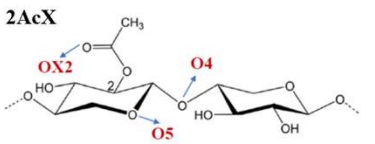
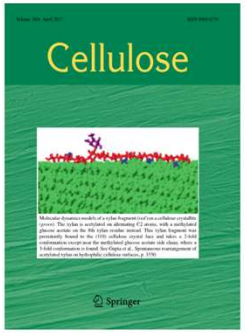
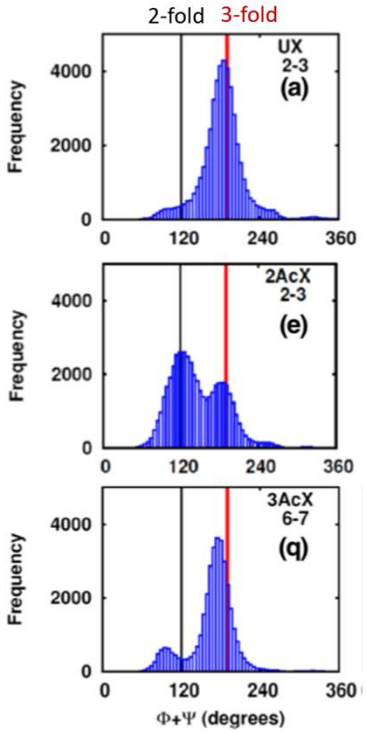
Xylan-cellulose interactions revealed from molecular simulations

Scientific Achievement

Identified the molecular interactions that stabilize cellulose-xylan binding and the effect of acetylation







Significance and Impact

The pattern of acetylation of xylans alters xylan binding to cellulose and secondary cell wall strength, but why this is so has been unclear. Here we simulated xylans in spatially proximity to a cellulose surface: 1,2-linked acetyl xylans (2AcX) adopt rigid two-fold helical screw conformations and bind tightly to cellulose, whereas 1,3-linked acetyl xylans (3AcX) maintain three-fold helical screw conformations and bind cellulose less strongly. The data demonstrate how chemical modifications affect plant cell wall polymer interactions and conformations.

Research Details

- Xylan conformations determined by unbiased molecular dynamics simulations.
- The 2AcX conformations are stabilized by interactions between the acetylated oxygen and the glycosidic linkage with C-O6 of cellulose.
- Results are consistent with previous ssNMR experiments.

Simulations were performed at the National Energy Research Scientific Computing Center (NERSC).
Gupta, M.; Rawal, T.B.; Dupree, P., Smith, J. C.; Petridis, L. Spontaneous rearrangement of acetylated xylan on hydrophilic cellulose surfaces. Cellulose 28, 3327–3345 (2021). https://doi.org/10.1007/s10570-021-03706-z