Supporting Information

Free Energy Profile and Mechanism of Self-Assembly of Peptide Amphiphiles Based on a Collective Assembly Coordinate

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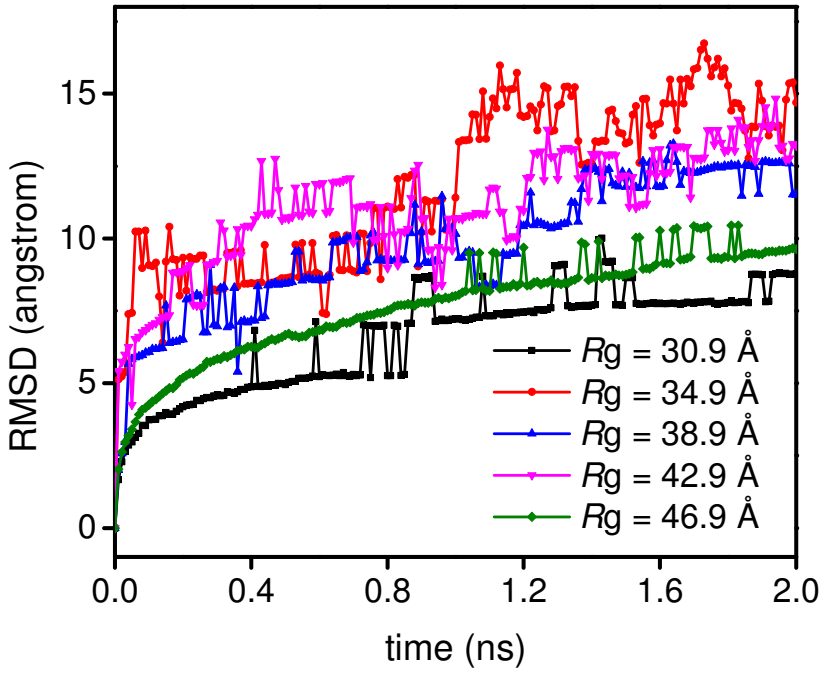

Figure S1. The RMSD values for the 2 ns equilibrium process after TMD calculation based on MD calculations in which the radius of gyration of the PAs is constrained to the TMD result. The RMSD was calculated by comparing configurations in the equilibrating calculations with the TMD-generated intermediate structure for various R_g values.

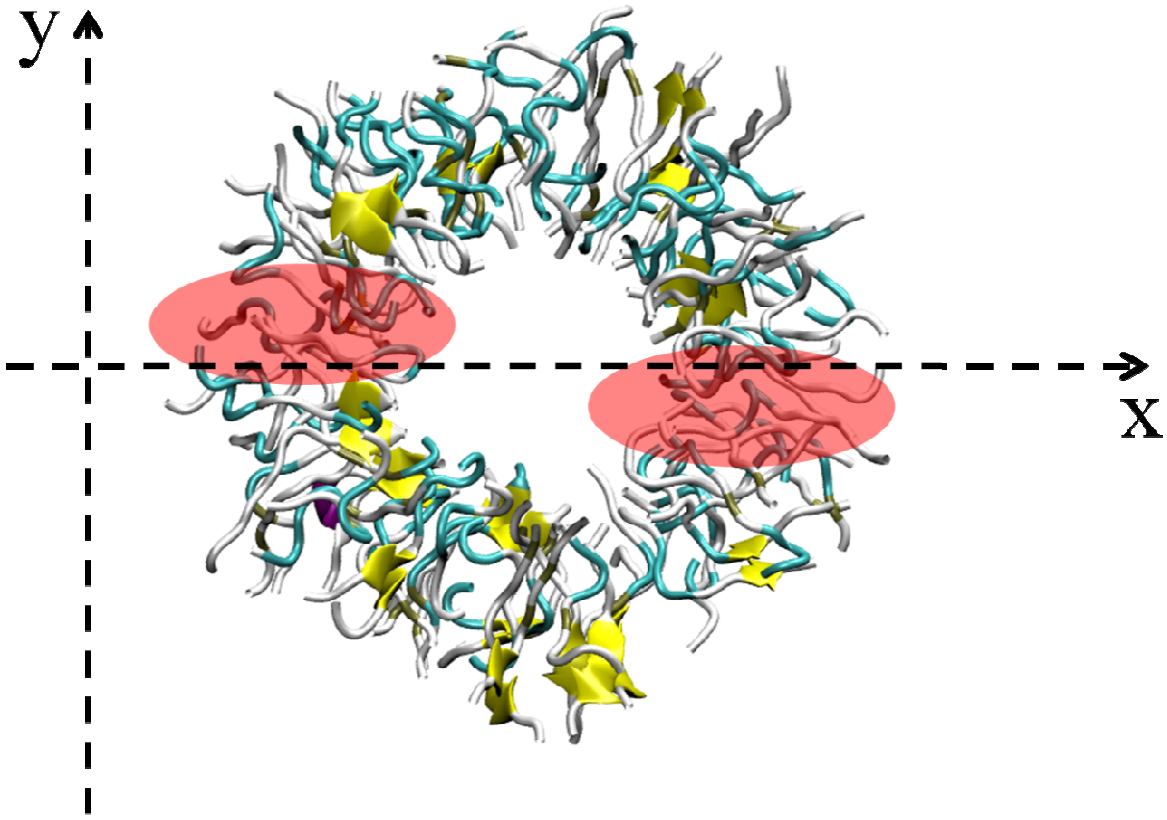

Figure S2. The spatial secondary structure (yellow: beta-sheet strand, green: turn, purple: alpha-helix, and white: rand coil) distribution of the bound state (top view), and the pink oval areas highlight the range where locates the PAs with mostly random coil structure.

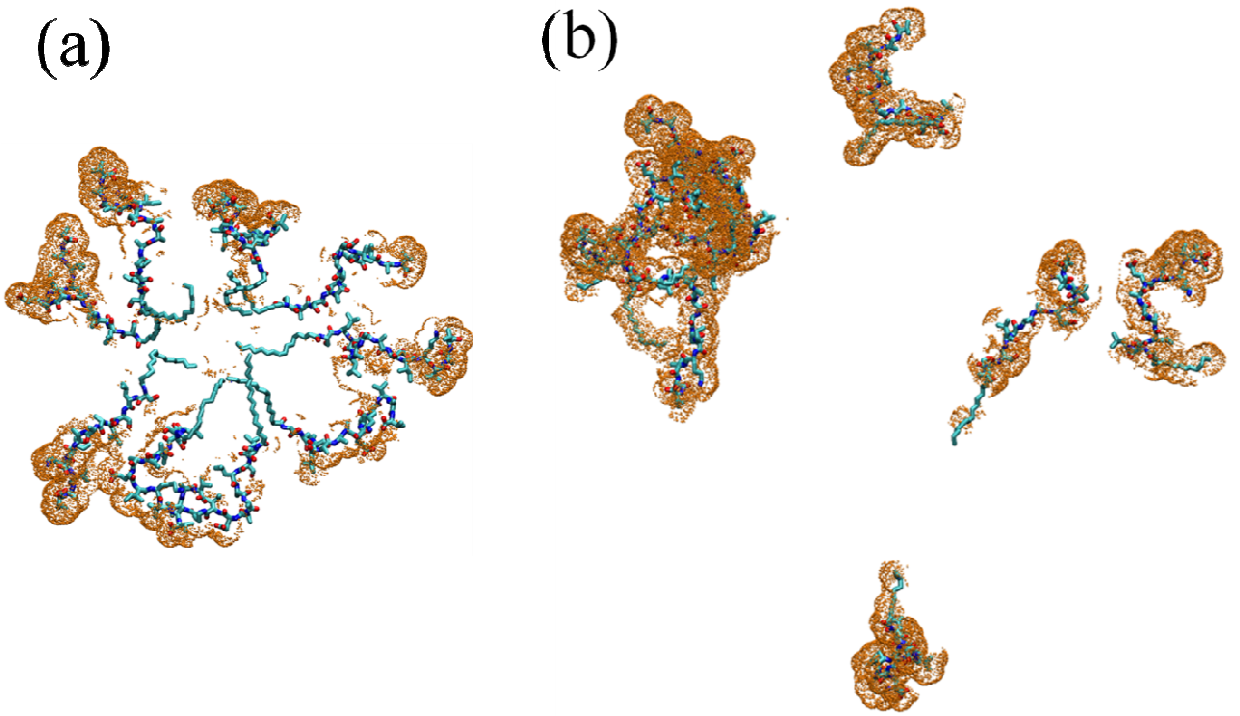

Figure S3. The solvent accessible surface area (SASA) of a group of PAs in the (a) bound state and (b) free state. The SASA is represented by orange dots.

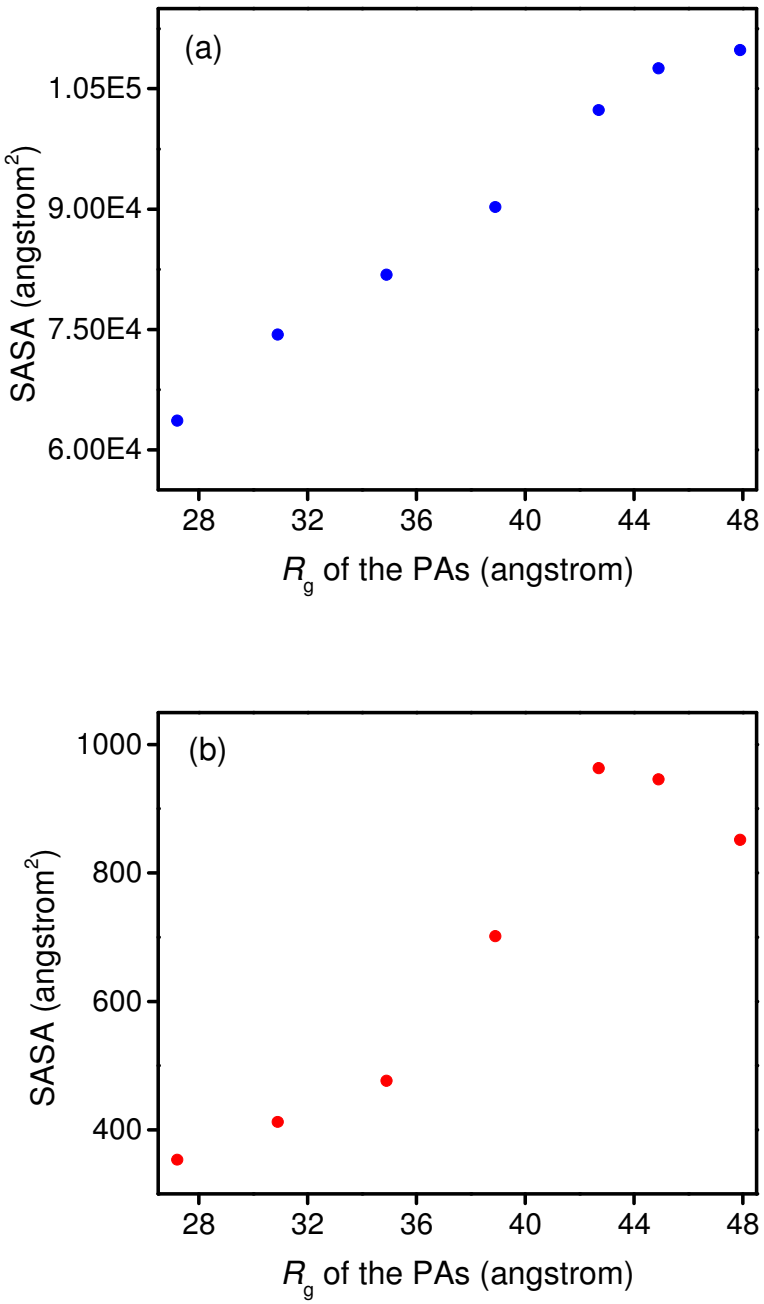

Figure S4. The averaged solvent accessible surface area (SASA) of PAs for the head (a) and tail (b) segment along the reaction coordinate.