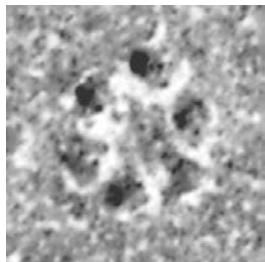
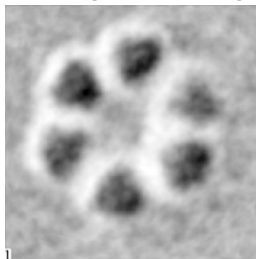


Combined Imaging and Computational Modeling Support a Maximum of 18 Cellulose Synthase Proteins in the Cellulose Synthesis Complex

Superior image of a 6-lobed rosette CSC



Triangular lobes in an image average



Significance and Impact

A maximum of 18 cellulose synthases (CESAs) in the membrane-bound cellulose synthesis complex (CSC) implies that the fundamental cellulose microfibril contains at most 18 glucan chains, providing a flexible platform for higher order cellulose and cell wall assembly.

Scientific Results

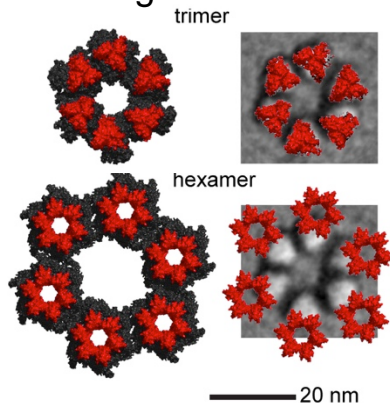
- *Triangular lobes were visible in original images and image averages of rosette CSCs.*
- *A more complete CESA model was computationally assembled into various oligomers, then hexameric assemblies of the oligomers. The hexamer of trimers was most stable in silico.*
- *The negatively-stained recombinant AtCESA1 catalytic domain was triangular. Its size and shape were similar to trimeric models derived from small angle scattering data or in silico.*

Research Details

- *We used optimized methods for freeze fracture electron microscopy previously applied only to animal research.*
- *We analyzed large in-silico protein assemblies inclusive of water and ions (1.6 – 3 million atoms per assembly).*

Nixon BT, Mansouri K, Singh A, Du J, Davis JK, Lee JG, Slabaugh E, Vandavasi VG, O'Neill H, Roberts EM, Roberts AW, Yingling YG, Haigler CH (2016) Comparative structural and computational analysis supports eighteen cellulose synthases in the plant cellulose synthesis complex. *Scientific Reports* 6, 28696

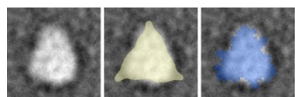
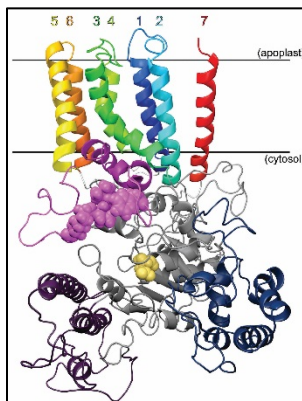
Image average overlaid with oligomeric models



The *in-silico* hexamer of trimers shows greatest stability.

Assembly level	Potential energy per monomer (kcal/mol x 10 ⁻⁵)				
	dimer	trimer	tetramer	pentamer	hexamer
single oligomer	-1.03	-1.65	-1.51	-1.59	-1.69
six-fold assembly	-1.42	-2.50	-1.89	-1.68	-2.20

Optimized CESA model



Spatial match between AtCESA1 catalytic trimer and models



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