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## Supporting information for

## *In silico* Studies of Solvated F19W Amyloid β (11-40) Trimer

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The temperature replica exchange molecular dynamics simulation was carried out with 48 different temperatures including 295, 296.68, 298.37, 300.07, 301.78, 303.49, 305.22, 306.95, 308.68, 310.42, 312.17, 313.92, 315.68, 317.45, 319.23, 321.01, 322.8, 324.6, 326.4, 328.25, 330.07, 331.89, 333.72, 335.57, 337.42, 339.28, 341.14, 343.02, 344.9, 346.79, 348.68, 350.59, 352.5, 354.42, 356.35, 358.29, 360.23, 362.18, 364.14, 366.11, 368.09, 370.07, 372.07, 374.07, 376.08, 378.1, 380.13, and 382.16 K. The temperatures were chosen based on previous study.<sup>1</sup>



**Figure S1.** The secondary structure terms, SASA, and CCS of the mutation F19W trimer in different replicas at 250 ns of REMD simulations.



**Figure S2.** Structure terms of the three 19<sup>th</sup> residues in the wild-type  $3A\beta_{11-40}$  (F19) (black) and F19W mutant trimer (red). The distributions were obtained between 300-417 ns for wild-type trimer and 250-400 ns for F19W mutant trimer. RMSD is comparted to the first snapshot when the simulation converged (300<sup>th</sup> ns for the wild-type trimer and 250<sup>th</sup> ns for the F19W mutant trimer).



Figure S3. The secondary structure terms per residue of F19W 3A $\beta_{11-40}$ 



**Figure S4.** The distributions of intramolecular polar contacts from D23 to V24, G25, S26, N27, K28, and G29, as well as intermolecular polar contacts  $H13_A$ -Q15<sub>B</sub> and  $H13_B$ -Q15<sub>C</sub> of F19W  $3A\beta_{11-40}$ .

## Reference

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