Supporting Material for: Surfactant effects on amyloid aggregation kinetics

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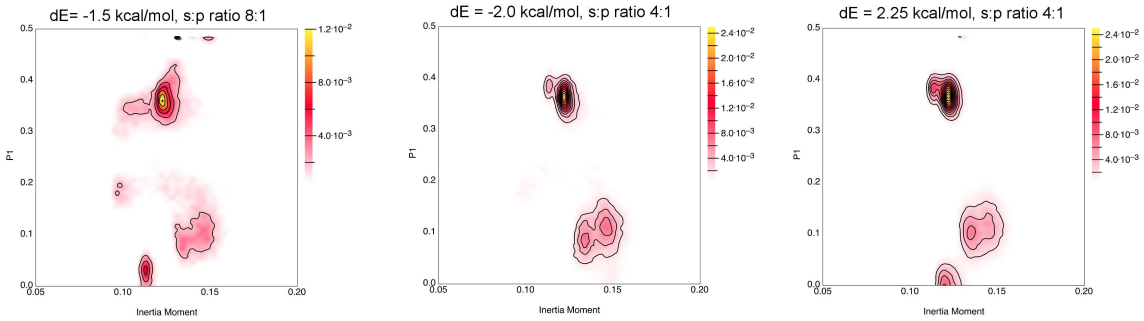

Figure S1: **Quantification of fibril morphologies**. Two-dimensional frequency histograms of the order parameter P1 and the minimum inertia moment (both described in Ref. [1]) calculated for the runs at dE=-1.5 kcal/mol and surfactant:peptide ratio 8:1 (left), dE=-2.0 kcal/mol and 4:1 (middle), and dE=-2.25 kcal/mol and 4:1 (right). Highest frequency is colored in yellow. The Figures can be compared with Figure S3 of [1]. Apparently, the morphologies of the fibrils are not effected by the presence of surfactants. The lack of a peak corresponding to a relatively rare morphology (4PF3) for the simulation at dE=-2.0 kcal/mol is likely due to the smaller number of runs (20 simulations here and 100 in Ref. [1]).

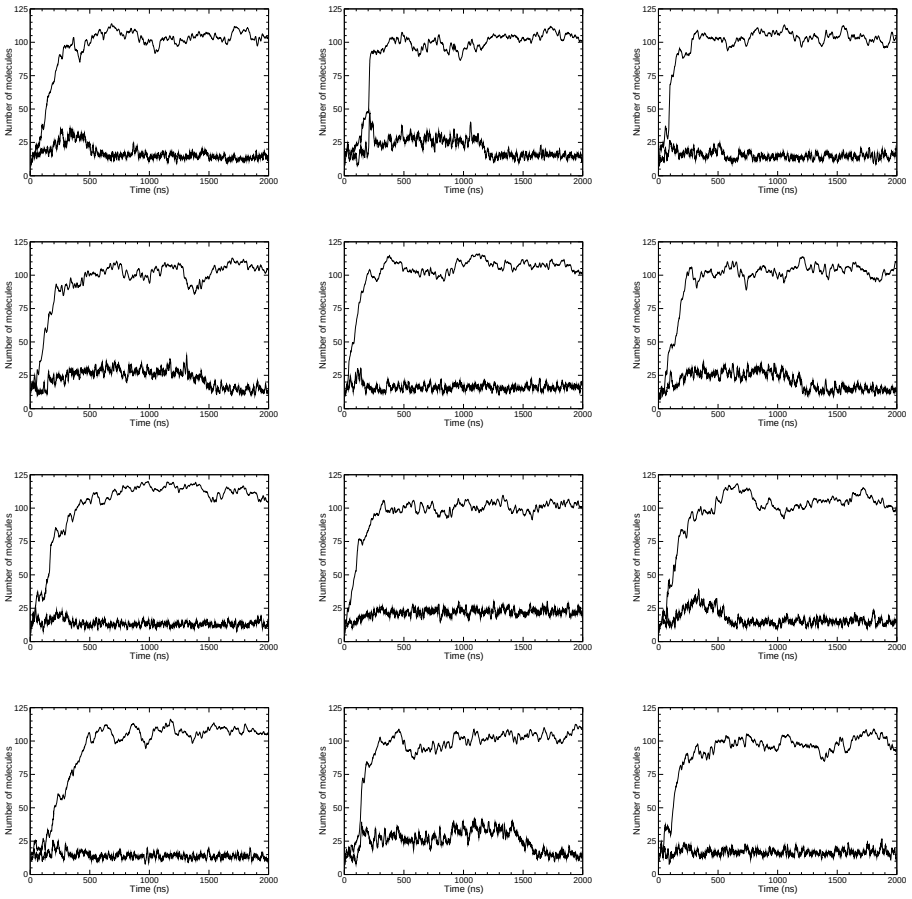

Figure S2: **Temporal evolution of number of molecules in the largest cluster (dE=-2.0 kcal/mol)**. The number of peptides (thin lines) and surfactants (thick lines) in the largest cluster, i.e., globulomer or fibril, are shown for all simulations with dE=-2.0 kcal/mol and 4:1 surfactant:peptide ratio.

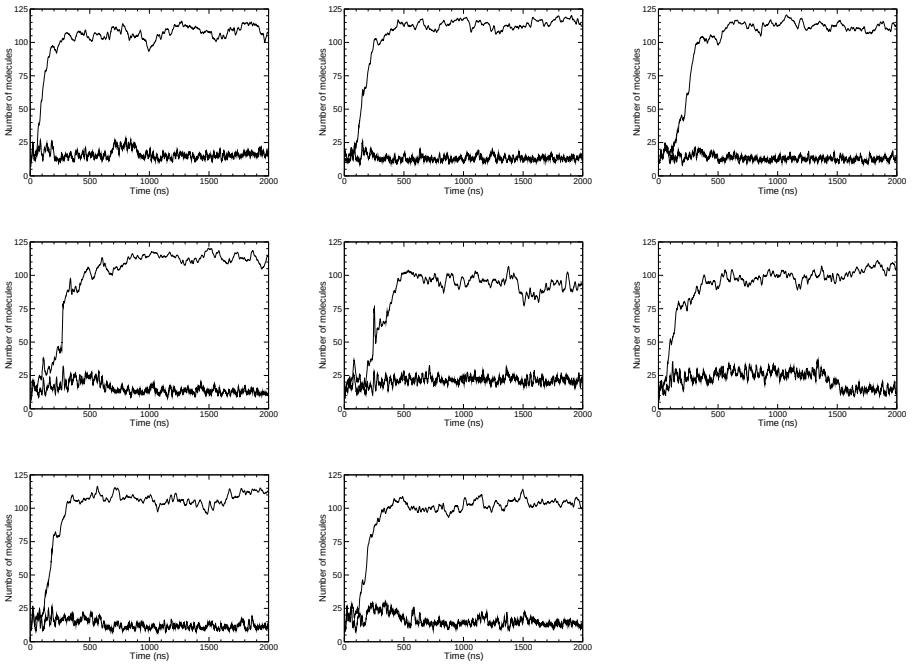

Figure S2 (continued)

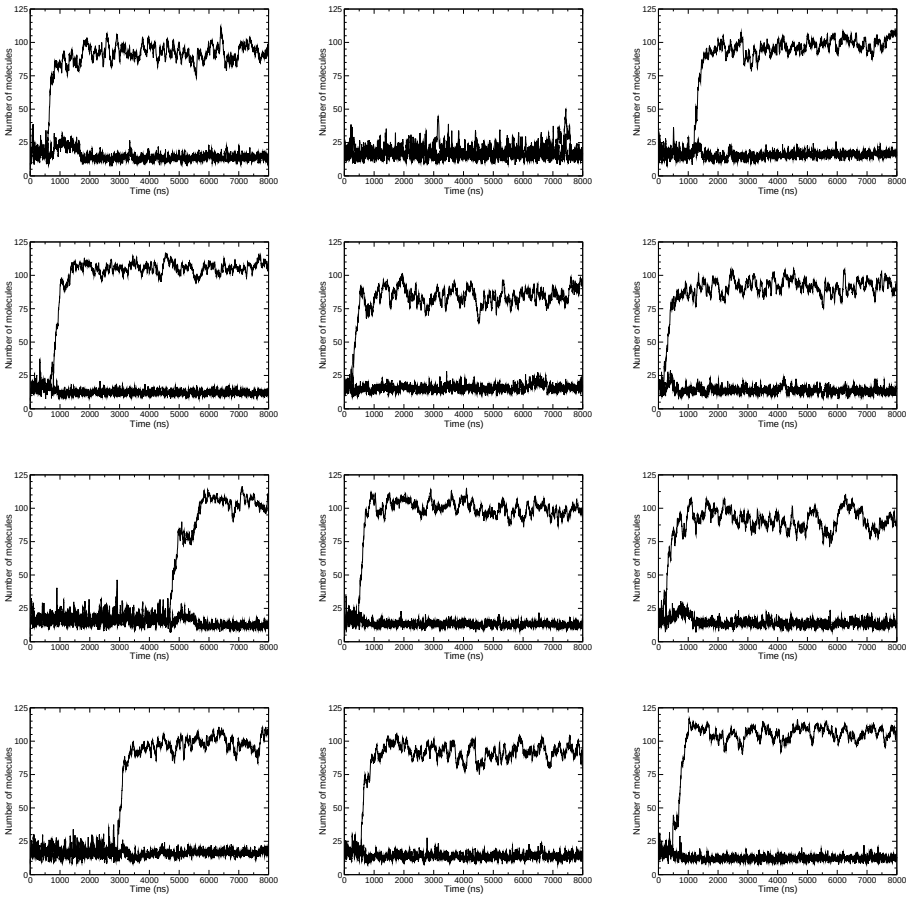

Figure S3: **Temporal evolution of number of molecules in the largest cluster (dE=-2.25 kcal/mol)**. The number of peptides (thin lines) and surfactants (thick lines) in the largest cluster, i.e., globulomer or fibril, are shown for all simulations with dE=-2.25 kcal/mol and 4:1 surfactant:peptide ratio. Fibril formation does not take place in one of the 16 runs (top, middle panel), and in a few cases the fibrils do not reach their finite size after 8 μs. Note the difference in the x-axis scale in comparison to Figure S2.

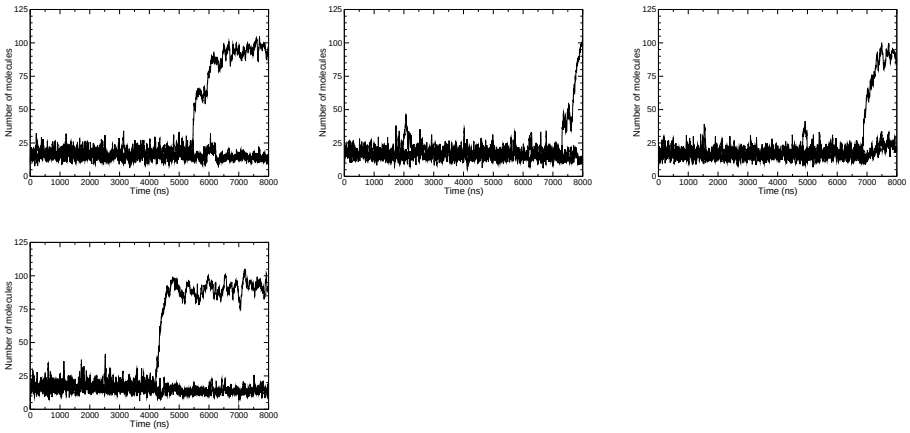

Figure S3 (continued)

[1] R. Pellarin, P. Schuetz, E. Guarnera, A. Caflisch, Amyloid fibril polymorphism is under kinetic control, J Am Chem Soc 132 (2010) 14960–14970.