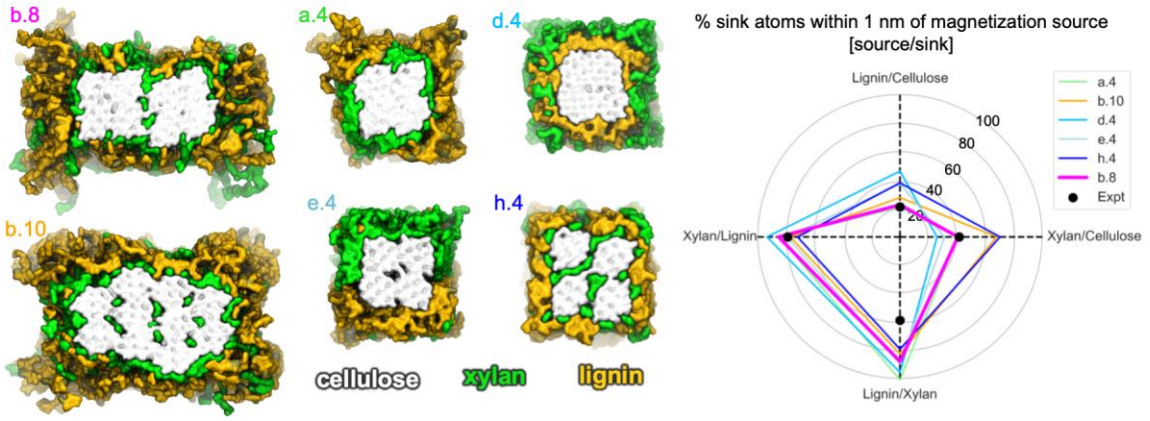
Solid State NMR informs the selection of atomistic secondary cell wall molecular models

Background

- Plant secondary cell walls (SCW) are composed of a heterogeneous interplay of three major biopolymers: cellulose, hemicelluloses, and lignin.
- Most depictions of the relative polymeric arrangements are cartoon-style and not computationally accessible. The few large-scale atomistic molecular models of the lignified plant SCW are extremely sparse.
- A major impediment to atomistic simulations of SCW biopolymer assemblies is the lack of experimentally validated, quantitative details describing the relative positions, and conformations of molecules necessary to construct realistic molecular models.



Atomistic SCW periodic model variants (left) and their inter-polymer proximity analyses (right, polar plot) are compared with ssNMR spin diffusion experiments (black dots). Model b.8 represents the best overall fit to experimental data.

Approach

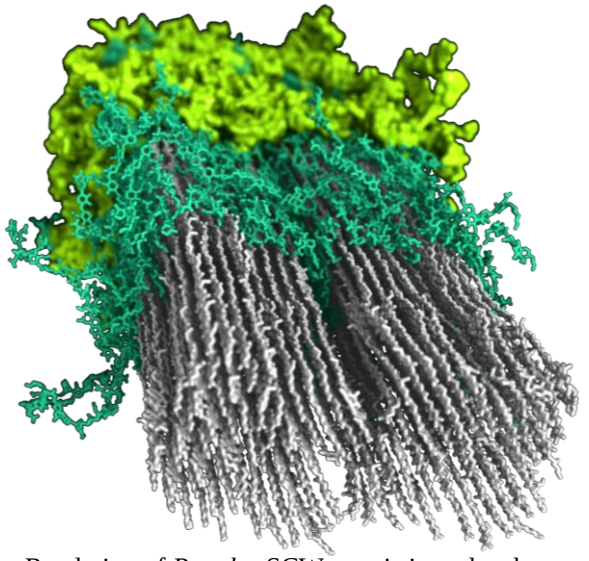
- We use solid-state Nuclear Magnetic Resonance (ssNMR) measurements to infer refined quantitative metrics about the structural configuration, intermolecular interactions, and relative proximity of all three major biopolymers in *Populus* cell walls. NMR observables are then articulated into atomistic, macromolecular models for biopolymer assemblies within the SCW.

Results

- ssNMR observables on ^{13}C-enriched *Populus* woody stems provide quantitative bounds on the length scales and extent of inter-polymer interactions. By comparing simulated metrics from multiple SCW models to experimental ssNMR data (top figure), we find that model b.8 best represents SCW polymeric arrangements.

Significance

- This effort represents the first quantitatively informed and computationally accessible atomistic molecular model of the plant secondary cell wall. These experimentally supported atomistic models lay the foundations for future *in silico* explorations to gain insights into the molecular level determinants of the emergent properties of naturally occurring, treated and engineered biomass feedstocks.
- It is the first ever plant cell wall model deposited in PDB-Dev.



Rendering of *Populus* SCW atomistic molecular model variant b.8, which represents the best overall fit of ssNMR restraints. Cellulose-gray, xylan-teal, lignin–green.

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