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Data Article

Data for ion and seed dependent fibril assembly of a spidroin core domain



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ABSTRACT

This data article includes size exclusion chromatography data of soluble eADF4(C16), an engineered spider silk variant based on the core domain sequence of the natural dragline silk protein ADF4 of *Araneus diadematus*, in combination with light scattering; the protein is monomeric before assembly. The assembled mature fibrils were visualized by transmission electron microscopy (TEM) and atomic force microscopy (AFM). Sonicated fibrils were used as seeds to by-pass the nucleation lag phase in eADF4(C16) assembly. We also provide data on the sedimentation kinetics of spider silk in the presence of different NaCl concentrations revealing very slow protein aggregation in comparison to the fast assembly triggered by phosphate ions published previously [1]. Experiments in the Data article represent supporting material for our work published recently [1], which described the assembly mechanism of recombinant eADF4(C16) fibrils.

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Specifications Table

Subject area	Biochemistry
More specific subject area	Structural proteins, fibril assembly
Type of data	Microscopy images, chromatograms, sedimentation kinetic data
How data was acquired	TEM, AFM, UV protein absorption, fluorescence spectroscopy multi-angle light scattering
Data format	Analyzed and processed in CorelDraw
Experimental factors	Experiments were based on soluble eADF4(C16) and tetramethylrhodamine modified eADF4(C16) in aq. buffers and assembled fibrils thereof
Experimental features	Assembly of eADF4(C16) under different salt concentration
Data source location	Biomaterials, Faculty of Engineering Science, University of Bayreuth, D-95440 Bayreuth, Germany
Data accessibility	The data are supplied with this article

Value of the data

Published work [1] and this additional material provide insights into how to analyze the nucleated assembly mechanism of recombinant spider silk protein eADF4(C16). The assembly mechanism of the silk compares to that of many other fibril forming proteins such as human A β peptides [2], huntingtin peptides [3] or yeast prion Sup35-NM [4] which all of them possess cross- β fibril structures. Data in the article and in the related publication [1] provide evidences that potassium and phosphate ions specifically trigger both nucleus formation as well as fibril growth. Both potassium and phosphate are strong kosmotropic ions and they also play a crucial role in the assembly of natural spider silks [5] in the spinning duct, whereas less kosmotropic NaCl is present in the ampulla stabilizing the protein during the storage. Therefore, the provided data could trigger further studies with amyloidogenic proteins concerning the influence of kosmotropic salts on fibril formation. In contrast, NaCl shows only marginal effect on the assembly of recombinant eADF4 (C16). Nevertheless, kinetic data suggest that the self-assembly of the cross- β fibrils as described here and in [1] is not related to the assembly of natural spider silk fibers. Nucleation is accompanied by a long lag phase (hours) followed by fibril elongation possessing perpendicularly oriented β -sheets [6,7]. Natural silk assembly is very fast (in the millisecond regime) and leads to β -sheet alignment along the fiber axis [5,8].

1. Data

In the data we included size exclusion chromatography data of soluble eADF4(C16) in a combination with light scattering revealing that the protein is monomeric before assembly (Fig. 1). A defined structural state is important before starting any kinetic study, since assemblies may significantly influence the kinetics by accelerating the nucleation (Fig. 2). The assembled mature fibrils were visualized by transmission electron microscopy (TEM) (Fig. 3) and atomic force microscopy (AFM) (Fig. 4), revealing fibrils typically 10 nm in diameter and 1 μ m in lengths. Sonication led to significantly shorter fibrils, as shown by AFM, increasing the number of the active fibril ends. Sonicated fibrils can be used as seeds to by-pass nucleation in eADF4(C16) assembly (Fig. 5). We further show sedimentation kinetics of spider silk in the presence of different NaCl concentrations revealing very slow protein aggregation (Fig. 6) in comparison to the fast assembly triggered by phosphate ions [1], which indicates that ion masking events are less important for the protein-protein interaction during spider silk assembly.

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