Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Distinct Oligomerization and Fibrillization Dynamics of Amyloid Core Sequences of Amyloid-beta and Islet Amyloid Polypeptide

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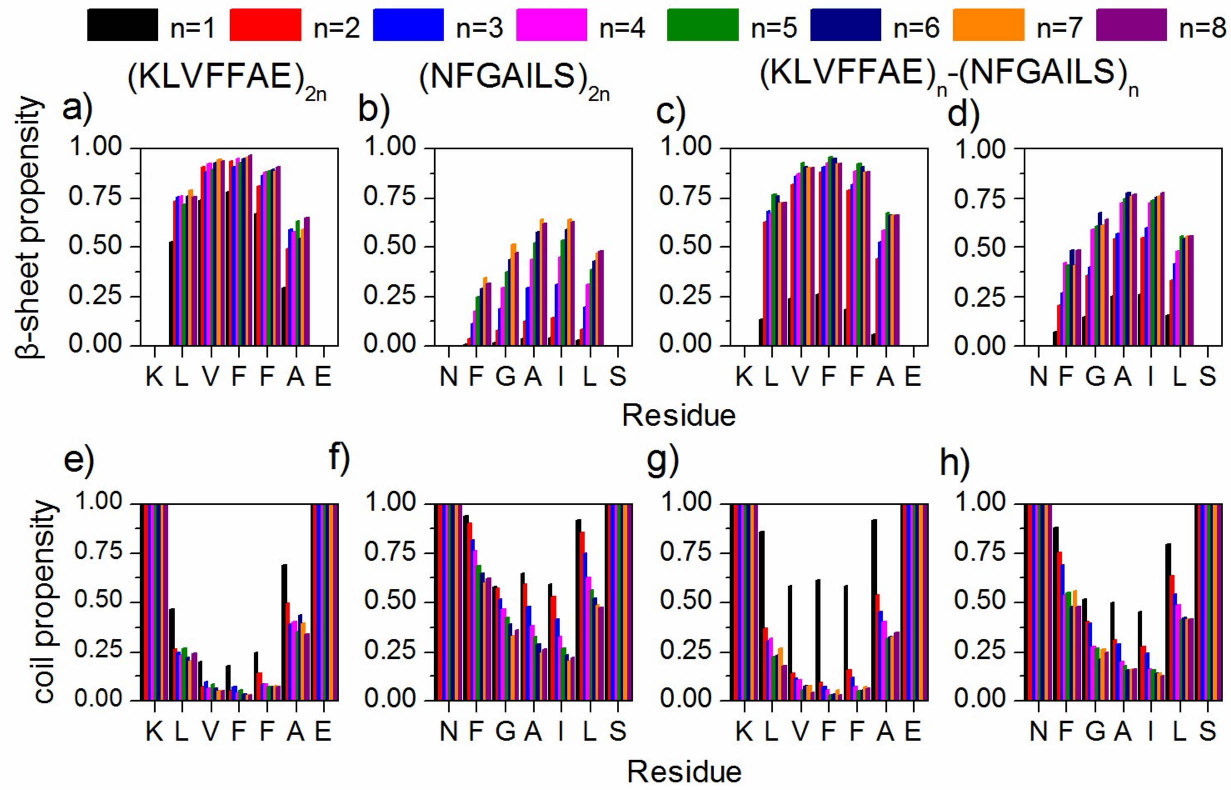

Figure S1. The averaged β-sheet and coil propensity for each residue using last 100 ns based on 10 independent DMD simulations for each system.

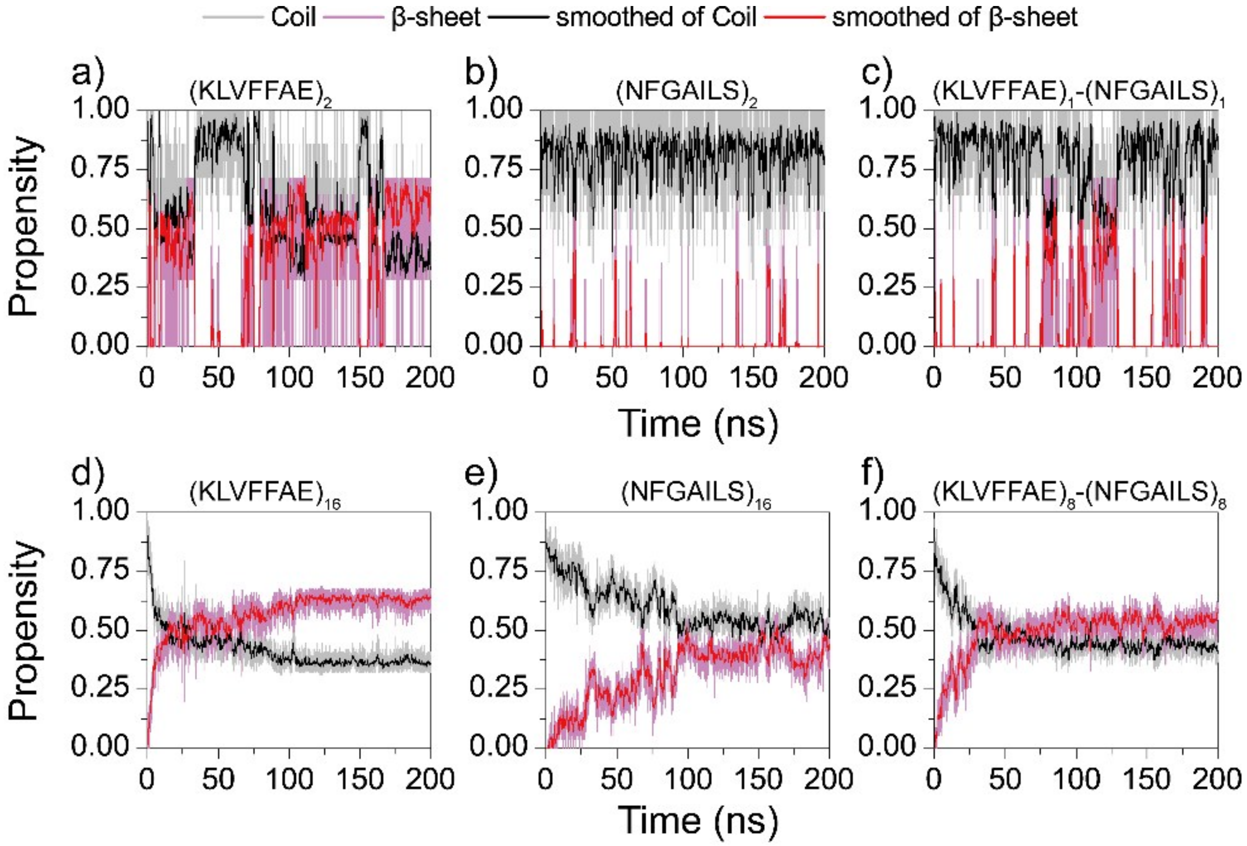

Figure S2. The time evolution of coil and β-sheet secondary structure propensities for $(KLVFFAE)_{2n}$, $(NFGAILS)_{2n}$ and $(KLVFFAE)_n$-$(NFGAILS)_n$. For each system we only show one representative trajectory from ten independent DMD simulations.

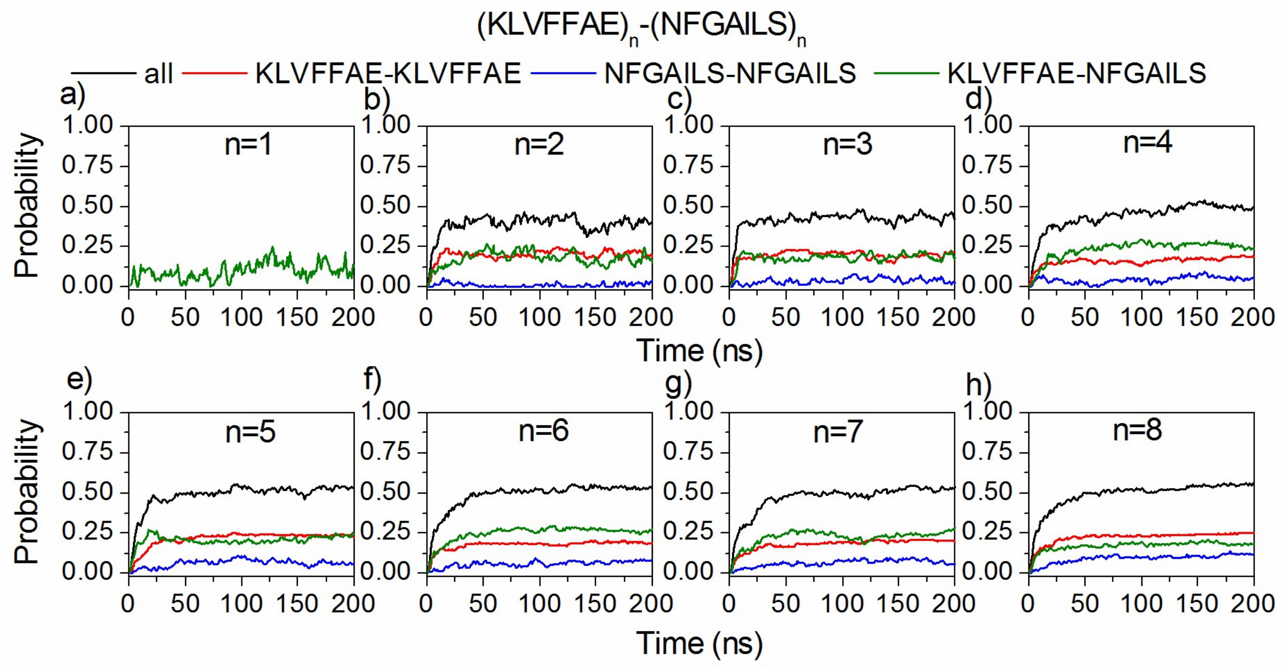

Figure S3. The time evolution of averaged probability of all of the β-sheet (black line), KLVFFAE-KLVFFAE (red line), NFGAILS-NFGAILS (blue line), and KLVFFAE-NFGAIL (green) β-sheet in the (KLVFFAE)$_n$-(NFGAILS)$_n$ systems using 10 independent MD simulation trajectories.

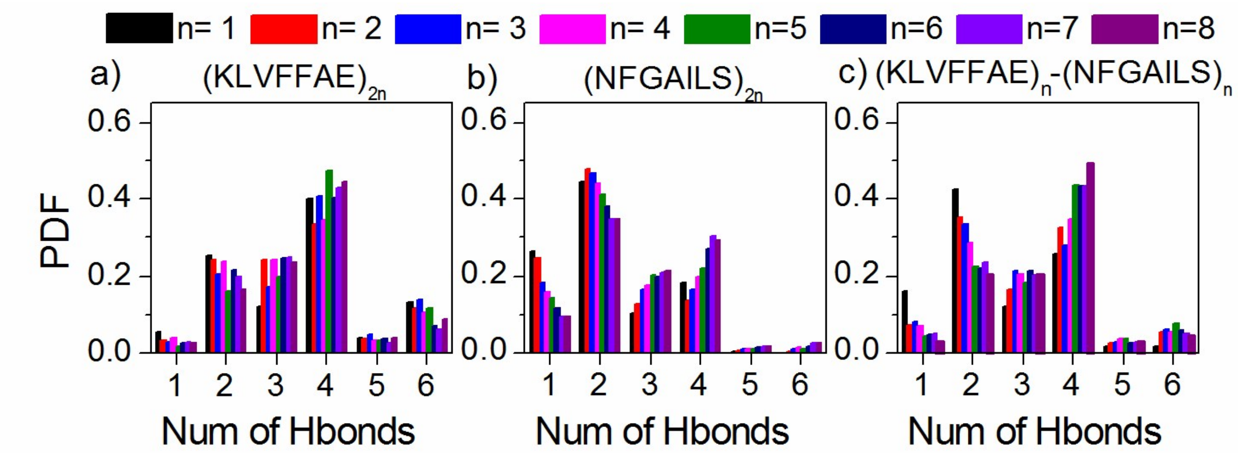

Figure S4. The probability distribution function of the hydrogen bonds between the main chains of connected peptides in each system.

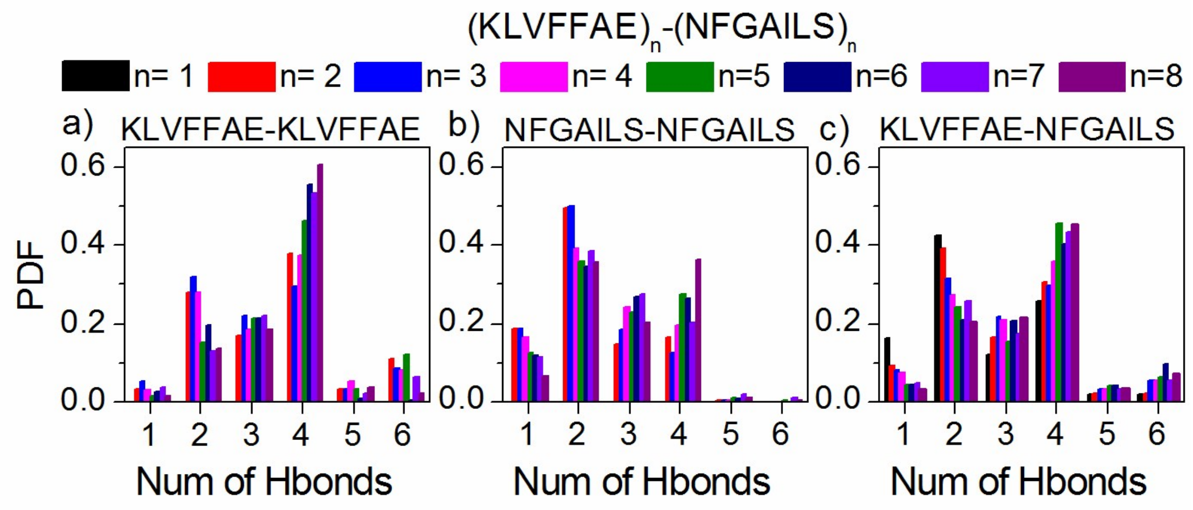

Figure S5. The probability distribution function of the hydrogen bonds between the main chain of each type connected peptides in $(KLVFFAE)_n$-$(NFGAILS)_n$ systems.

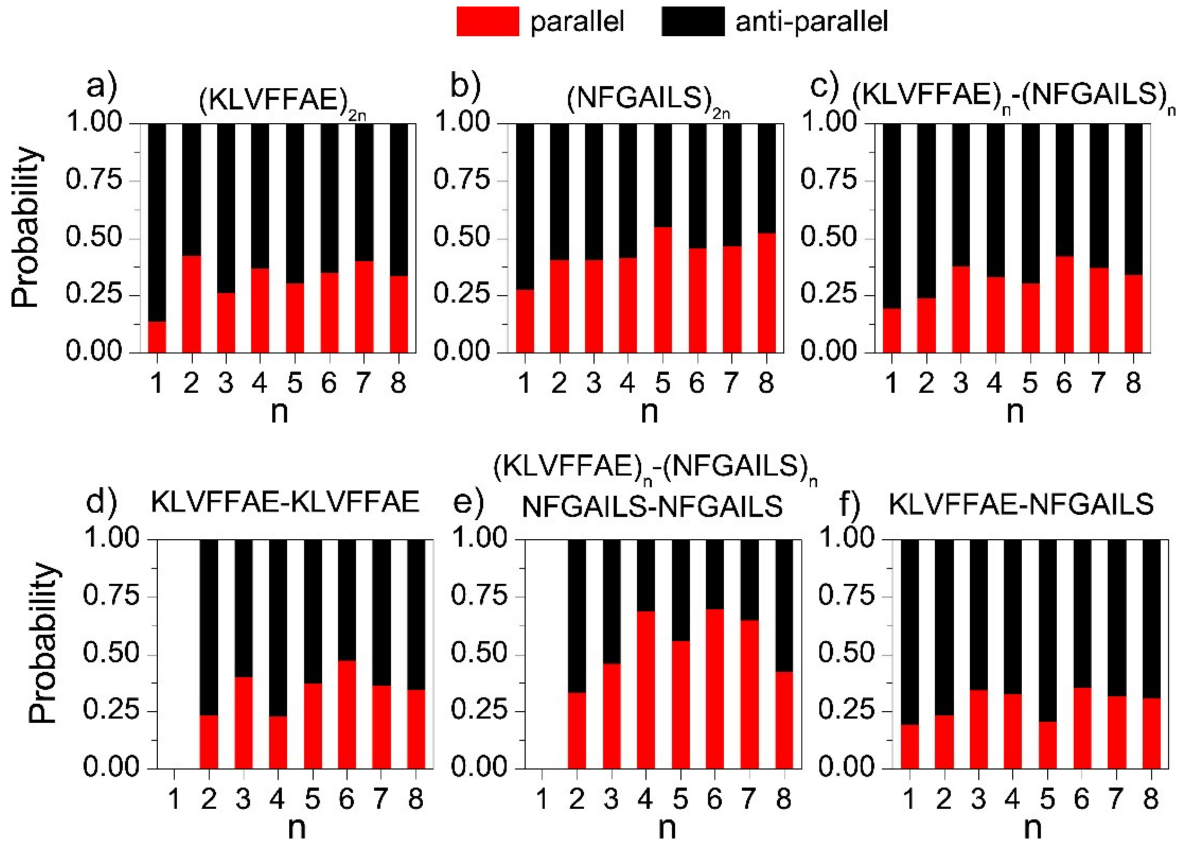

Figure S6. The probability of parallel and anti-parallel β-sheet observed in each system: $(KLVFFAE)_{2n}$ a), $(NFGAILS)_{2n}$ b) and $(KLVFFAE)_n$-$(NFGAILS)_n$ c), and the parallel and anti-parallel ratio in the β-sheet formed by KLVFFAE-KLVFFAE d), NFGAILS-NFGAILS e), and KLVFFAE-NFGAILS f) in $(KLVFFAE)_n$-$(NFGAILS)_n$ systems.

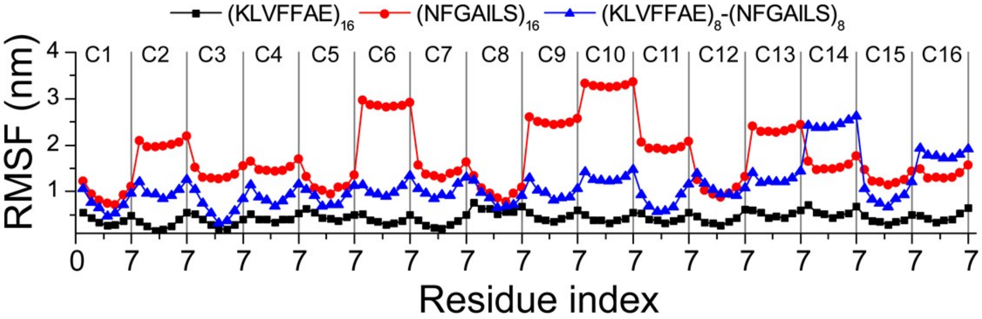

Figure S7. The root-mean-square fluctuation (RMSF) per residue computed during the last 100 ns simulation trajectories. The chain index was labeled as C_i (e.g., C5 denotes the fifth chain). For the (KLVFFAE)$_8$-(NFGAILS)$_8$ system, C1~C8 and C9~C16 represented the eight Aβ16-22 and eight IAPP22-28 peptides, respectively,.