Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information

Analytical model and multiscale simulations of aggregation amyloid β peptide in lipid membranes: Toward a unifying description for conformational transitions, oligomers and membrane damage

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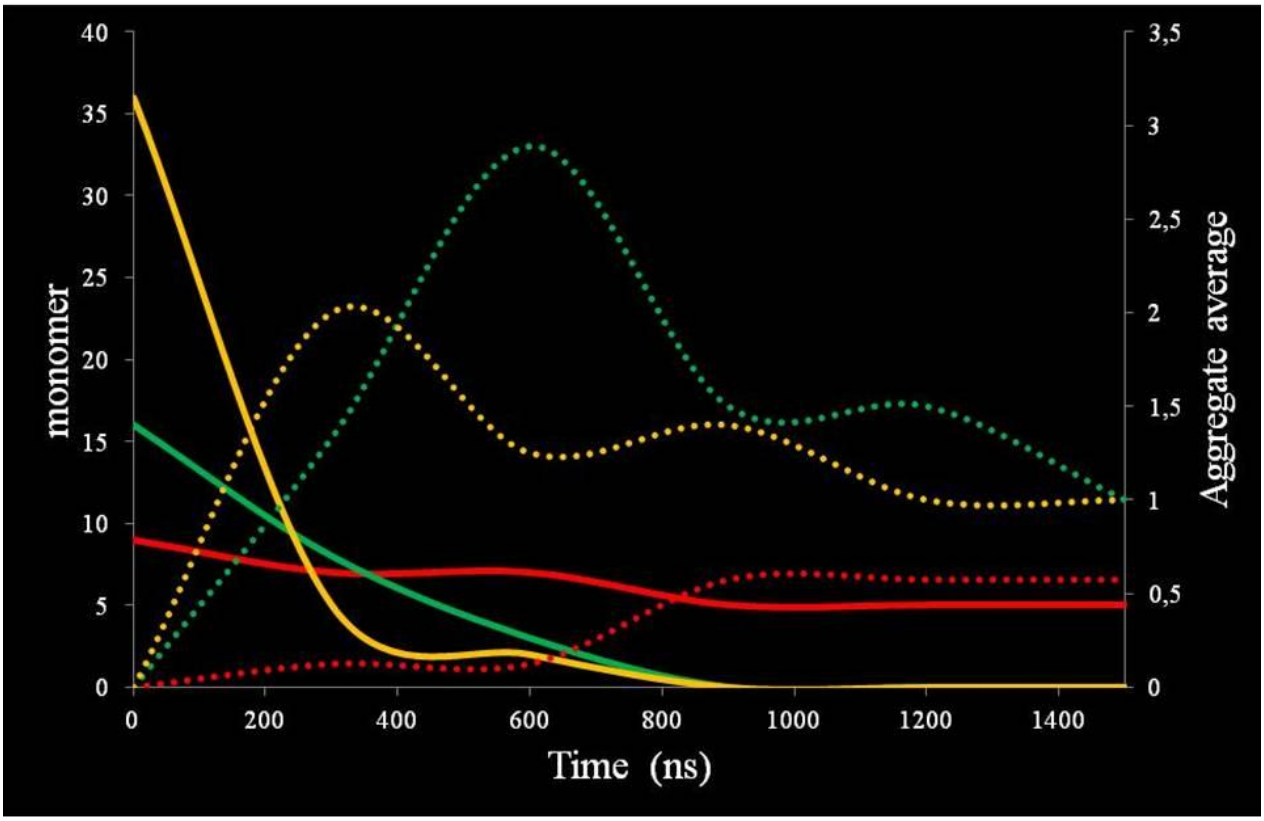

Fig. S1. Analysis of the evolution of the size and number of Aβ aggregates over of three 1.4 μs independent CG simulations performed at different lipid/peptide ratios. Solid lines represent the number of monomers, while dotted curves report the number of aggregates with an average size <*n*> defined as:

$< n >= \frac{\sum_{n>1} nP_n(t)}{\sum_{n>1} P_n(t)}$, where *n* is the aggregate number and $P_n(t)$ is the probability of finding an n-meric aggregate at time *t*. Color codes refer to the different lipid/peptide ratio: 192:1 (red lines), 100:1 (green lines) and 36:1 (yellow lines).

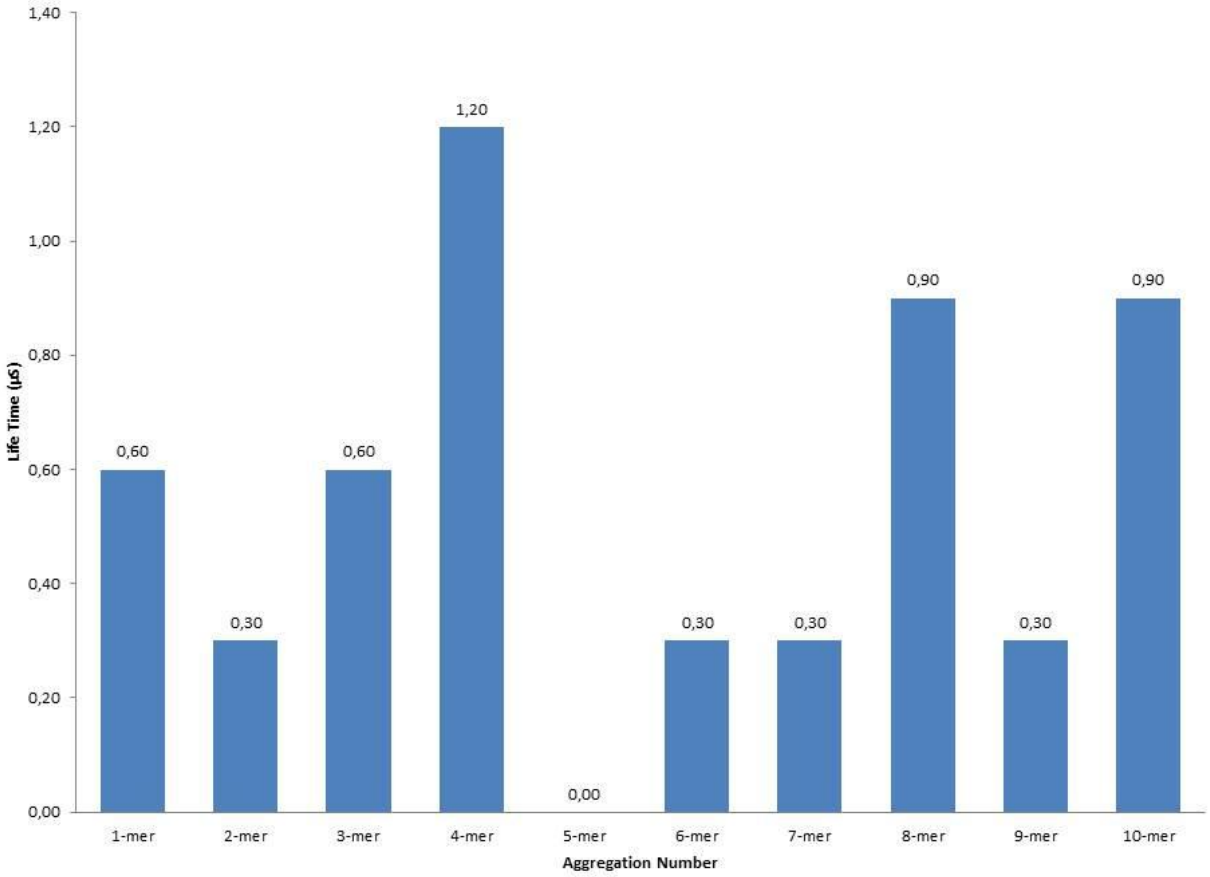

Fig. S2. Lifetime vs. aggregation number during 1.5 μs CG simulations of 36 molecules Aβ40 embedded in POPC bilayer. Life time was calculated by sampling over 300 frame of two independent simulations.

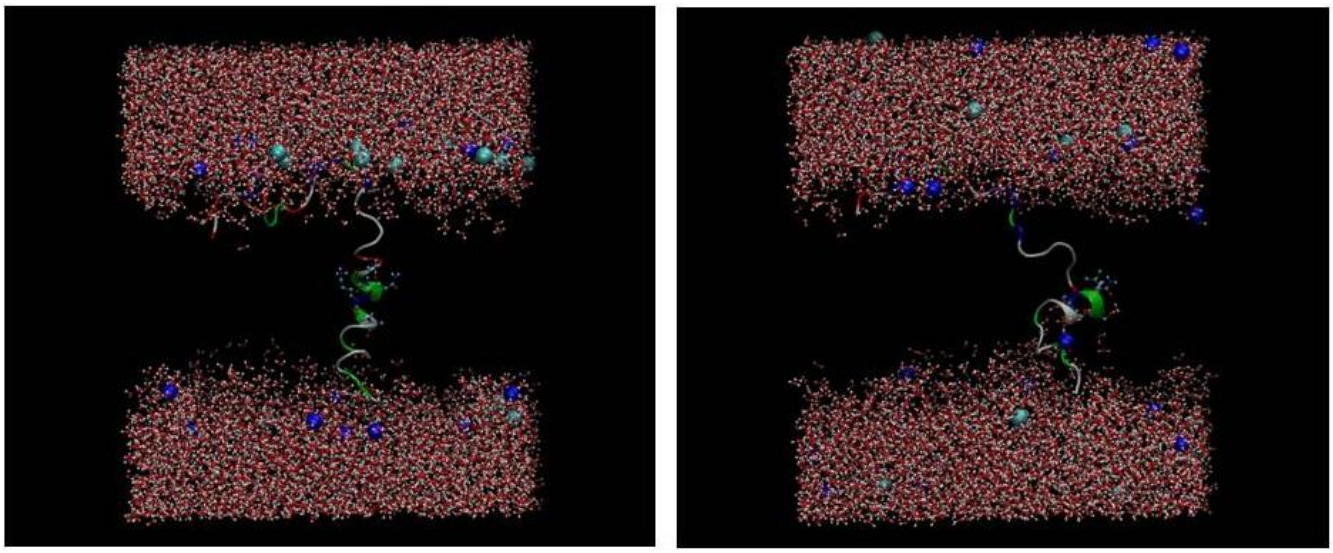

Fig S3. Snapshots from the 40 ns of AA simulation of a single Aβ (1-40) within a POPC bilayer. For the sake of clarity lipids were omitted. Left panel: 0ns, ; right panel: 40ns. Color code: blue spheres: sodium ions; cyan sphere, Chlorine ions; white: non-polar residues; green: polar residues; red: acidic residue; blue: basic residues.

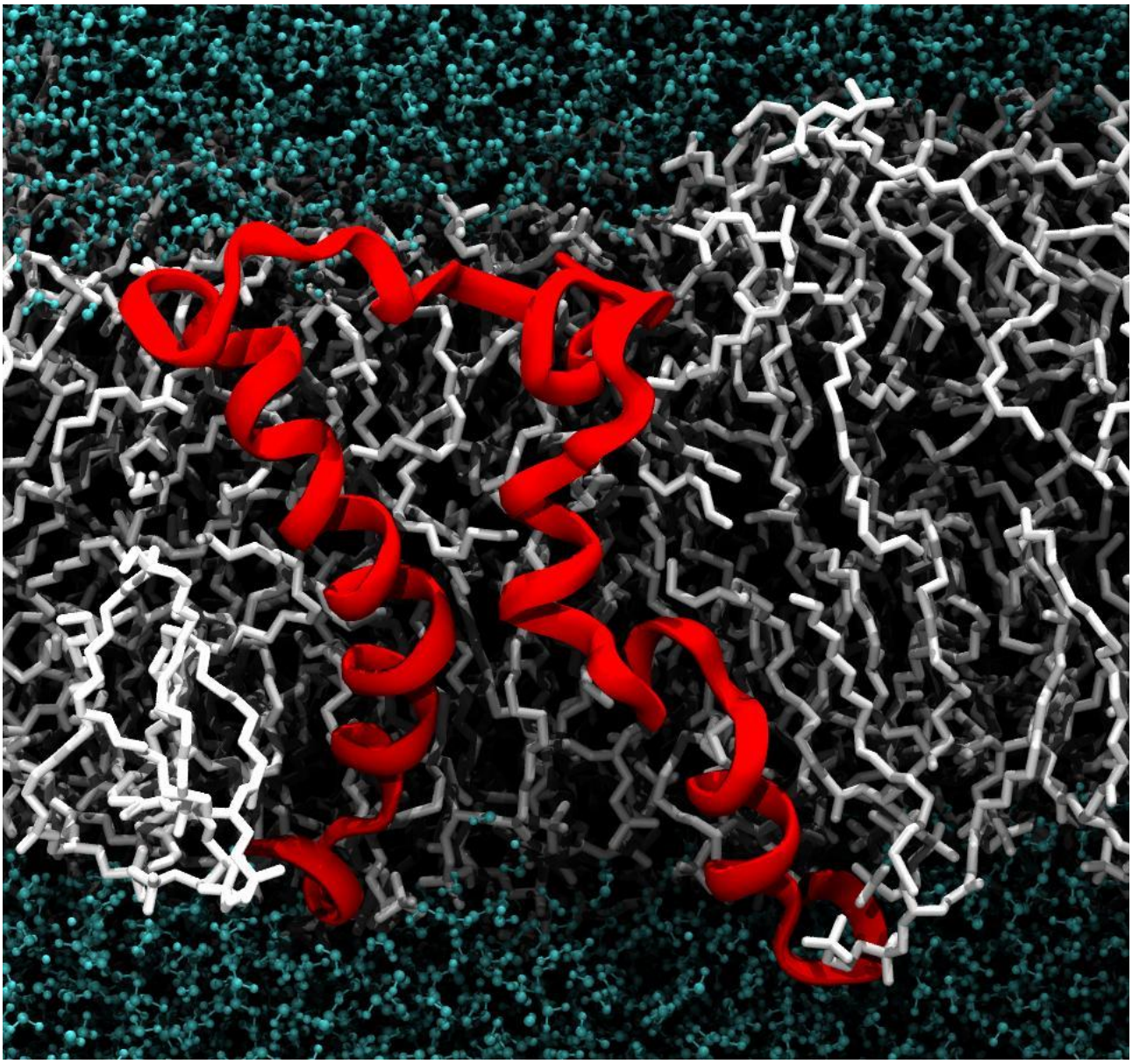

Fig S4. Snapshots from the 350 ns of AA simulation of two dimers of Aβ (1-40) within POPC bilayer. For sake of clarity, solvent and ions were omitted. Left panel, start; right panel end. Color code: white non polar residue; green polar residue; red acidic residue; blue basic residue.