Supporting information for:

The C-terminal Plays as the Possible Nucleation of the Self-Aggregation of S-shape $A\beta_{11-42}$ Tetramer in Solution: Intensive MD Study

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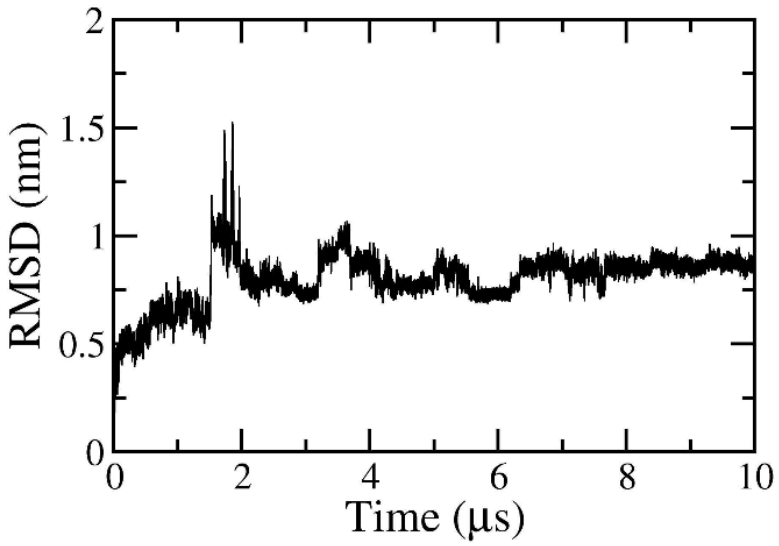

Figure S1. Backbone RMSD of S4Aβ$_{11-42}$ peptide in time evolution.

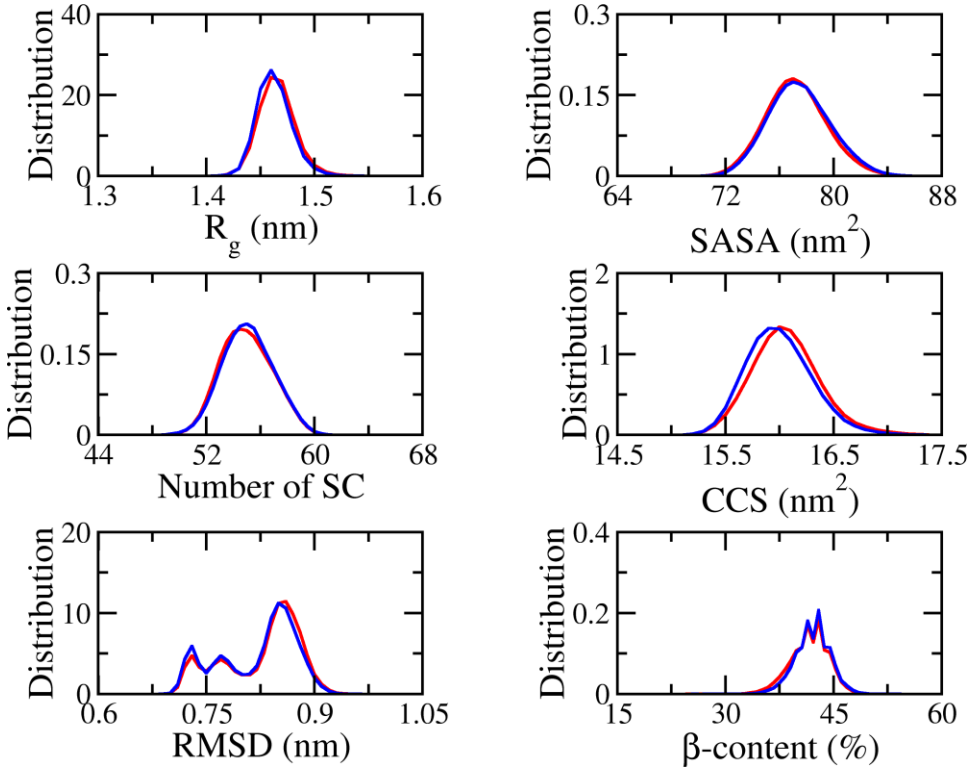

Figure S2. The calculated metrics over different simulation time intervals including 4-10 μs (red color) and 5.2-8.8 μs (blue color). The convergence of simulations was validated according to the superposition of these curves mentioned.

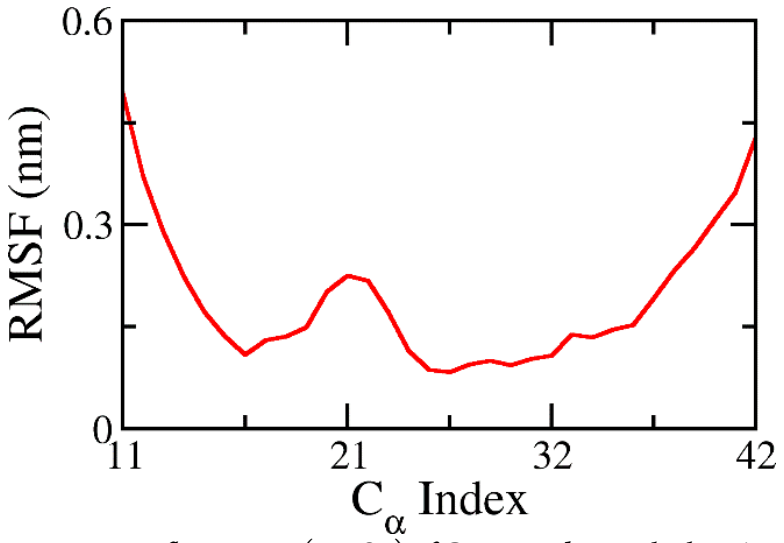

Figure S3. The root mean square fluctuation (RMSF) of C_α atoms during the last 6 μs of MD simulations. Measured results were obtained every 10 ps using GROMACS tools.[1]

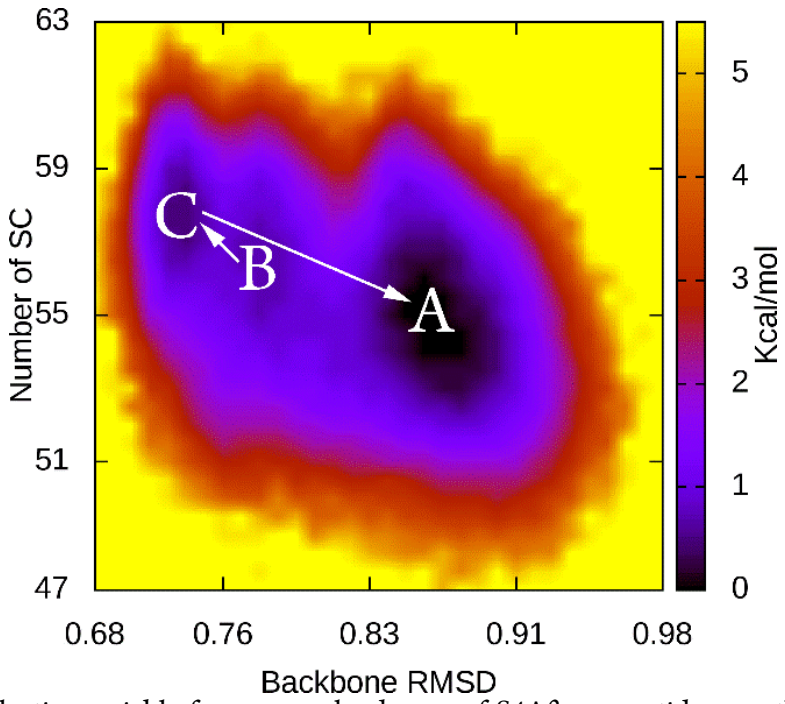

Figure S4. The collective-variable free energy landscape of S4A$\beta_{11\text{-}42}$ peptide over the last 6 μs of MD simulations. The backbone RMSD and number of non-bonded contacts between constituting chains of the peptide are used as the reaction coordinates. The white arrow mentioned the probable self-aggregation pathway of the tetramer.

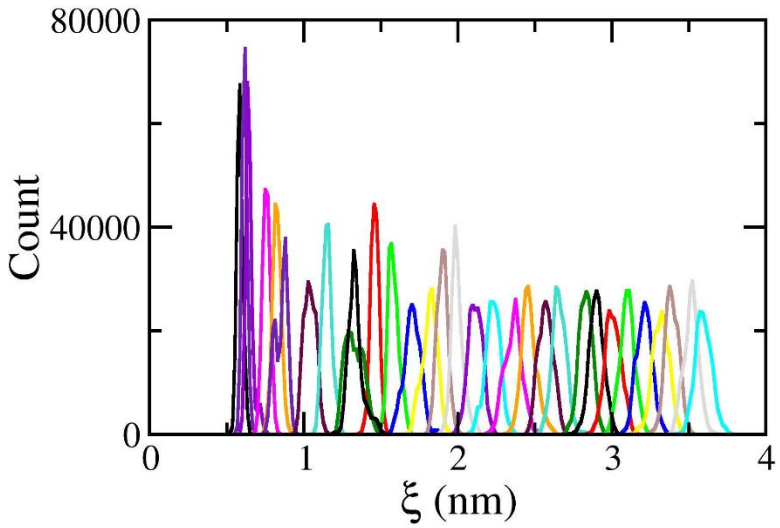

Figure S5. The histograms of 31 different windows of the umbrella sampling simulations.

References

1. Abraham, M. J.; Murtola, T.; Schulz, R.; Páll, S.; Smith, J. C.; Hess, B.; Lindahl, E., GROMACS: High Performance Molecular Simulations through Multi-Level Parallelism from Laptops to Supercomputers. *SoftwareX* **2015,** *1–2*, 19-25.