Combined Analytics and Modeling Probing Polymer-Polymer Interactions Within Secondary Cell Walls leads to better structural insights

**Background**

- The molecular-level architecture of the plant Secondary Cell Wall (SCW) is elusive due to the amorphous and heterogeneous nature of lignocellulosic biomass.
- A combined experimental and computational approach is presented to bridge this gap.

**Selected Conclusions**

- Polymer-Polymer interactions are probed in detail with solid-state NMR measurements (ssNMR) on $^{13}$C-enriched poplar stems.
- Extent of the lignin/hemicellulose interaction is quantified for the first time: ~70 – 75% of all acetylated xylan share surface contact with lignin.
- Evidence of preferential xylan/lignin binding: S-lignin > G-lignin.
- Xylan $\text{Ac}_{\text{Me}}$/Lignin inter-polymer distance is in the order of 0.4 – 0.5 nm
- Molecular dynamics simulations can illuminate the underlying atomistic architectures dictating specific ss-NMR signatures.

**Significance**

- Investigating plant SCW superstructure using a combined ssNMR and MD approach will greatly improve our molecular-level understanding of cell wall recalcitrance. Experimental data (ssNMR) will inform detailed atomistic cell wall models (MD), together providing better tools capable of predicting deconstruction performance and biomass structure.
