

## **Supplementary Materials**

**for**

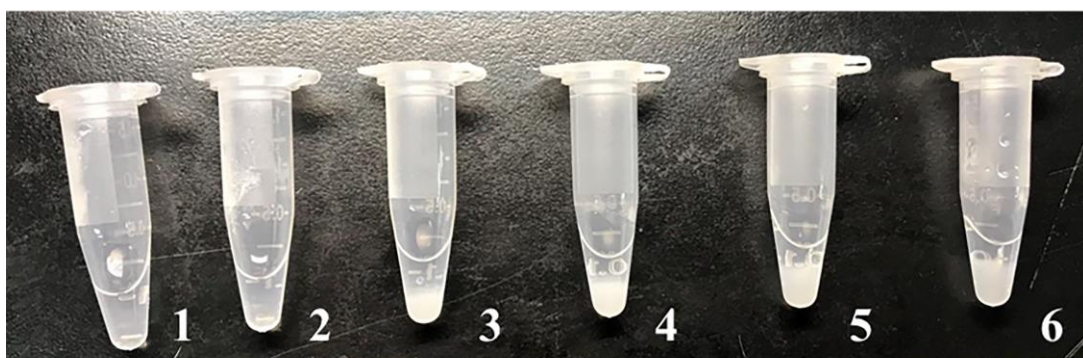
### **Structural insights for the stronger ability of shrimp ferritin to coordinate with heavy metal ions as compared to human H-chain ferritin**

*Yingjie Wang<sup>1</sup>, Jiacheng Zang<sup>1</sup>, Chengtao Wang<sup>2</sup>, Xiuqing Zhang<sup>1,\*</sup>, Guanghua Zhao<sup>1,\*</sup>*

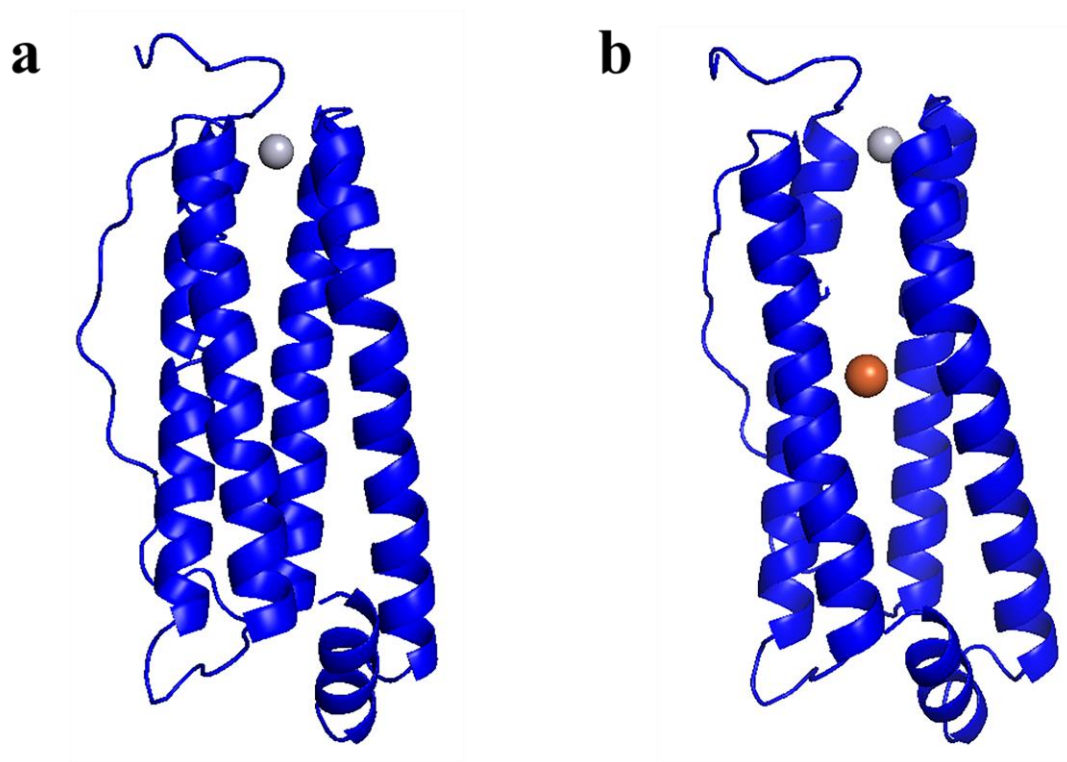
<sup>1</sup>College of Food Science and Nutritional Engineering, China Agricultural University, Beijing Key Laboratory of Functional Food from Plant Resources, Beijing, 100083, China.

<sup>2</sup>Beijing Engineering and Technology Research Center of Food Additives, Beijing Technology & Business University, No. 11 Fucheng Road, Haidian District, Beijing 100048, China.

\* Corresponding authors: E-mail: [xiuqingzhang@cau.edu.cn](mailto:xiuqingzhang@cau.edu.cn); [gzhao@cau.edu.cn](mailto:gzhao@cau.edu.cn)



**Figure S1.** Solution images of HuHF plus  $\text{Hg}^{2+}$ . Tube 1: untreated HuHF sample; tubes 2, 3, 4, 5 and 6 correspond to HuHF upon treated with  $\text{Hg}^{2+}$  at a metal/protein ratio of 50/1, 100/1, 250/1, 500/1 and 1000/1, respectively.



**Figure S2.** (a) The crystal structure of the complex of MjF and  $\text{Hg}^{2+}$  without iron near the ferroxidase site. (b) The crystal structure of the complex of MjF and  $\text{Hg}^{2+}$  with iron near the ferroxidase site. Iron is highlighted in red.

**Table S1.**

Parameters	MjF-Hg <sup>2+</sup>	MjF-Cd <sup>2+</sup>	MjF-Hg <sup>2+</sup> (remove Fe)
<b>Data collection</b>			
Beamline	SSRF BL19U	SSRF BL19U	SSRF BL19U
Wavelength (Å)	0.9789	0.9789	0.9785
Space group	<i>I4</i>	<i>P6322</i>	<i>I4</i>
Unit cell	125.372, 125.372, 176.189, 90, 90, 90	155.613, 155.613, 162.729, 90, 90, 90,	126.285, 126.285, 177.247, 90, 90, 90
<sup>a</sup> Resolution (Å)	29.55-2.30	30.02-3.00	30.02-2.70
<sup>a</sup> Redundancy	3.4	10.4	3.5
<sup>a</sup> Completeness (%)	99.8	99.6	99.9
<sup>a</sup> <i>I</i> / $\sigma$ <i>I</i>	5.8	8.7	6.6
<sup>a,b</sup> <i>R</i> <sub>pim</sub>	0.072	0.056	0.063
<sup>c</sup> CC <sub>1/2</sub>	0.982	0.990	0.976
<b>Refinement</b>			
Unique reflections	60408	23717	37908
Measured reflections	119004	43884	74922
<sup>d</sup> <i>R</i> <sub>work</sub> / <i>R</i> <sub>free</sub>	0.195 / 0.237	0.240 / 0.275	0.254 / 0.332
<i>Wilson B-factor</i> (Å <sup>2</sup> )	29.45	43.53	47.05
<i>B-factors</i> (Å <sup>2</sup> )	31.12	37.59	49.44
Rms. deviations			
Bond lengths (Å)	0.001	0.009	0.011
Bond angles (°)	1.01	1.145	1.311
Ramachandran plot (%)			
Favored	98.38	97.46	92.41
Outliers	0.10	0.15	1.83

<sup>a</sup>Highest resolution shell is shown in parentheses.

<sup>b</sup> $R_{pim} = \sum_{hkl} [1/(N-1)]^{1/2} \sum_j |I_j(hkl) - \langle I(hkl) \rangle| / \sum_{hkl} \sum_j I_j(hkl)$ , where N is the redundancy of the dataset.

<sup>c</sup>CC<sub>1/2</sub> is the correlation coefficient of the half datasets.

<sup>d</sup> $R_{work} = \sum_{hkl} | |F_{obs}| - |F_{calc}| | / \sum_{hkl} |F_{obs}|$ , where *F*<sub>obs</sub> and *F*<sub>calc</sub> is the observed and the calculated structure factor, respectively. *R*<sub>free</sub> is the cross-validation R factor for the test set of reflections (5% of the total) omitted in model refinement.