Electronic Supplementary Information

Elevated Amyloidoses of Human IAPP and Amyloid Beta by Lipopolysaccharide and Their Mitigation by Carbon Quantum Dots

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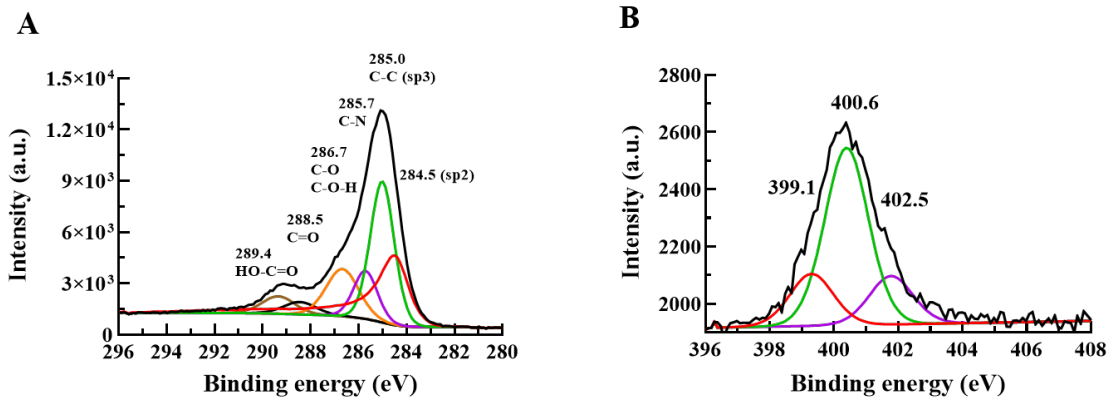

Figure S1. High-resolution XPS spectra of CQDs. (A) C 1 s and (B) N 1 s.

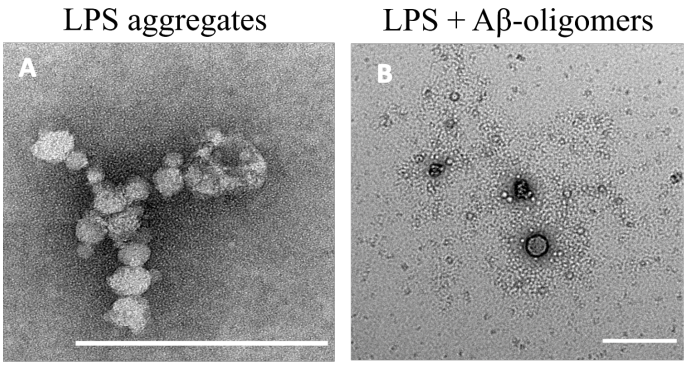

Figure S2. TEM imaging of LPS and Aβ interacting with LPS of different conformations. LPS aggregates (A), LPS micelles surrounded by Aβ monomers (B). Scale bars: 200 nm.

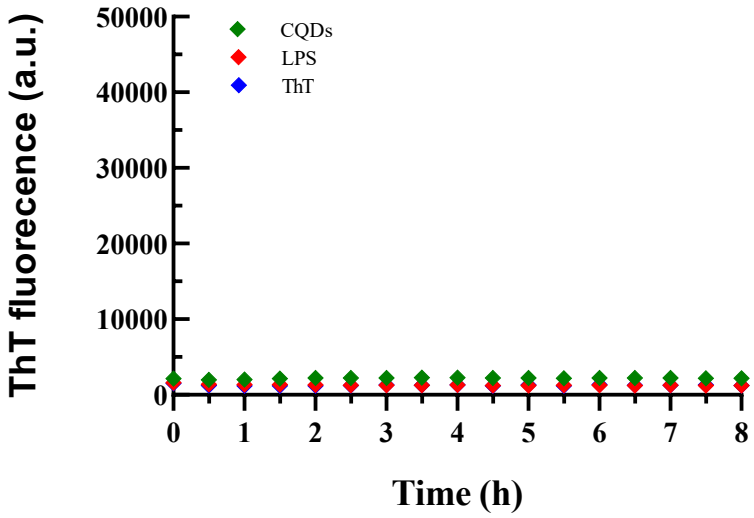

Figure S3. ThT fluorescence of CQDs, LPS and ThT dye. CQDs, LPS and ThT concentrations are as follows: 200 µg/mL, 0.78 µg/mL and 100 µM. Excitation/emission: 440/484 nm.

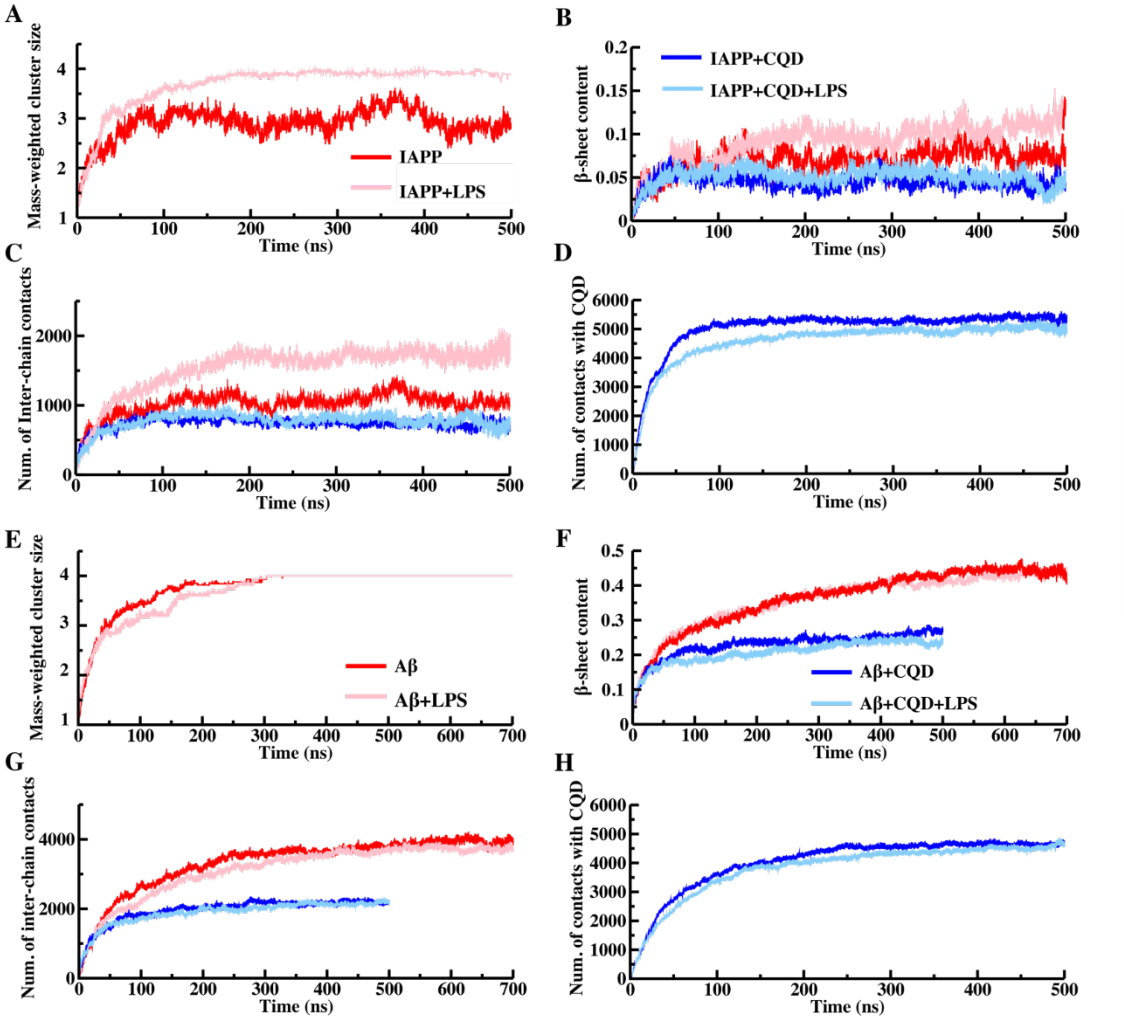

Figure S4. Dynamics of the aggregation processes of IAPP (A-D) and Aβ (E-H). The mass-weighted cluster size (**A**), β-sheet content (**B**), number of inter-chain contacts (**C**) and number of contacts between peptides and a CQD (**D**) for the systems with IAPP. The mass-weighted cluster size (**E**), β-sheet content (**F**), number of inter-chain contacts (**G**) and number of contacts between peptides and the CQD (**H**) for the systems with Aβ.

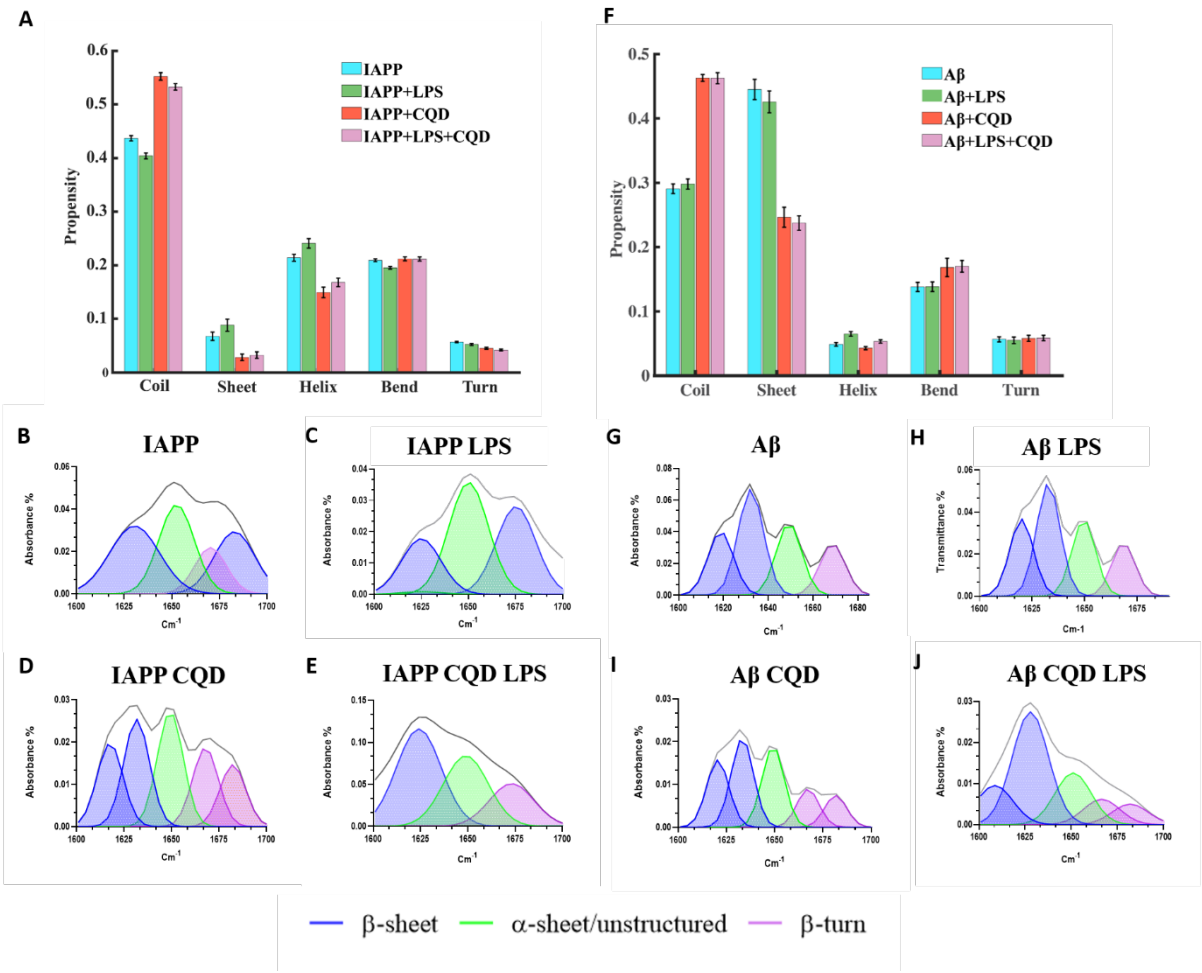

Figure S5. Analysis of the secondary structures of IAPP and Aβ in the presence of LPS and CQDs. DMD simulations (top row) and FTIR spectral deconvolution analysis (bottom row).

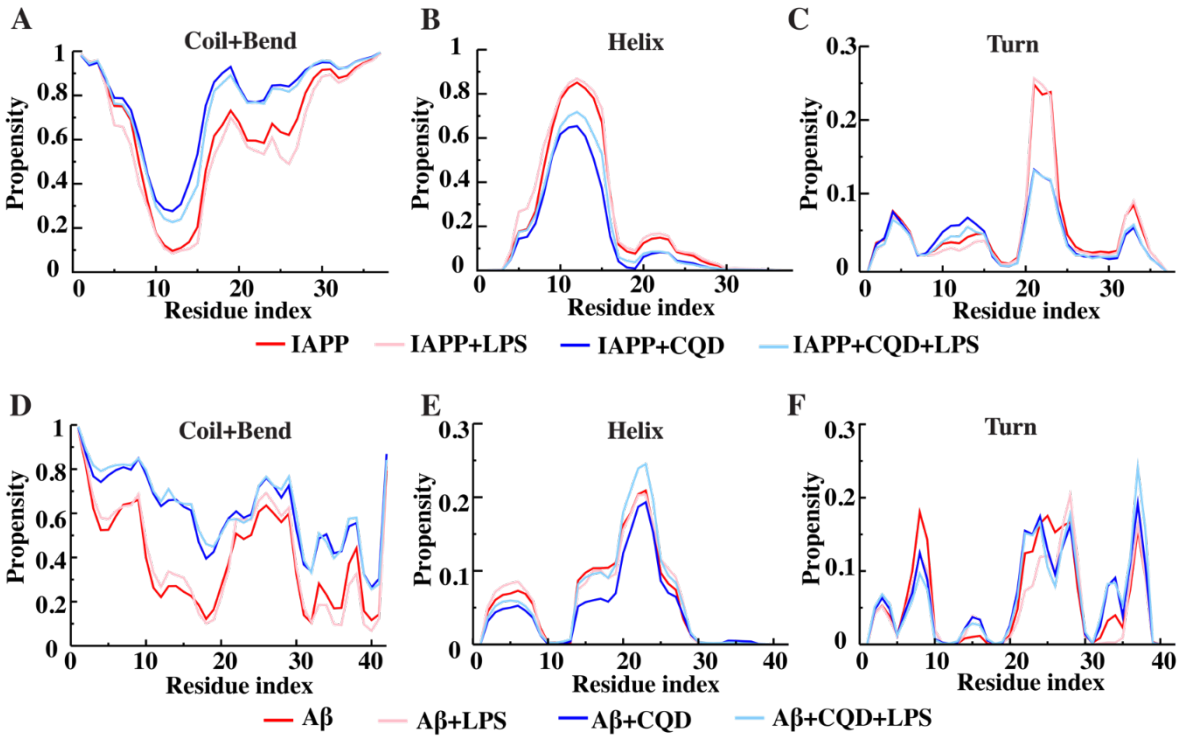

Figure S6. *In silico* IAPP and Aβ secondary structure analyses. The rises in the β-sheet contents in the peptides in the presence of LPS at residues 16-20 and 24-32 were due to the reduction in the propensity of unstructured coils and bends (**A-C, Fig. 3C**). For Aβ, its β-sheet content was specifically promoted in the regions with strong LPS binding (residues 16-21 and 31-40), and reduced in other regions (**D-F, Fig. 3D**). The reduction was likely a result of additional electrostatic interactions between the negatively charged Aβ and LPS. For both IAPP (**A-C**) and Aβ (**D-F**), CQDs reduced their β-sheet propensities by increasing the coil and bend structures.

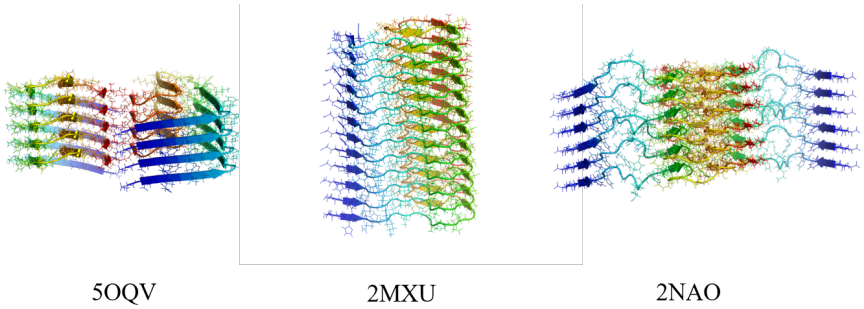

Figure S7. Examples of solved Aβ fibril structures. For each of the PDB structures, the individual peptide is shown in cartoon and colored in rainbow, highlighting the formation of in-registered parallel β-sheet between adjacent peptides in the fibril.

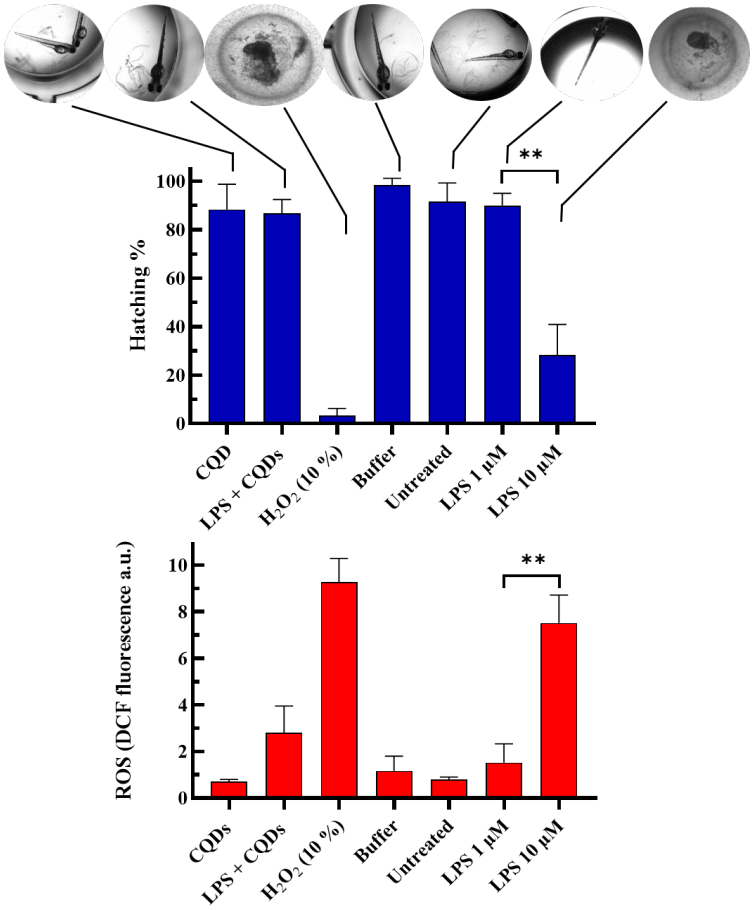

Figure S8. Hatching rates and ROS levels of zebrafish exposed to control treatments. LPS (10 and 1 µM), CQDs (0.5 µg/mL), and LPS (1 µM) with CQDs (0.5 µg/mL), IAPP (10 µM) or Aβ (10 µM) were microinjected to the embryos. The embryos were imaged at 3 h post injection under the green and bright field channels of a fluorescence microscope. ROS production was measured 12 h after injections. Hatching of the embryos was calculated at 3 days post injection. P<0.005 **

Table S1. Band assignments in FTIR spectroscopy[1]

Secondary structure	**Band wavenumber (cm^{-1})**
α-helix	1648 - 1657
β-sheet	1623 - 1641, 1674 - 1695, 1615 - 1627
β-turns	1622 - 1686
Unstructured	1642 - 1657

References

1. B. Srour, S. Bruechert, S. L. A. Andrade and P. Hellwig, *Methods Mol. Biol.*, 2017, **1635**, 195-203.