

Supporting Information

for

Re-designing Ferritin Nanocage for Mercuric Ion Detection

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      10      20      30      40      50      60      70      80      90
HuHF-MBP  .....|.....|.....|.....|.....|.....|.....|.....|.....|
            AGAAGGAGATATACATCTGATGGGCATGACCTGTGCCCGCTGTACGACCCGGTCCACCTCGCAGGTGCGCCAGAACTACCACCAGGACTC
HuHF      .....|.....|.....|.....|.....|.....|.....|.....|.....|
            .....|.....|.....|.....|.....|.....|.....|.....|.....|
            M G M T C A A C T T A S T S Q V R Q N Y H Q D S
            .....|.....|.....|.....|.....|.....|.....|.....|.....|
            M T T A S T S Q V R Q N Y H Q D S

      100     110     120     130     140     150     160     170     180
HuHF-MBP  .....|.....|.....|.....|.....|.....|.....|.....|.....|
            AGAGGCCGCAATCAACCGCCAGATCAACCTGGAGCTCTACGCCCTCCACGTTTACCTGTCCATGTCTTACTACTTTGACCGCATGATGT
HuHF      .....|.....|.....|.....|.....|.....|.....|.....|.....|
            AGAGGCCGCAATCAACCGCCAGATCAACCTGGAGCTCTACGCCCTCCACGTTTACCTGTCCATGTCTTACTACTTTGACCGCATGATGT
            E A A I N R Q I N L E L Y A S Y V Y L S M S Y Y F D R D D V

      190     200     210     220     230     240     250     260     270
HuHF-MBP  .....|.....|.....|.....|.....|.....|.....|.....|.....|
            GGCTTTGAAGAACTTTGCCAAATACCTTCTCACCAATCTCATGAGGAGAGGGAAACATGCTGAGAAACTGATGAAGCTGCAGAACCAACG
HuHF      .....|.....|.....|.....|.....|.....|.....|.....|.....|
            GGCTTTGAAGAACTTTGCCAAATACCTTCTCACCAATCTCATGAGGAGAGGGAAACATGCTGAGAAACTGATGAAGCTGCAGAACCAACG
            A L K N F A K Y F L H Q S H E E R E H A E K L M K L Q N Q R

      280     290     300     310     320     330     340     350     360
HuHF-MBP  .....|.....|.....|.....|.....|.....|.....|.....|.....|
            AGGTGGCCGAATCTTCCTCAGGATATCAAGAAACCCAGACTGTGATGACTGGGAGAGCGGGCTGAATGCAATGGAGTGTGCATTACATTT
HuHF      .....|.....|.....|.....|.....|.....|.....|.....|.....|
            AGGTGGCCGAATCTTCCTCAGGATATCAAGAAACCCAGACTGTGATGACTGGGAGAGCGGGCTGAATGCAATGGAGTGTGCATTACATTT
            G G R I F L Q D I K K P D C D D W E S G L N A M E C A L H L

      370     380     390     400     410     420     430     440     450
HuHF-MBP  .....|.....|.....|.....|.....|.....|.....|.....|.....|
            GGAAAAAATGTGAATCAGTCACCTACTGGAACCTGCACAAACTGGCCACTGACAAAAATGACCCCAATTTGTGTGACTTCATTGAGACACA
HuHF      .....|.....|.....|.....|.....|.....|.....|.....|.....|
            GGAAAAAATGTGAATCAGTCACCTACTGGAACCTGCACAAACTGGCCACTGACAAAAATGACCCCAATTTGTGTGACTTCATTGAGACACA
            E K N V N Q S L L E L H K L A T D K N D P H L C D F I E T H

      460     470     480     490     500     510     520     530     540
HuHF-MBP  .....|.....|.....|.....|.....|.....|.....|.....|.....|
            TTACCTGAATGAGCAGGTGAAAGCCATCAAAGAAATGGGGTGACCACGTGACCAACTTGCGCAAGATGGGAGCGCCGAACTGGCTTGGC
HuHF      .....|.....|.....|.....|.....|.....|.....|.....|.....|
            TTACCTGAATGAGCAGGTGAAAGCCATCAAAGAAATGGGGTGACCACGTGACCAACTTGCGCAAGATGGGAGCGCCGAACTGGCTTGGC
            Y L N E Q V K A I K E L G D H V T N L R K M G A P E S G L A

      550     560     570     580     590     600     610     620     630
HuHF-MBP  .....|.....|.....|.....|.....|.....|.....|.....|.....|
            GGAATATCTCTTTGACAAGCACACCCCTGGGAGACAGTGATAATGAAAGCTAAGGATCCGGCTGCTAACAAAGCCCGAAAGGAAGCTGAGT
HuHF      .....|.....|.....|.....|.....|.....|.....|.....|.....|
            GGAATATCTCTTTGACAAGCACACCCCTGGGAGACAGTGATAATGAAAGCTAAGGATCCGGCTGCTAACAAAGCCCGAAAGGAAGCTGAGT
            E Y L F D K H T L G D S D N E S * G S G C * Q S P K G S * V
            E Y L F D K H T L G D S D N E S *

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Figure S1. Complete nucleotide sequences of HuHF-MBP and HuHF. The chain of hybrid gene were prepared by grafting a mercury binding peptide gene, grafted extra codons are highted within a red box.

Table S1. Crystallographic properties and data collection and model refinement statistics.

Parameters	HuHF-MBP
X-ray source	Shanghai Synchrotron Radiation Facility SSRF (BL19U)
Wavelength (Å)	0.9789
Space group	P42
Resolution range (Å)	47.75 - 3.503 (3.628 - 3.503)
Unit cell	217.524, 217.524, 146.821, 90, 90, 90
Unique reflections	85322 (8499)
Completeness (%)	98
Mean I/sigma (I)	1.5
Wilson B-factor	46.27
CC1/2	0.945
Reflections used in refinement	84692(8479)
Reflections used for R-free	1997 (198)
R-work	0.3397 (0.3697)
R-free	0.3967 (0.4561)
Number of non-hydrogen atoms	33912
macromolecules	33912
Protein residues	4128
RMS (bonds)	0.003
RMS (angles)	0.50
Ramachandran favored (%)	98
Ramachandran allowed (%)	1.9
Ramachandran outliers (%)	0.44
Rotamer outliers (%)	1.2
Clashscore	5.32
Average B-factor	34.03
macromolecules	34.03