SURFACE EFFECTS ON THE KINETICS OF PEPTIDE AGGREGATION

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Abstract

The presence of surfaces influences aggregation kinetics of peptides and proteins. We studied acceleration or retardation of amyloidogenic peptides caused by different surfaces using molecular simulations of model peptides represented by patchy spherocylinders. We show that increasing the monomer-surface attraction affects nucleation and growth of small oligomers in a non-linear manner: Weakly attractive surfaces lead to retardation; strongly attractive surfaces lead to acceleration. Further, the same type of surface either accelerates or retards growth, depending on the bulk propensity of the peptide to form fibrils: An attractive surface retards fibril formation of peptides with a high tendency for fibril formation, while the same surface accelerates fibril formation of peptides with a low propensity for fibril formation. The surface effect is thus determined by the relative association propensity of peptides for the surface compared to bulk, and by the surface area to protein concentration ratio. Our results are supported by thioflavin T fluorescence experiments with increasing surface area introduced in a controlled way in the form of nanoparticles to solutions of alpha-synuclein from Parkinson or amyloid beta peptide from Alzheimer disease. These findings offer molecular insight into fibril formation kinetics in complex environments and may be used to tune fibrillation properties in diverse systems.

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