

Supporting information

The self-assemble mechanism of tetra-peptides from the motif of β -amyloid peptide: a combined coarse grain and all atom molecular dynamics simulation.

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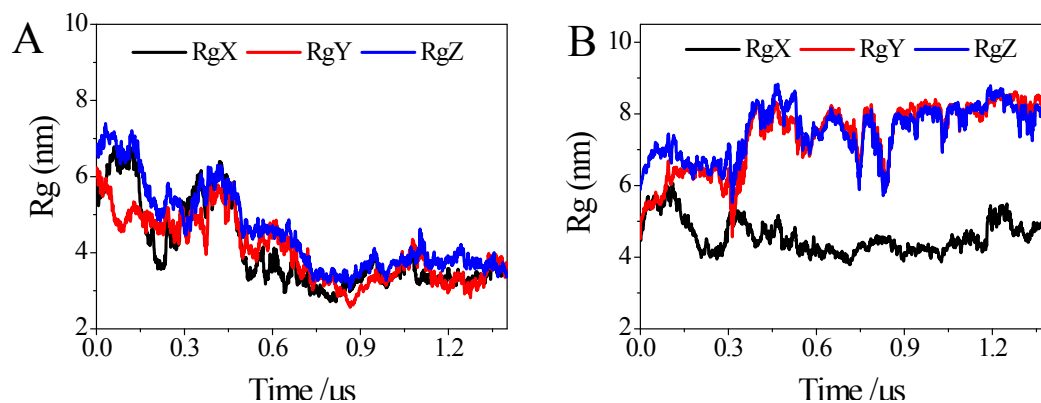


Figure S1. The evolution of radius of gyration (Rg) in the self-assembly process of two different types of tetra-peptides: (A) VFFA and (B) KFFA. Change of the x , y and z components of Rg are represented by black line, red line and blue line, respectively.

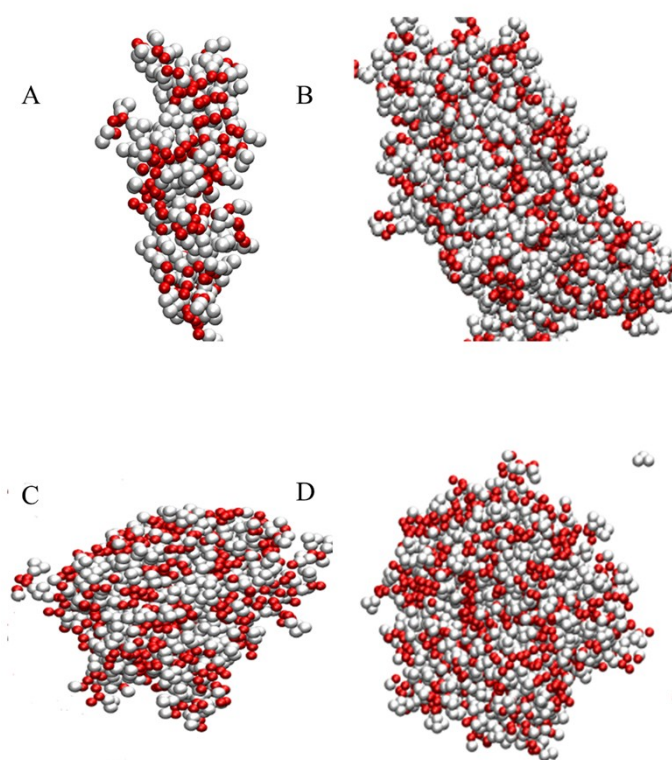


Figure S2. The configuration at the concentration of (A) 10 mg/mL and (B) 40 mg/mL for KFFA, and concentration of (C) 10 mg/mL and (D) 40 mg/mL for VFFA at the end of CG simulations.

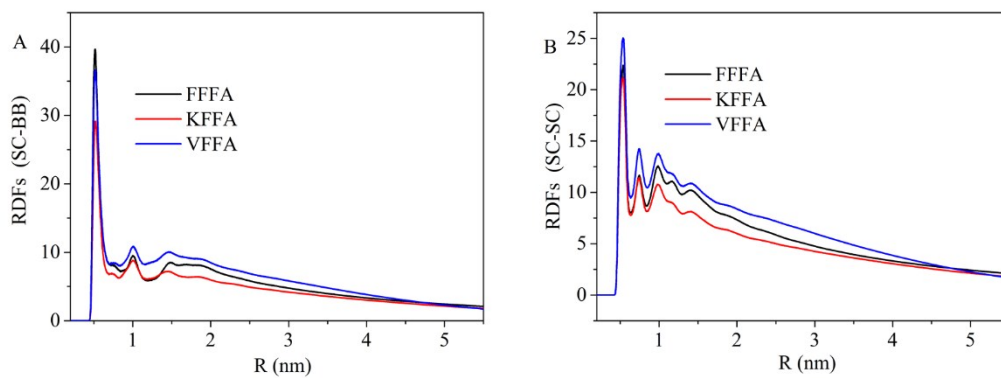


Figure S3. The radial distribution functions of (A): side chains beads to main chain beads and (B) side chains beads to side chains beads from last 1 μ s simulation in three different systems: FFFA (black line), KFFA (red line), and VFFA (blue line).