Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for:

The structure of chromophore-grafted Amyloid-β_{12-28} dimers in the gas-phase: FRET-experiments guided modelling

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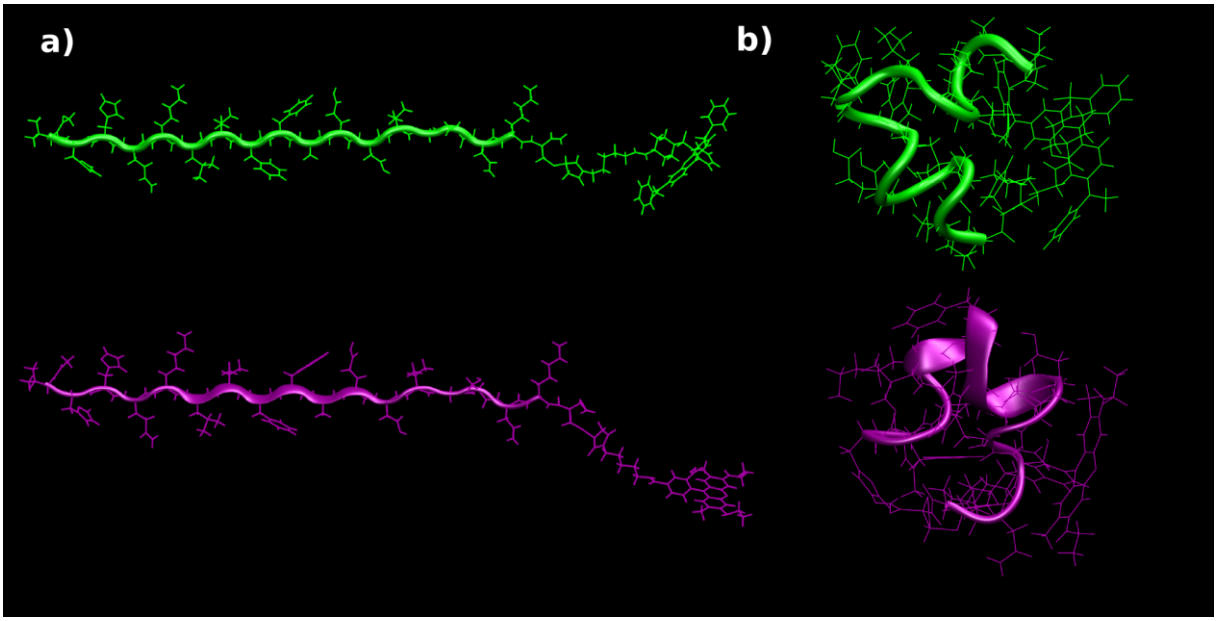

Fig. S1 Starting structures and optimized monomer configurations a) extended peptide conformation b) lowest-energy optimized structures after 4 REMD of cycles of 10 ns (green: c-terminally QSY7-grafted strand, purple Rh575-grafted strand, peptide backbone configuration in cartoon representation).

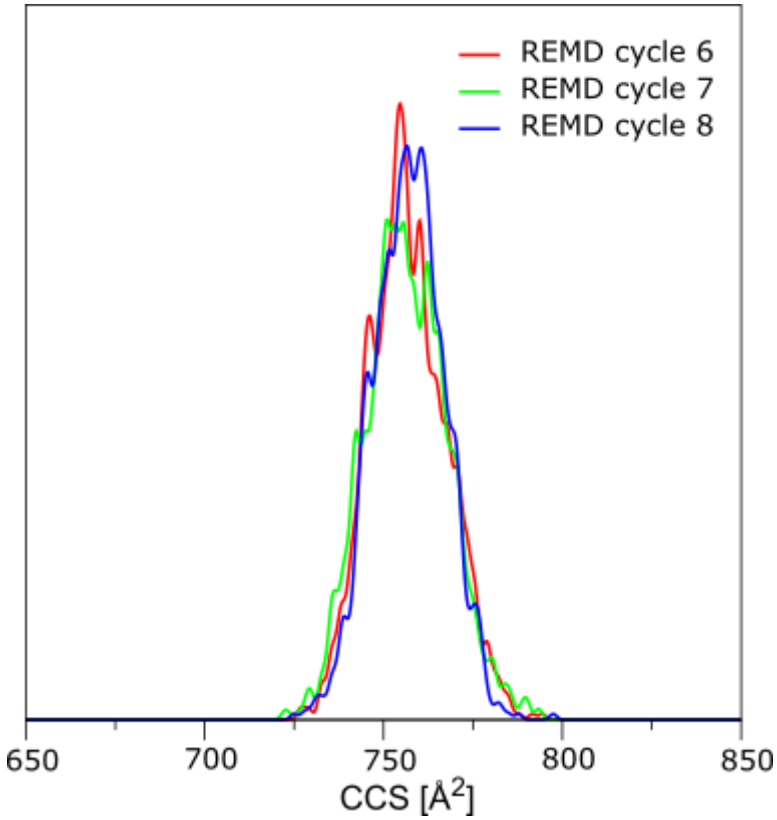

Fig. S2 Convergence of the metrics "collisional cross section" (CCS) used for comparison with the experiment as a function of the REMD cycles (after initial restraint has been removed). The last three cycles (yielding very similar samples) are shown.

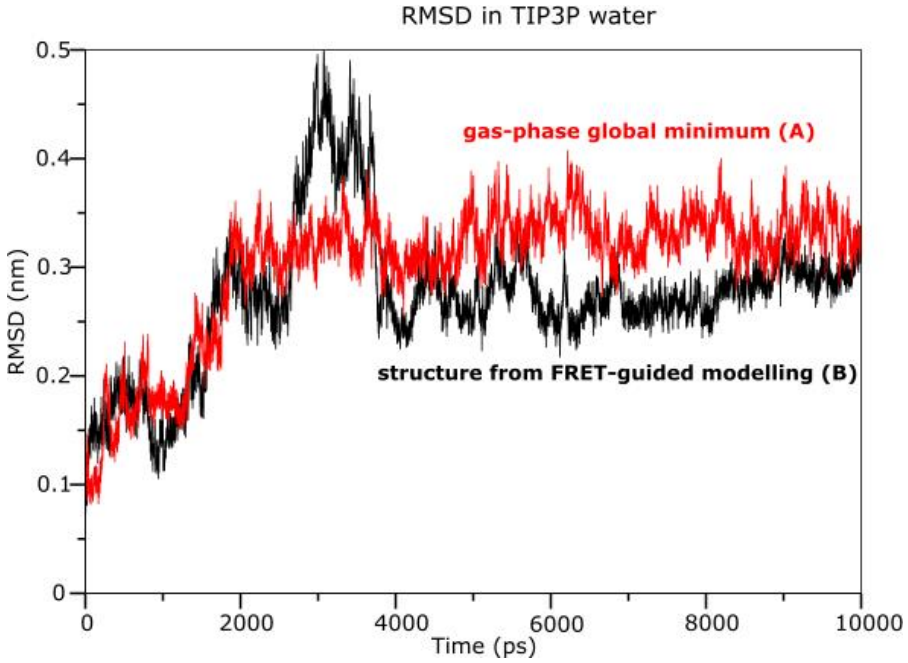

Fig. S3 Equilibration (root mean square deviation from the initial structures, RMSD) of the global gas-phase minimum (red) and the final structure from gas-phase FRET-guided modelling performed in water. MD simulations were performed without any constraints using the same parameter set as for the gas-phase (notice that for quantitative conformational analyses, more suitable solution-phase parameters are recommended). Explicit water (TIP3P, cubic box, length of 5 nm) was added to the cantered final structures of the gas-phase treatment and steepest descent relaxation (1000 steps), NVT equilibration (Nosé-Hoover thermostat 200 K, 0.25 ns), and finally NPT equilibration (Parinello-Rahman pressure coupling, 1 bar, T=300 K, 10 ns) was performed. Cutoffs for nonbonded interactions are 1 nm, Electrostatics were treated with the PME method[1]. Both starting structures converge to a RMSD of 0.3 nm within 10 ns indicating that these structural families may present also structural populations in solution. The final structures were optimized using the semi-empirical PM7 method in implicit solvent (COSMO method, ε=78.4, SCF calculations used the MOZYME function). The PM7 energies in water are -13567 kJ/mol for A and -13566 for B (single point calculations upon the optimized geometries). The respective gas-phase energies are -12906 kJ/mol for A and -12837 kJ/mol for B.

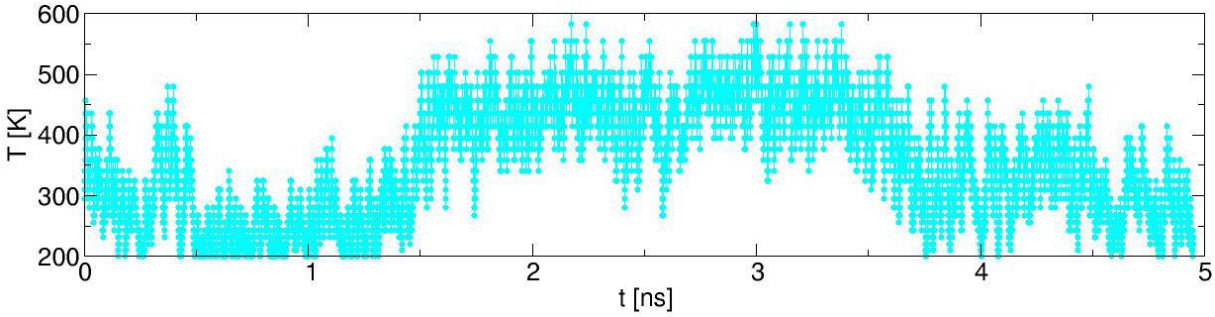

Fig. S4 Mobility of nuclear trajectory (295 K starting temperature) in temperature space during REMD.

References

1. Essmann, U. *et al.* A smooth particle mesh Ewald method. *J Chem Phys* **103,** 8577–8593 (1995).