## Effect of arabinose side-chains on xylan rigidity and selfaggregation



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## Significance and Impact

We show that xylans with a low degree of arabinose substitution are stiffer and form larger aggregates in water than their highly substituted counterparts. These results rationalize xylan's function in the plant cell wall: Highly substituted xylan acts as a spacer, keeping cellulose microfibrils apart, whereas low substitution xylan is localized in plant cell walls and promotes cellulose bundling.

## **Scientific Results**

- SANS: Low substitution xylans have a larger radius of gyration.
- MD simulation: Low substitution xylans have a larger persistence length, *i.e.* are stiffer.
- Rationalize findings: Entropic penalty of xylan binding to cellulose is smaller for the stiffer, low substitution xylan.

## **Research Details**

Synergistic approach combining small-angle neutron scattering experiments with Hamiltonian Replica Exchange Molecular Dynamics Simulations.

