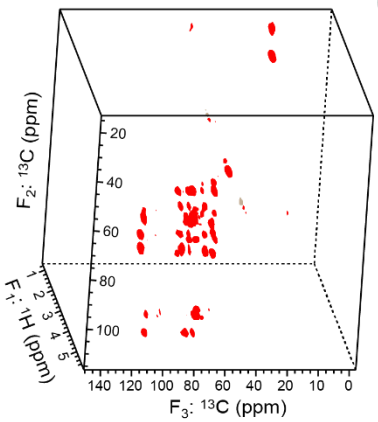
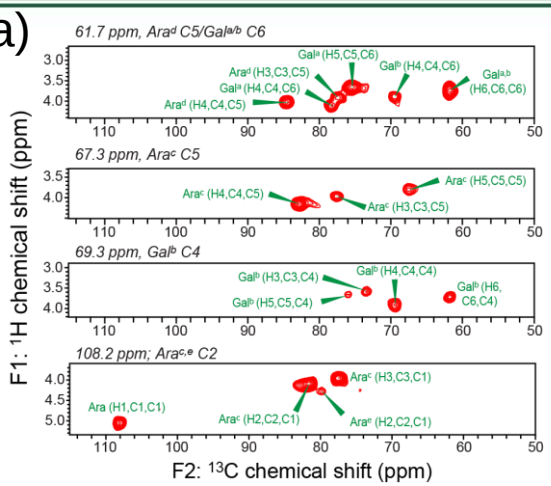
^{1}H-^{13}C Correlation NMR for Structural Investigation of Primary Cell Walls



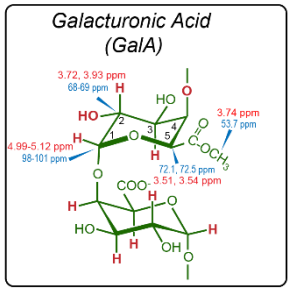
(a)

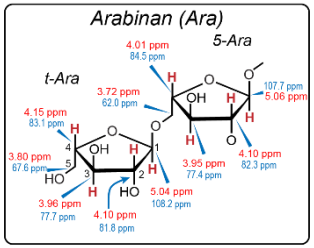


Significance and Impact

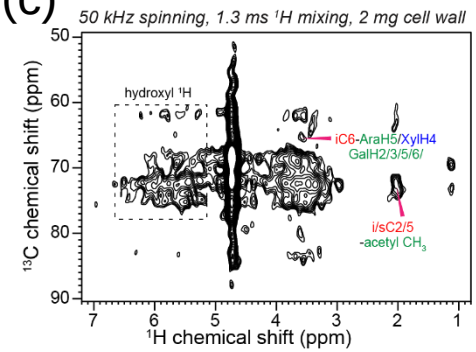
Until recently, studies of plant cell walls by solid-state NMR mostly relied on ^{13}C chemical shifts. By resolving the ^{1}H chemical shifts of polysaccharides, we add a new molecular probe of cell wall polysaccharides. Knowledge of the ^{1}H chemical shifts allows us to use ^{1}H spin diffusion NMR to detect nanometer intermolecular contacts, which is difficult to achieve by ^{13}C spin diffusion NMR.

(b)





(c)



Phyo P and Hong M: Fast MAS ^{1}H-^{13}C correlation NMR for structural investigations of plant cell walls. J. Biomol. NMR, 73, 661-674 (2019) Work carried out at MIT based on cell walls produced at Penn State (Gu lab)

Scientific Results

A 3D NMR method is developed to measure ^{1}H chemical shifts and intermolecular interactions of plant cell wall polysaccharides.

Research Details

(a) A 3D ^{1}H-^{13}C-^{13}C correlation experiment at 37 kHz MAS gives high-resolution spectra of matrix polysaccharides in *Arabidopsis* cell walls. (b) The ^{1}H and ^{13}C chemical shifts combine to resolve all polysaccharides in cell walls. (c) Using these ^{1}H chemical shifts, and spinning at 50 kHz, we detected cellulose-pectin correlations using only 2 mg of cell wall material and a short mixing time of 1.3 ms. This is much more efficient than ^{13}C spin diffusion NMR.

U.S. DEPARTMENT OF ENERGY | Office of Science | OAK RIDGE National Laboratory | NC STATE UNIVERSITY | UNIVERSITY of VIRGINIA | Massachusetts Institute of Technology | UNIVERSITY OF RHODE ISLAND | PENNSTATE | CLSF