Supplementary information for

Unveiling the inhibition mechanism of host-defense peptide cathelicidin LL-37 on the amyloid aggregation of human islet amyloid polypeptide

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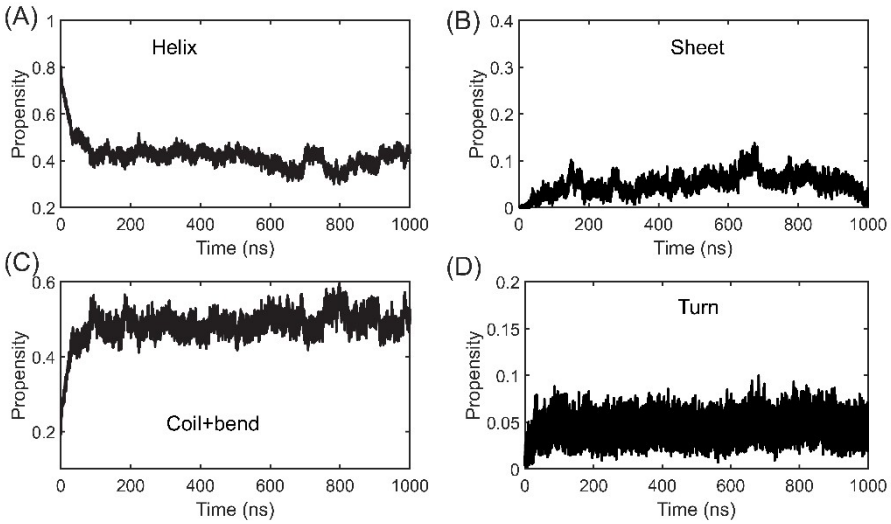

Figure S1. **Variations of the secondary structure propensities of LL37 monomer as a function of time.** (A) Helix, (B) β-sheet, (C) coil and bend, and (D) turn structures.

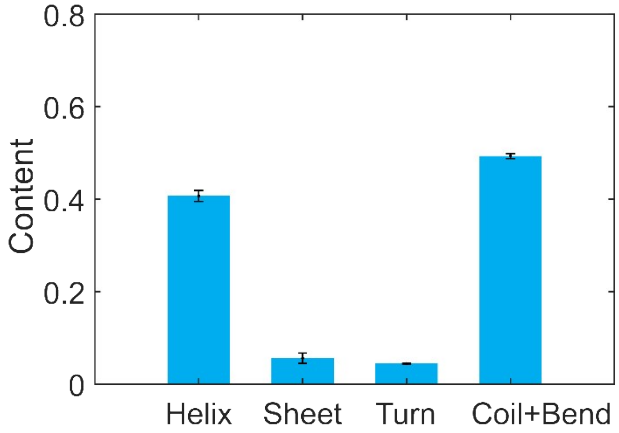

Figure S2. **Secondary structure contents of the monomeric LL37 peptide**.

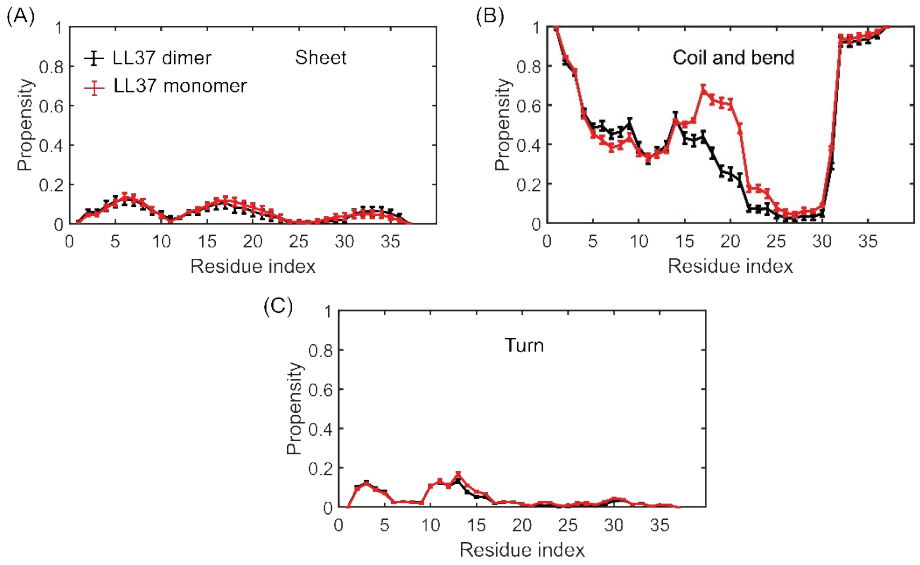

Figure S3. **Secondary structure propensities of each LL37 residue for the LL37 monomer and dimer.** (A) β-sheet; (B) coil and bend; (C) turn structure.

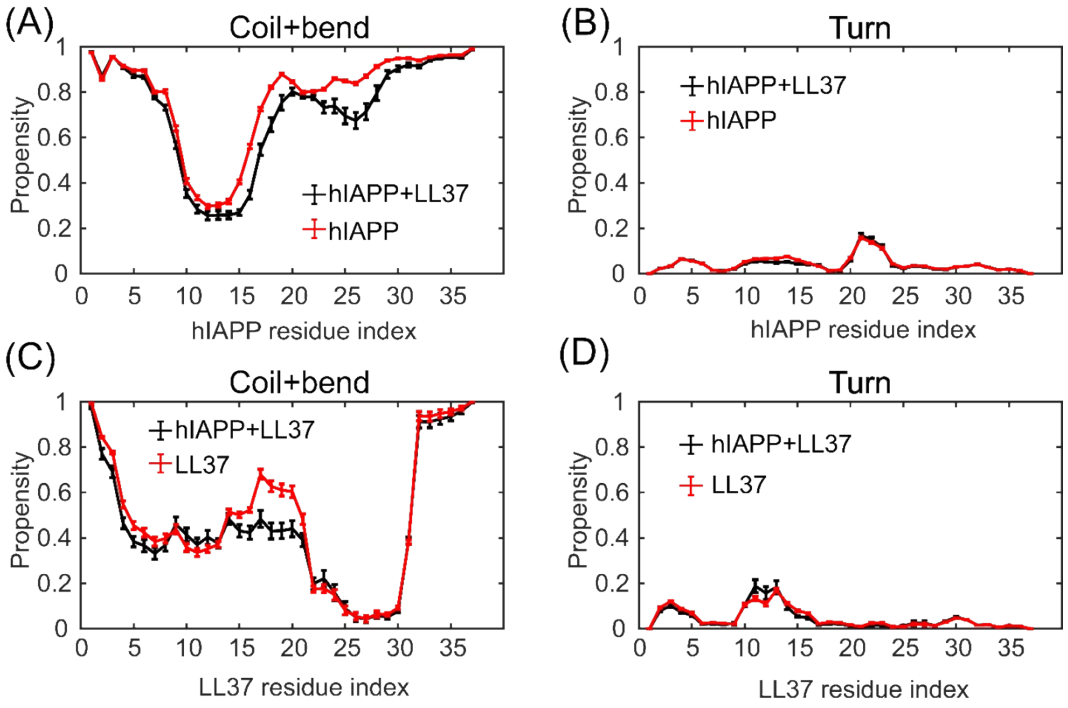

Figure S4. **Secondary structure propensities of each residue**. (A) Coil and bend, and (B) propensities of each hIAPP residue for the system with hIAPP:LL37=1:1 and monomeric hIAPP. (C) Coil and bend, and (D) propensities of each LL37 residue for the system with hIAPP:LL37=1:1 and monomeric LL37.

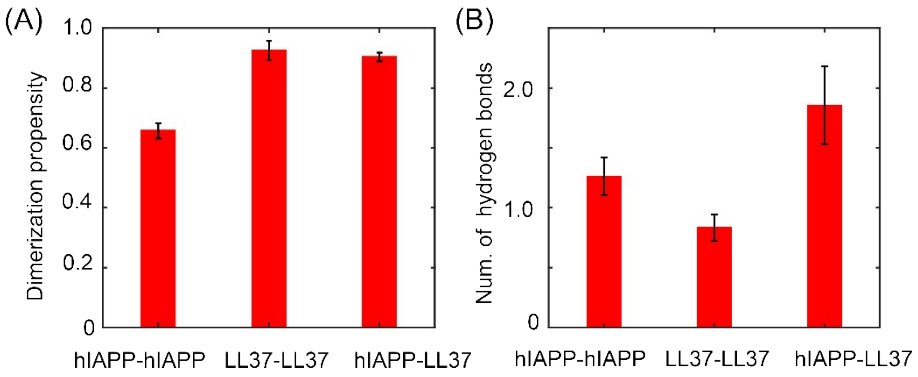

Figure S5. (A) Dimerization propensities of hIAPP-hIAPP, LL37-LL37, and hIAPP-LL37 systems. (B) Ensemble-averaged Number of hydrogen bonds for the systems with hIAPP-hIAPP, LL37-LL37, and hIAPP-LL37.

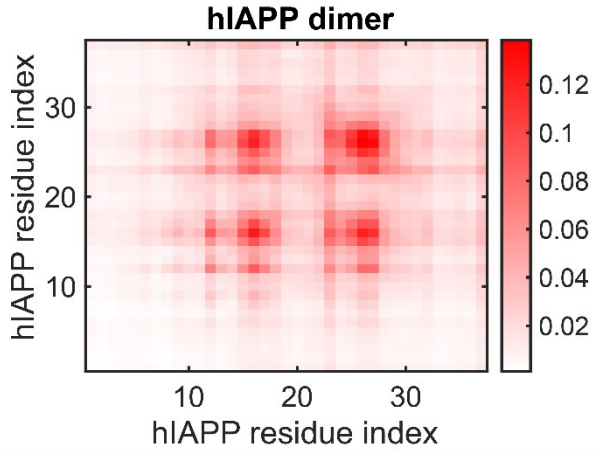

Figure S6. Inter-peptide contact frequency between each hIAPP residue during the dimerization of hIAPP peptides.