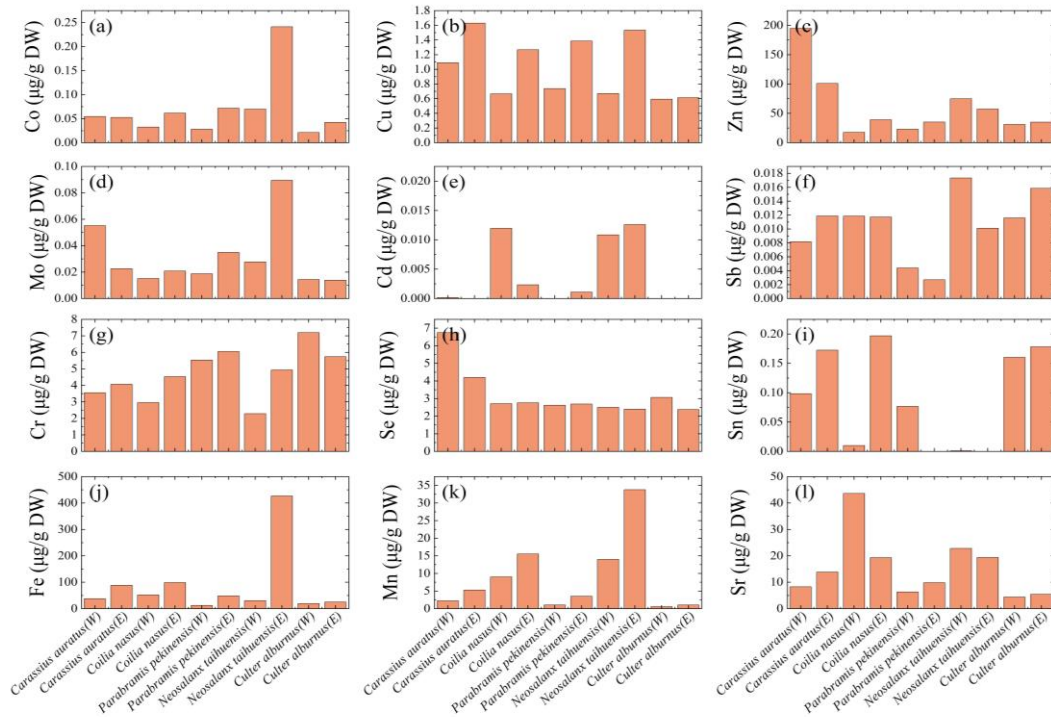


Fig. S1 The spatial distribution of trace elemental concentrations ( $\mu\text{g/g DW}$ ) in different fish species of lake area.

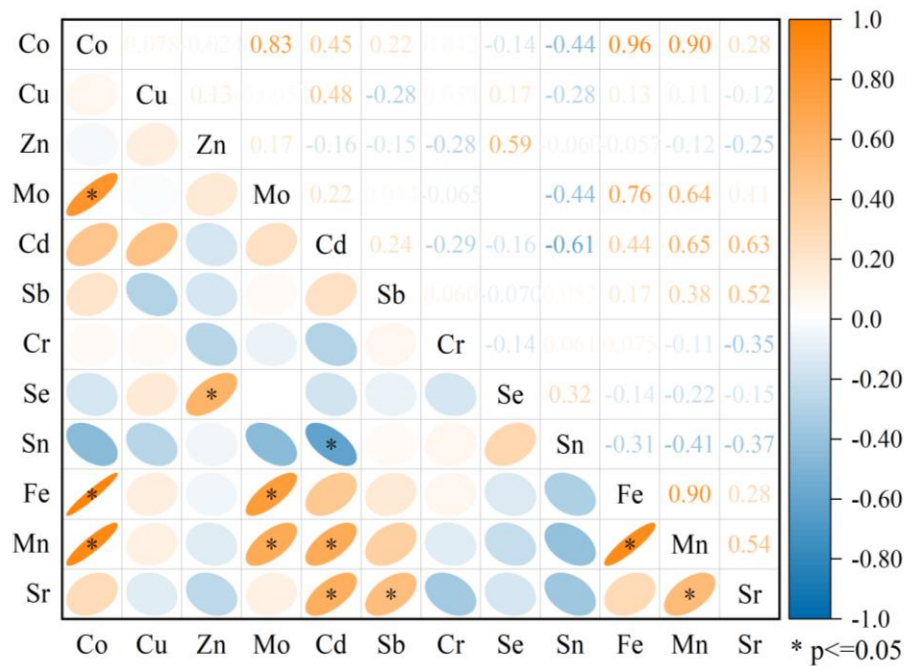


Fig. S2 The correlation analysis of trace element in fish.

Table S1 Indicators used in species of Zn in the process of PHREEQC simulation.

Index	R1	R2	R3	R4	R5	L1	L2	L3	L4	L5	L6	L7
pH	8.07	9.25	8.59	8.21	8.49	9.01	8.65	8.69	8.67	8.7	8.33	8.61
T	34.9	36.5	36.8	34	36.4	17.8	20.8	15.6	16.4	15.5	16.3	15.9
Zn( $\mu\text{g/L}$ )	0.2500	0.6790	0.4250	0.2500	0.2500	5.6400	4.5560	4.4180	4.3710	4.1160	4.2890	3.9950
Li <sup>+</sup> (mg/L)	0.0001	0.0010	0.0004	0.0002	0.0001	0.0013	0.0000	0.0000	0.0003	0.0007	0.0004	0.0000
Na <sup>+</sup> (mg/L)	32.8624	107.7578	82.6267	60.4588	57.5070	97.9322	71.4448	65.1932	61.6002	61.9415	67.6405	65.5912
NH <sub>4</sub> <sup>+</sup> (mg/L)	0.0009	0.0000	0.0064	0.0000	0.0036	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0024
K <sup>+</sup> (mg/L)	0.0396	0.4816	0.3142	0.0613	0.1978	1.3833	0.1716	0.2253	0.4883	0.6077	0.2844	0.0270
Mg <sup>2+</sup> (mg/L)	0.0515	0.5076	0.3521	0.0717	0.1386	0.6808	0.1025	0.2510	0.6208	0.5643	0.2148	0.0668
Ca <sup>2+</sup> (mg/L)	0.1587	2.0155	1.2757	0.1806	0.5402	2.3215	0.2911	0.9311	2.4588	2.1297	0.6341	0.1258
F <sup>-</sup> (mg/L)	0.3258	0.5166	0.5441	0.4937	0.5563	0.3689	0.3039	0.3672	0.3691	0.3668	0.3846	0.3771
BrO <sub>3</sub> <sup>-</sup>	0.0000	0.0000	0.0000	0.1265	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cl <sup>-</sup> (mg/L)	10.5072	40.6611	34.9736	16.0342	25.8087	52.6192	34.5439	28.9313	26.5885	26.2632	27.9067	26.8455
NO <sub>2</sub> <sup>-</sup> (mg/L)	0.1122	0.0000	0.1448	0.0892	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Br <sup>-</sup> (mg/L)	0.0000	0.2520	0.0000	0.2252	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
NO <sub>3</sub> <sup>-</sup> (mg/L)	5.1604	10.7691	9.1297	4.3887	6.0369	12.3100	8.7210	6.3388	4.1761	4.6071	4.9785	4.2566
SO <sub>4</sub> <sup>2-</sup> (mg/L)	0.0000	0.0000	0.0000	0.0000	0.0000	36.6626	25.4586	22.9792	21.5893	20.9362	22.9921	21.0828

Table S2 The mean concentrations and coefficient of variation of TEs in fish in Chaohu Lake Basin.

Elements	River		Lake	
	Mean concentrations ( $\mu\text{g/g DW}$ )	Coefficient of variation	Mean concentrations ( $\mu\text{g/g DW}$ )	Coefficient of variation
Co	0.029	16.20%	0.068	93.94%
Cu	1.495	103.22%	1.019	40.22%
Zn	80.807	63.23%	60.848	87.87%
Mo	0.021	84.37%	0.031	76.70%
Cd	0.003	223.61%	0.004	141.50%
Sb	0.003	88.66%	0.011	43.03%
Cr	3.871	32.39%	4.683	32.20%
Se	3.112	36.78%	3.207	42.12%
Sn	0.131	90.65%	0.089	92.64%
Fe	35.651	40.77%	83.906	147.39%
Mn	1.937	58.31%	8.598	120.58%
Sr	4.461	23.50%	15.319	77.51%

Table S3 Total concentration of trace elements in freshwater fish muscles worldwide ( $\mu\text{g/g DW}$ ).

		As	Cr	Mn	Fe	Ni	Cu	Zn	Cd	Se	
China	Chaohu Lake	0.412	4.292	6.096	75.510	0.551	1.243	62.327	0.007	3.058	This study
	Chaohu Lake		2.839			0.150	2.438	96.038	0.175		Yin et al., 2018
	Tai Lake	0.338	0.558	4.993	29.141			92.400	0.037		Chen et al., 2013
	Dongting Lake	0.480	1.010		4.614	0.479	0.683	18.227	0.007	1.020	Jiang et al., 2022
	Yangtze River	0.100	1.077				12.856	46.958	0.709		Yi et al., 2011
	Yellow River	0.388	1.235						0.053		Ai et al., 2022
	Pearl River	0.928	15.355						0.628		
	Huai River	0.145	1.575						1.598		
	Southeast basin	0.158	0.200						0.015		
	China	0.228	0.310						0.034		
Other countries	Bangladesh	1.040	0.760				4.970		0.110		Ahmed et al., 2019
	South Africa	<0.02	0.105				1.963	19.925	0.025	1.757	C. Plessl et al., 2019
	Poland	5.660	0.680			6.800	2.110	0.730			Szara-Bak et al., 2021
	Turkey	0.291	0.061		6.700	0.039	0.358	6.600	0.003		Varol et al., 2022
	France	0.410							0.025		Noël et al., 2013
	India		3.480				15.750	85.735	2.995		Maurya et al., 2019
	Peru	0.205					1.070	12.715			Condor et al., 2021

Table S4 Original results of mass molality of Zn species output by PHREEQC model.

	BAF		Mass molality													
	Zn	Zn <sup>2+</sup>	ZnOH <sup>+</sup>	Zn(OH) <sub>2</sub>	Zn(OH) <sub>3</sub> <sup>-</sup>	Zn(OH) <sub>4</sub> <sup>2-</sup>	ZnCl <sup>+</sup>	ZnOHCl	ZnF <sup>+</sup>	ZnCl <sub>2</sub>	ZnCl <sub>3</sub> <sup>-</sup>	ZnCl <sub>4</sub> <sup>2-</sup>	ZnBr <sup>+</sup>	ZnBr <sub>2</sub>	ZnSO <sub>4</sub>	Zn(SO <sub>4</sub> ) <sub>2</sub> <sup>2-</sup>
<i>Cyprinus carpio</i> (HB)	41043.92	2.75E-09	6.56E-10	4.12E-10	1.59E-13	3.31E-18	2.89E-12	2.63E-12	6.47E-13	8.63E-16	3.04E-19	5.25E-23	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<i>Cyprinus carpio</i> (ZG)	62031.66	2.42E-09	7.28E-10	6.66E-10	3.58E-13	1.06E-17	3.60E-12	4.66E-12	8.23E-13	1.61E-15	8.60E-19	2.29E-22	1.49E-15	1.52E-21	0.00E+00	0.00E+00
<i>Cyprinus carpio</i> <i>Cyprinus carpio</i> (NF)	15581.49	1.92E-09	1.64E-09	2.91E-09	3.80E-12	2.79E-16	6.70E-12	1.83E-11	7.11E-13	6.44E-15	7.63E-18	4.62E-21	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<i>Cyprinus carpio</i> (Z)	60830.86	1.43E-09	9.65E-10	1.42E-09	1.45E-12	8.26E-17	3.75E-12	8.35E-12	5.58E-13	2.70E-15	2.36E-18	1.03E-21	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<i>Cyprinus carpio</i> (SWL)	48908.2	2.90E-10	1.08E-09	8.94E-09	5.37E-11	1.84E-14	1.13E-12	1.42E-11	9.88E-14	1.24E-15	1.71E-18	1.22E-21	1.86E-16	2.05E-22	0.00E+00	0.00E+00
<i>Carassius auratus</i> (W)	8549.228	2.08E-08	6.22E-09	4.16E-08	6.23E-11	5.26E-15	3.60E-11	2.25E-10	3.54E-12	3.21E-14	3.42E-17	1.81E-20	0.00E+00	0.00E+00	7.79E-10	1.72E-12
<i>Carassius auratus</i> (E)	4901.075	1.64E-08	3.67E-09	4.21E-08	7.04E-11	6.58E-15	1.72E-11	1.55E-10	3.20E-12	1.15E-14	9.03E-18	3.45E-21	0.00E+00	0.00E+00	5.00E-10	9.42E-13
<i>Coilia nasus</i> (W)	774.7502	2.08E-08	6.22E-09	4.16E-08	6.23E-11	5.26E-15	3.60E-11	2.25E-10	3.54E-12	3.21E-14	3.42E-17	1.81E-20	0.00E+00	0.00E+00	7.79E-10	1.72E-12
<i>Coilia nasus</i> (E)	1785.139	1.91E-08	4.28E-09	4.26E-08	6.65E-11	5.80E-15	2.11E-11	1.70E-10	3.79E-12	1.44E-14	1.15E-17	4.46E-21	0.00E+00	0.00E+00	6.03E-10	1.16E-12
<i>Parabramis pekinensis</i> (W)	815.7959	7.36E-09	3.87E-09	7.41E-08	2.57E-10	5.14E-14	1.62E-11	2.64E-10	1.40E-12	2.13E-14	3.40E-17	2.72E-20	0.00E+00	0.00E+00	3.53E-10	1.14E-12
<i>Parabramis pekinensis</i> (E)	1704.638	1.64E-08	3.67E-09	4.21E-08	7.04E-11	6.58E-15	1.72E-11	1.55E-10	3.20E-12	1.15E-14	9.03E-18	3.45E-21	0.00E+00	0.00E+00	5.00E-10	9.42E-13
<i>Neosalanx taihuensis</i> (W)	3384.975	1.82E-08	4.00E-09	4.44E-08	7.27E-11	6.66E-15	2.11E-11	1.84E-10	3.55E-12	1.55E-14	1.34E-17	5.64E-21	0.00E+00	0.00E+00	6.07E-10	1.26E-12
<i>Neosalanx taihuensis</i> (E)	2671.141	4.09E-08	4.14E-09	1.90E-08	1.36E-11	5.42E-16	4.71E-11	1.74E-10	8.41E-12	3.35E-14	2.81E-17	1.15E-20	0.00E+00	0.00E+00	1.37E-09	2.83E-12
<i>Culter alburnus</i> (W)	1103.26	7.36E-09	3.87E-09	7.41E-08	2.57E-10	5.14E-14	1.62E-11	2.64E-10	1.40E-12	2.13E-14	3.40E-17	2.72E-20	0.00E+00	0.00E+00	3.53E-10	1.14E-12
<i>Culter alburnus</i> (E)	1749.721	2.09E-08	3.92E-09	3.54E-08	4.81E-11	3.65E-15	2.29E-11	1.64E-10	4.22E-12	1.57E-14	1.26E-17	4.92E-21	0.00E+00	0.00E+00	6.50E-10	1.24E-12

Table S5 Correlation analysis between BAF and the mass molarity and proportion of Zn species.

BAF	the mass molarity of Zn morphologies				the proportion of Zn morphologies			
	Zn <sup>2+</sup>	Zn(OH) <sub>2</sub>	ZnOH <sup>+</sup>	ZnCl <sup>+</sup>	ZnOHCl	ZnF <sup>+</sup>	ZnSO <sub>4</sub>	Zn(SO <sub>4</sub> ) <sub>2</sub> <sup>2-</sup>
BAF	-0.659**	-0.770**	0.744**	0.529*	-0.785**	0.635*	-0.686**	-0.719**

\*\* . At level 0.01 (two-tailed), the correlation was significant.

\* . At level 0.05 (two-tailed), the correlation was significant.

Table S6 BCR extraction fractions of Zn.

	<b>Exchangeble</b>	<b>Reducible</b>	<b>Oxidisable</b>	<b>Residual</b>	<b>Recovery</b>	<b>Total</b>
	<b>(µg/g)</b>	<b>(µg/g)</b>	<b>(µg/g)</b>	<b>(µg/g)</b>	<b>rate</b>	<b>(µg/g)</b>
<b>L1</b>	91.28	118.63	22.05	50.29	1.05	269.94
<b>L2</b>	12.77	17.70	10.08	34.79	0.96	78.24
<b>L3</b>	12.56	22.14	10.74	42.31	0.83	106.06
<b>L5</b>	10.24	20.84	12.72	66.75	0.96	115.12
<b>L6</b>	11.62	11.50	12.29	57.81	0.82	113.25

Table S7 Trophic levels of the different fish.

Fish species	TL
<i>Cyprinus carpio</i> (HB)	3.957872
<i>Cyprinus carpio</i> (ZG)	3.416238
<i>Cyprinus carpio</i> (NF)	2.657757
<i>Cyprinus carpio</i> (Z)	3.25933
<i>Cyprinus carpio</i> (SWL)	2.93252
<i>Carassius auratus</i> (W)	5.483565
<i>Carassius auratus</i> (E)	4.582826
<i>Coilia nasus</i> (W)	6.166775
<i>Coilia nasus</i> (E)	5.095905
<i>Parabramis pekinensis</i> (W)	5.234156
<i>Parabramis pekinensis</i> (E)	3.702229
<i>Neosalanx taihuensis</i> (W)	5.638742
<i>Neosalanx taihuensis</i> (E)	4.835281
<i>Culter alburnus</i> (W)	5.794129
<i>Culter alburnus</i> (E)	5.459926

Table S8 The feeding habits, food sources, and habitat of different fish species.

Species	Feeding habits	Food Source	Habitat
<i>Cyprinus carpio</i>	Herbivorous(main) omnivorous	Plant foods (aquatic grasses, algae, moss, corn, sorghum, rice); Animal food (fish, shrimp, shellfish, earthworms)	The bottom water
<i>Carassius auratus</i>	Herbivorous(main) omnivorous	Plant food (plant debris, aquatic grasses, algae, etc.); Animal food (cladicorns, copepods, bryozoans, rotifers, freshwater shells, clams, midge larvae, shrimp, etc.)	The bottom water
<i>Coilia nasus</i>	Carnivorous(main) omnivorous	Fish, shrimp, squid, earthworms, insects, frogs	The surface water
<i>Parabramis pekinensis</i>	Herbivorous(main)	Aquatic vascular plants (bitter grass, black algae of wheel leaf, eye seed, etc); Terrestrial grasses, vegetable leaves; Plant debris in sediment and zooplankton	The bottom water
<i>Neosalanx taihuensis</i>	Carnivorous(main) omnivorous	Plankton, shrimp and fry	The middle and lower layers of the water
<i>Culter alburnus</i>	Carnivorous(main)	Fish, shrimp, aquatic insects, plankton, aquatic plants	The middle and upper layers of the water

Table S9 The body length and weight of sampling fish.

Scientific name	Body length/cm	Weight/g
<i>Cyprinus carpio</i>	33±9.4	395.0±176.3
<i>Carassius auratus</i>	18.2±1.4	173.4±39.0
<i>Coilia nasus</i>	34.9±0.8	128.2±15.0
<i>Parabramis pekinensis</i>	20.1±1.5	197.8±48.0
<i>Neosalanx taihuensis</i>	6.7±0.4	2.7±0.5
<i>Culter alburnus</i>	32±1.8	370.4±20.0

## Section 1

In this study, an improved BCR extraction method was adopted extracted and analyzed the chemical fractions of trace elements in sediments, and the extraction methods were as follows (Mossop & Davidson, 2003):

Step 1-Extractable fraction: Put 1 g freeze-dried and 100-mesh sieved sediment in tube, and add 40 mL 0.11 mol/L CH<sub>3</sub>COOH (AR, Sinopharm Chemical Reagent, China) and shake at 25°C for 16h. The supernatant was taken after centrifugation at 6000 r/min for 15 min, filtered by 0.45μm membrane, and stored in a refrigerator at 4°C for test.

Step 2-Redusible fraction: Add 40 mL 0.1mol /L NH<sub>2</sub>OH·HCl (AR, Sinopharm Chemical Reagent, China) to the residues of step 1, repeat the above operations, and put the filtered supernatant into the refrigerator at 4°C for storage to be measured.

Step 3-Oxidizable fraction: Add 10 mL 8.8 mol/L H<sub>2</sub>O<sub>2</sub> (AR, Sinopharm Chemical Reagent, China) into the residues of Step 2 (add it 5 to 10 times to prevent the violently reacted liquid from erupting), after intermittent shock, dissolve it in a water bath at 85°C until the volume of the mixture is reduced to 2 to 3 mL, and then add 1 mol/L NH<sub>4</sub>Ac (AR, Sinopharm Chemical Reagent, China) into the mixture. After repeating the above steps of shock, centrifugation and filtration, the filtered supernatant is stored in the refrigerator at 4 ° C to be measured.

Step 4-Residual fraction: The residue obtained in step 3 is freeze-dried, and digested by microwave in a mixed acid solution of HNO<sub>3</sub> (AR, Sinopharm Chemical Reagent, China) -HClO<sub>4</sub> (AR, Sigma-Aldrich, USA)-HCl (AR, Sigma-Aldrich, USA), and then diluted and filtered with a 0.45-μm filter membrane.

The recovery rates were calculated as follows:

$$\text{The recovery rate} = \frac{F1 + F2 + F3 + F4}{\text{Total concentration}} \times 100\%$$

Where F1, F2, F3 are the concentration of trace elements in step 1, 2, 3, and F4 is the concentration of residuals, Total concentration is the concentrations of trace elements in sediment.

## Section 2:

Take the R1 water sample for example:

DATABASE phreeqc.dat

SOLUTION R1 FROM NORDSTROM AND OTHERS (1979)

units ppm

pH 8.07

Density 1.023

Temp 34.9

Li 0.0001

Na 32.8624  
K 0.0396  
Mg 0.0515  
Ca 0.1587  
F 0.3257  
Cl 10.5072  
N(3) 0.1122  
Br 0  
N(5) 5.1604  
S(6) 0  
N(-3) 0.0009 as NH4  
Zn 0.25 ppb N(5)/N(-3)  
SOLUTION\_MASTER\_SPECIES  
Zn Zn+2 0.0 65.409 65.409  
Zn(2) Zn+2 0.0 65.409  
SOLUTION\_SPECIES  
Zn+2 = Zn+2  
log\_K 0.0  
gamma 6.0 0.0  
SOLUTION\_SPECIES  
Zn+2 + Cl- = ZnCl+  
log\_k 0.43  
delta\_h 7.79 kcal  
gamma 4.0 0.0  
Zn+2 + 2Cl- = ZnCl2  
log\_k 0.45  
delta\_h 8.5 kcal  
Zn+2 + 3Cl- = ZnCl3-  
log\_k 0.5  
delta\_h 9.56 kcal  
gamma 4.0 0.0  
Zn+2 + 4Cl- = ZnCl4-2  
log\_k 0.2  
delta\_h 10.96 kcal  
gamma 5.0 0.0  
Zn+2 + F- = ZnF+  
log\_k 1.15  
delta\_h 2.22 kcal  
Zn+2 + H2O = ZnOH+ + H+  
log\_k -8.96  
delta\_h 13.4 kcal  
Zn+2 + 2H2O = Zn(OH)2 + 2H+

log\_k -16.9  
 $Zn^{+2} + 3H_2O = Zn(OH)_3^- + 3H^+$   
 log\_k -28.4  
 $Zn^{+2} + 4H_2O = Zn(OH)_4^{2-} + 4H^+$   
 log\_k -41.2  
 $Zn^{+2} + H_2O + Cl^- = ZnOHCl + H^+$   
 log\_k -7.48  
 $Zn^{+2} + SO_4^{2-} = ZnSO_4$   
 log\_k 2.37  
 delta\_h 1.36 kcal  
 $Zn^{+2} + 2SO_4^{2-} = Zn(SO_4)_2^{2-}$   
 log\_k 3.28  
 $Zn^{+2} + Br^- = ZnBr^+$   
 log\_k -0.58  
 $Zn^{+2} + 2Br^- = ZnBr_2$   
 log\_k -0.98  
 END

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 Beginning of initial solution calculations

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