

초청강연

STACKED BILAYER HELICES:

A NEW STRUCTURAL ORGANIZATION OF AMPHIPHILIC MOLECULES

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ABSTRACT

The spontaneous self-organization of amphiphilic molecules into complex aggregates was undoubtedly an important factor in the emergence of life on earth. We study the parameters governing the self-organization of a simple amphiphilic model system using electron cryomicroscopy of ice-embedded specimens in combination with extensive data analysis. Different stable helices can be generated reproducibly by changing the parameters controlling the molecular aggregation process. The repeating units of the helical aggregates in the micrographs can be found by multivariate statistical image analysis techniques, and these two-dimensional projection images suffice for calculating the three-dimensional density distribution of the fibers. We present a typical structure consisting of a narrow stack of compartmented bilayers twisted into a left-handed helix. Our new techniques directly elucidate the three-dimensional structure of helical assemblies and can complement or replace diffraction-based approaches.

FIGURE 2:

(a) The average of the repeating units of the 6-bilayer helix calculated from 450 individual helix repeats.

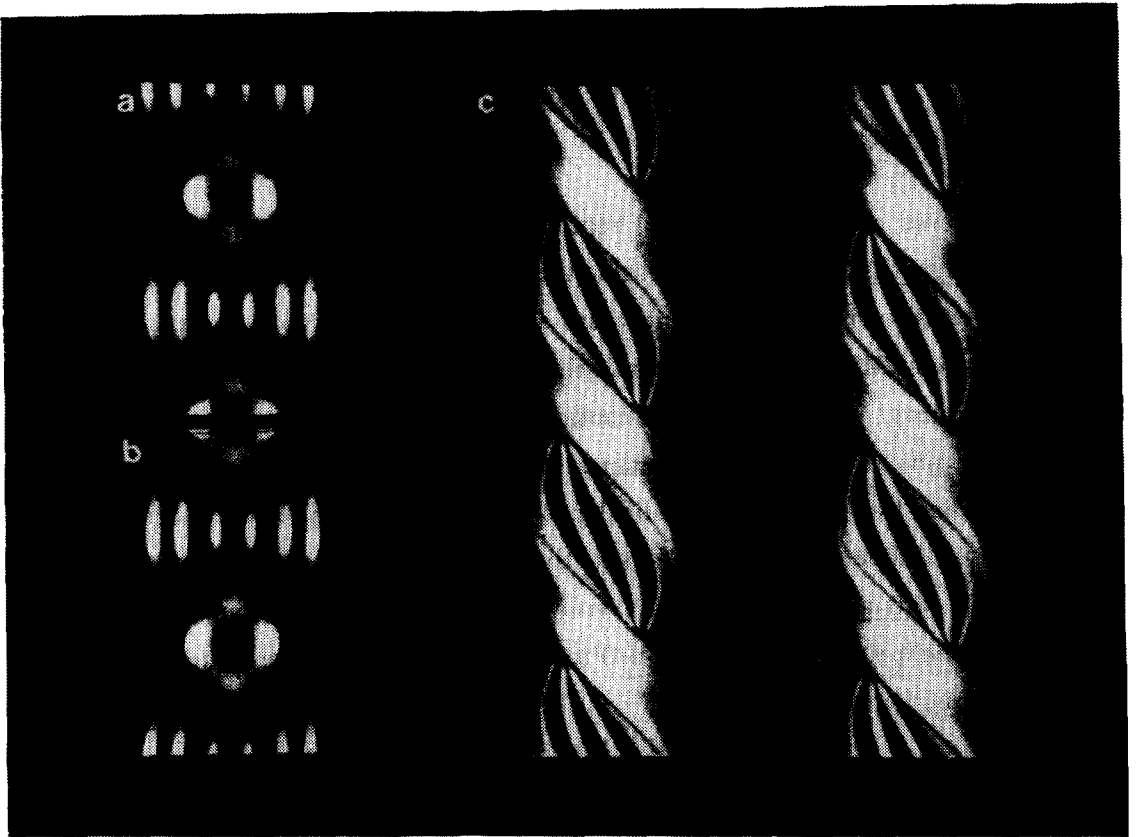
(b) The reprojection of the 3D density distribution of the reconstructed helix (c) showing an excellent similarity with the input data.

(c) Stereo pair of the 3D reconstruction of the 6-bilayer helix showing 1.5 helical repeats, each repeat corresponding to a full rotation of the helical motif over 360°.

Alignment and MSA

450 environments of the (half) helical repeat were extracted interactively from several digitized micrographs. All image processing was performed in the context of the IMAGIC V software system²⁴. The fiber segments were aligned and then submitted to multivariate data compression ("MSA")¹² and automatic classification¹³ to subdivide the data set into 20 classes. Apart from a few "bad" classes containing only a negligible number of images, the resulting classsums all exhibited mm symmetry indicating a twofold axis along the long axis of the helices and twofold axes perpendicular to the long axis of the helix, characteristic for a non-directional fiber. The resolution in the classsums as determined by the S-image technique²⁵ is ~2.0nm. The resulting overall sum of the helical fragments was used as input for the helical 3D reconstruction (Fig. 2c) which was performed using the "exact filter" reconstruction scheme²⁶.

Sofia



S. japonica
 1971

ETA
 1971

N-Oct, -D-β-monomide

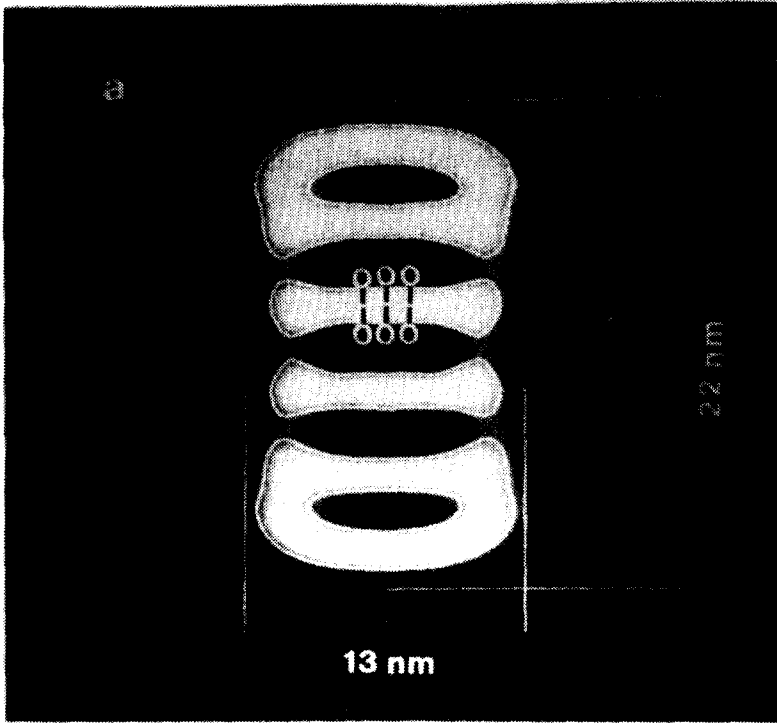


FIGURE 3:

(a) Cross section of the 3D-reconstruction of the 6-bilayer helix (Fig. 2c) with dimensions. The dotted line indicates the closed outer surface of the fiber, which surface is believed to consist of hydrophilic head groups of the D-Glu-8 molecules (all dark areas in this cross section are thought to consist mainly of head groups of the molecules). The orientation of the molecules within the bilayer stack is indicated schematically.

(b) Stereo pair of a small segment of the 6-bilayer helix.