

Electronic Supplementary Information (ESI)

Peroxynitrite scavenger FeTPPS bind with hCT to effectively inhibit its amyloid aggregation

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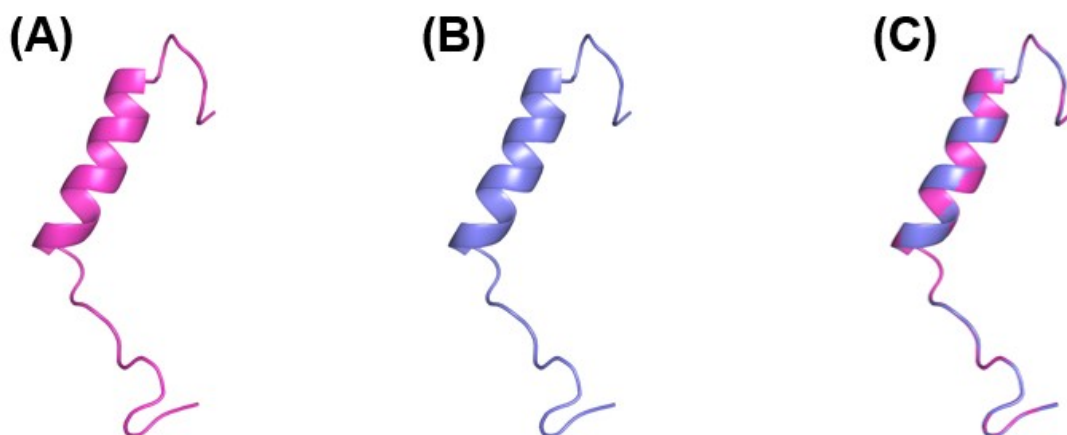


Figure S1. (A) 3D structure of template: 7TYH; (B) The structure model of hCT generated by homology modeling using template: 7TYH; (C) The superposition of template with hCT model.

Procedure for model construction:

The structure model of hCT was constructed on the Swiss-Model online server (<https://swissmodel.expasy.org/>). The templates search was firstly carried out according to the sequence of hCT (CGNLSTCMLGTYTQDFNKFHTFPQTAIGVGAP, disulfide bond: Cys1-Cys7). Among these search results, the template:7TYH with the largest GMQE value (0.8) and the 100% sequence identity, presenting the high quality of the model prediction, was chose for model construction. Then, the model of hCT was built based on the template.

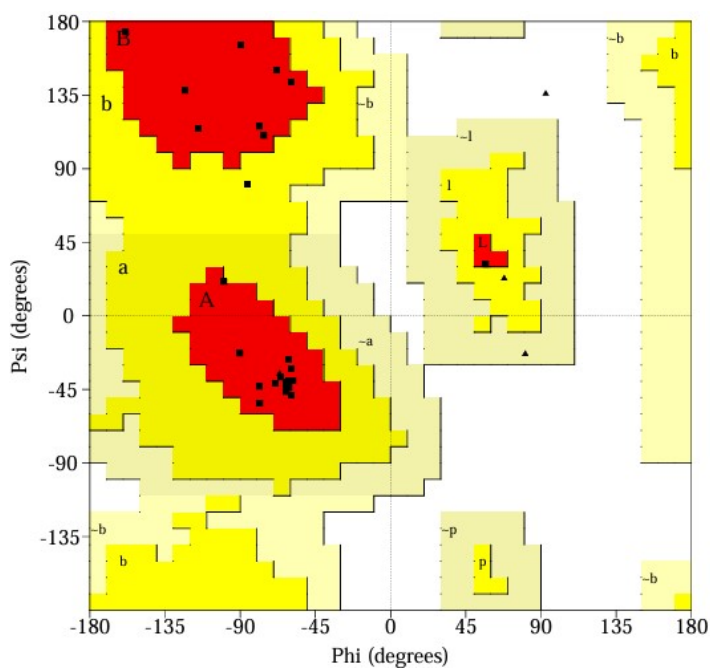


Figure S2. The Ramachandran plot of hCT model.

Evaluation for model construction:

The obtained structure model of hCT was evaluated using SAVES v6.0 (<https://servicesn.mbi.ucla.edu/SAVES/>). As shown in **Figure S2**, the number of residues within the reliable range (Residues in most favoured regions [A, B, L]) is 23, accounting for 92.0% of the total sequence, and two residues locate in the allowed range (Residues in additional allowed regions [a, b, l, p]), accounting for 8% of the total sequence. The residues within the reliable and allowed ranges account for 100% in total. This result suggests that the structure model of hCT generated by homology modeling is reasonable and credible.

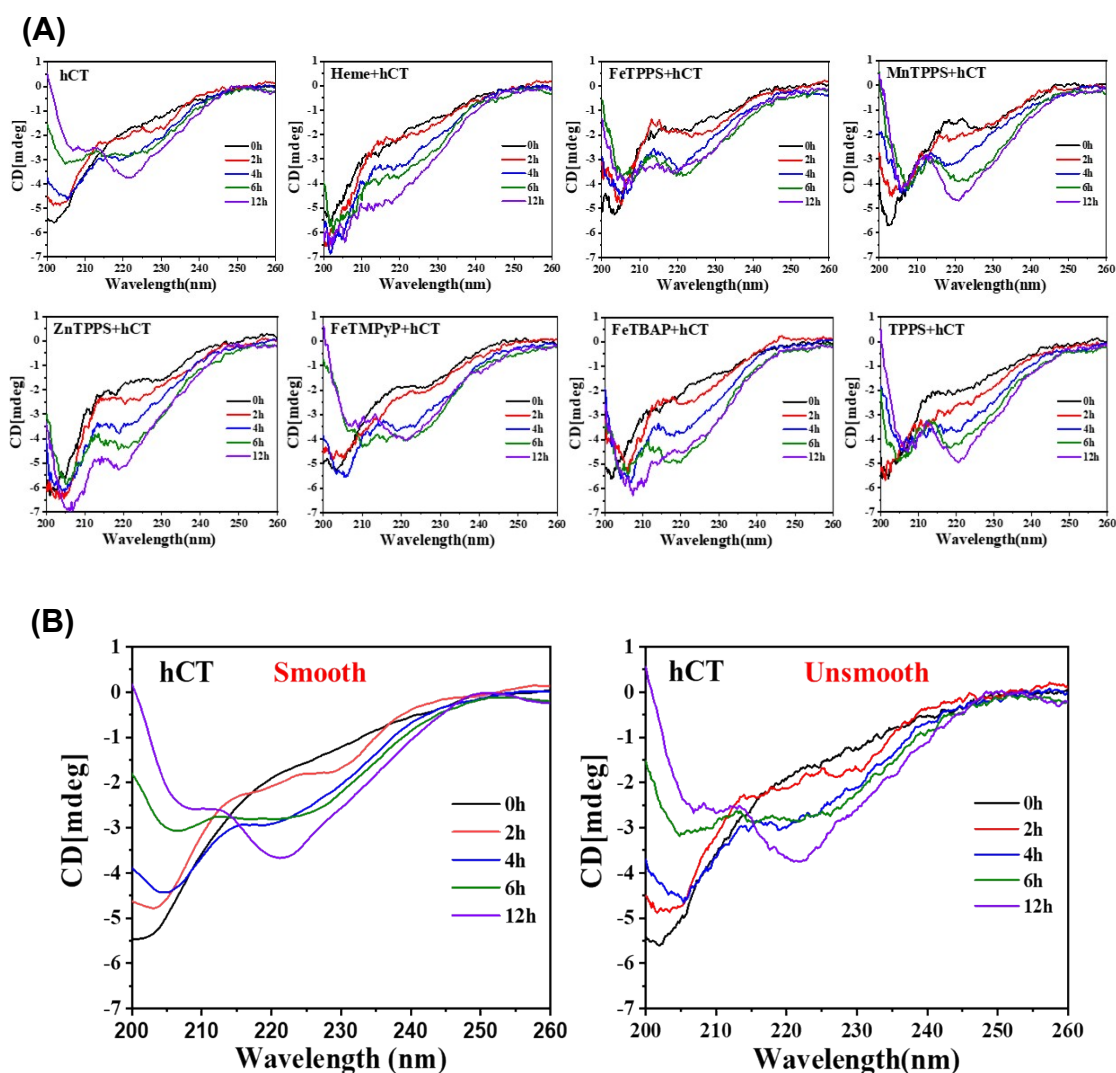


Figure S3. (A) The original time-dependent CD spectra for hCT (20 μ M) without or in presence of porphyrin (10 μ M) during 12 h; (B) The original spectra of hCT along with the smoothed one.