

STRUCTURAL MODEL OF PLANT CELLULOSE SYNTHASE AND CELLULOSE SYNTHASE COMPLEX

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Cellulose synthase (CESA) is an enzyme that polymerizes glucose into cellulose which is a principal component of plant cell walls and lignocellulosic biomass. Despite the importance of plant cellulose to nature and industry, we have little understanding of the 3D structure of proteins required for plant cellulose biosynthesis. However, manipulating the physical properties of cellulose through biochemical engineering of CESA structure offers many prospects for improved biomaterials, as reduction of cellulose crystallinity can increase the efficiency of saccharification, a process important for biofuels production from lignocellulosic biomass. To date the crystal structure of synthase protein is not known and the mechanism of how CESA produces cellulose is not completely understood.

Computational models can provide understanding of the CESA function and the assembly of CESAs into cellulose synthesis complex (CSC). We used de-novo protein structure modeling and molecular dynamics simulations to generate all-atom 3D model of CESAs protein structure of cotton. Using our 3D model we observed an agreement in the catalytic mechanisms between bacteria and plants and the specific roles of other conserved regions of CESA. To further understand the evolutionary relationships and the biochemical roles of various structural motifs, such as regions unique to plant CESA and Zn-finger, in regulating cellulose production, we predicted the assembly and stability of CESAs into CSC complex and show possible formation of oligomeric assemblies from dimers to hexamers. Our 3D model of complete CSC suggest that each rosette lobe preferably contains a trimer of Cesa producing 18 cellulose chains per rosette. Our 3D model allows for exploration and testing of the structure-to-function relationship of synthase proteins.