Supplementary Information

Replica Exchange Molecular Dynamics Study of the Amyloid beta (11-40) Trimer Penetrating the Membrane

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The Electronic Supporting Information file includes the temperature index of the REMD simulations. Additional figures consist of the mean exchange rates between neighboring replicas, the distribution of potential energy of all replicas, the diffusion of temperature space of 1st and 48th replicas, the RMSF of the trimer, and the RMSD of the solvate Aβ_{11-40} trimer.

The structure changed of transmembrane 3A$\beta_{11\text{-}40}$ peptide in explicit solvent inserting the membrane DPPC lipid bilayers has been investigated using replica exchange molecular dynamics simulations that the number of replicas is 48 as range from 290 to 417 K, such as 290.00, 292.34, 294.69, 297.06, 299.44, 301.83, 304.24, 306.67, 309.11, 311.56, 314.04, 316.52, 319.03, 321.54, 324.08, 326.63, 329.19, 331.77, 334.37, 336.99, 339.62, 342.26, 344.92, 347.6, 350.3, 353.01, 355.75, 358.49, 361.27, 364.05, 366.85, 369.67, 372.51, 375.37, 378.24, 381.14, 384.04, 386.97, 389.92, 392.88, 395.86, 398.87, 401.89, 404.93, 407.99, 411.07, 414.16, 417.28 K.

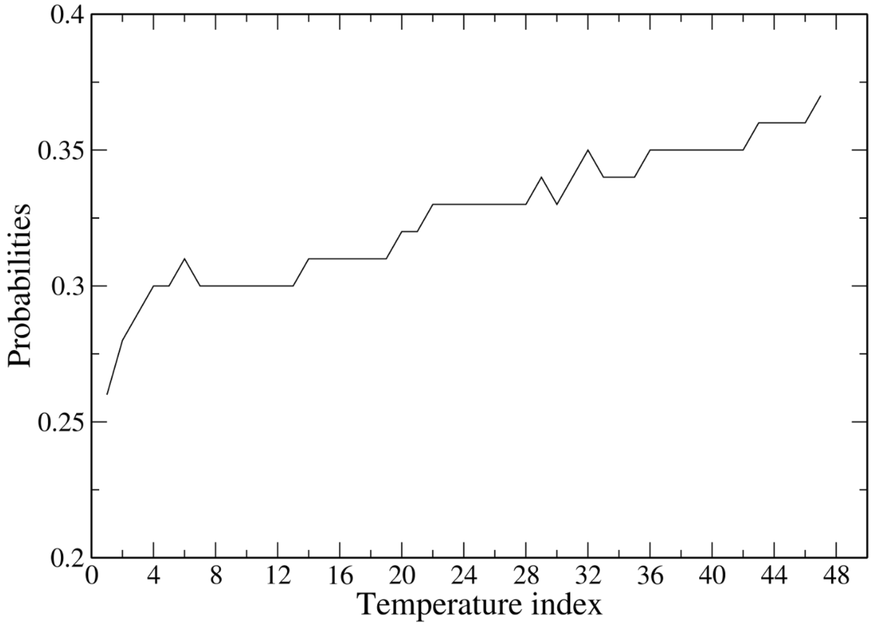

Fig. S1 The average of exchange rate between neighbor replicas that are almost higher than 26%.

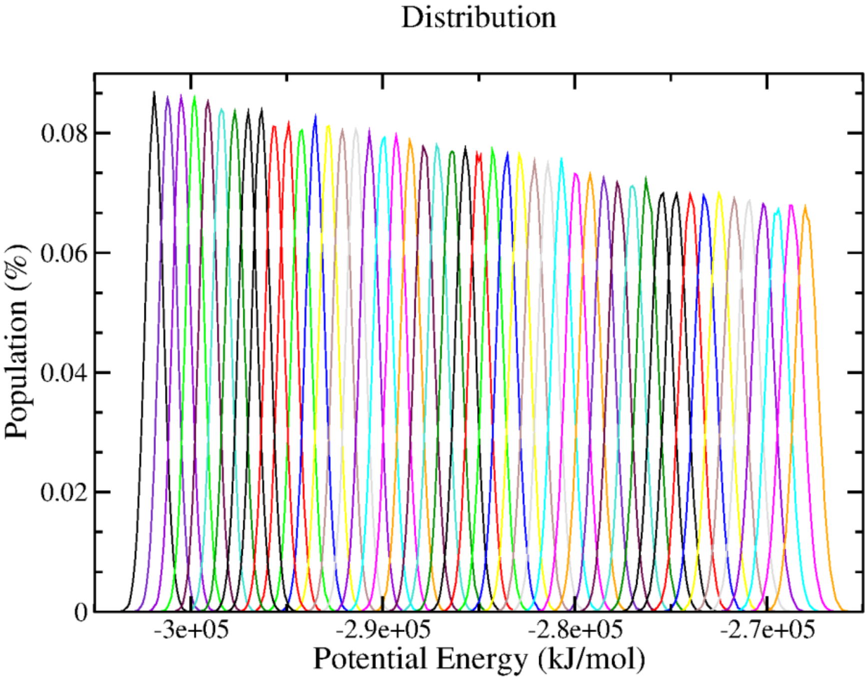

Fig. S2 The distribution of potential energy of 48 replicas of transmembrane truncated 3A$\beta_{11\text{-}40}$ oliomer with bilayer DPPC lipid bilayers at 324 K. The energetic overlap between neighboring replicas is good which keep effective exchange according the Metropolis Criterion.

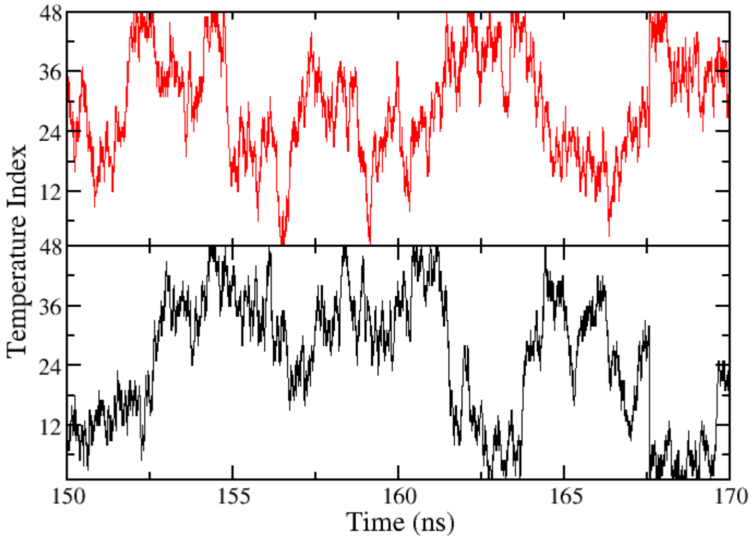

Fig. S3 The diffusion of temperature space of the REMD simulations is monitored by the replica temperature index that is exchanged between the 1st (black) and 48th (red) replicas.

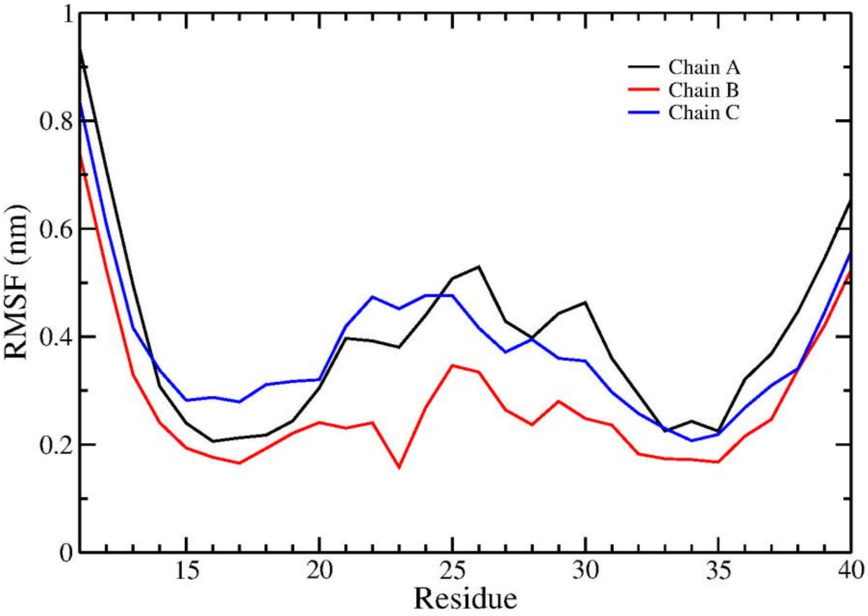

Fig. S4 The root mean square fluctuation of transmembrane 3A$\beta_{11\text{-}40}$ peptide at 324 K during last 300 ns REMD simulations.

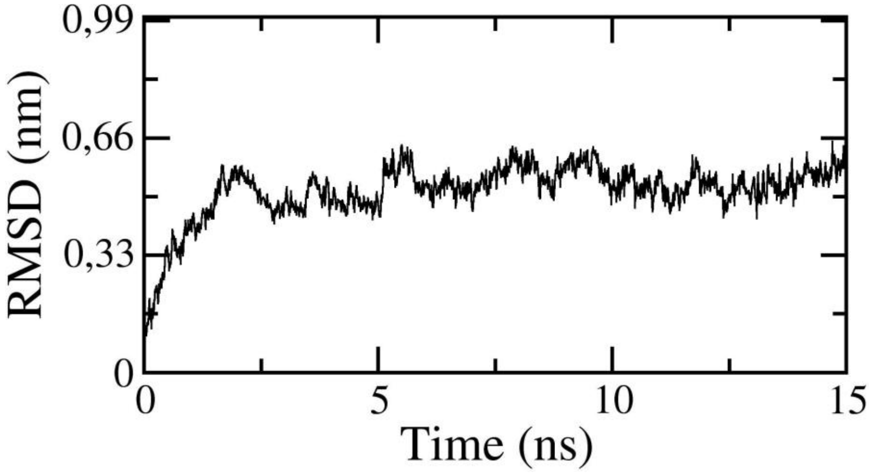

Fig. S5 The RMSD of the solvated A$\beta_{11\text{-}40}$ trimer in solution. The system get the equilibrium after 2.0 ns approximately.

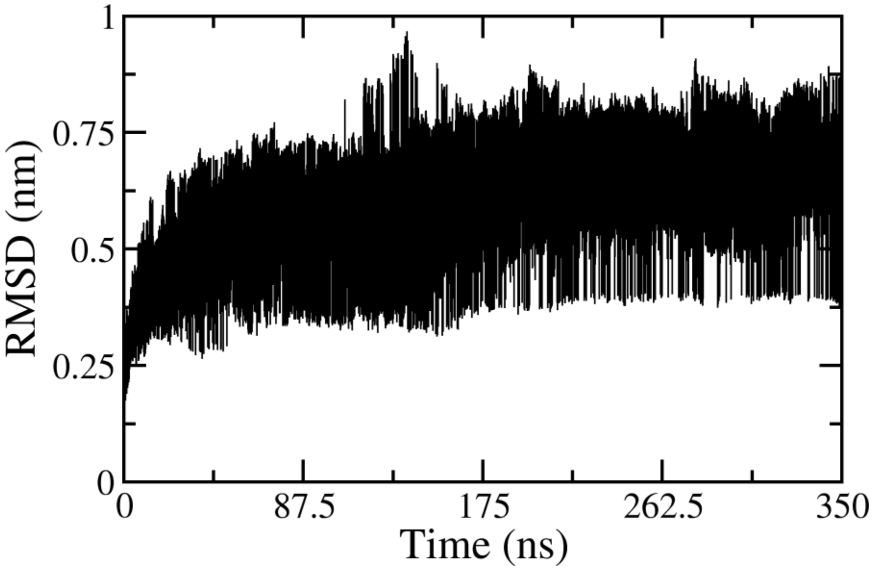

Fig. S6 The RMSD of the A$\beta_{11\text{-}40}$ trimer in the solution of the continuous trajectory of the 4th replica while diffusing in the temperature space.