

Effect of Deuteration on the Structure of Bacterial Cellulose

Approach: Bacterial Cellulose (BC) as a Model for Cellulose in Lignocellulosic Biomass

- A molecular structure similar to that of the plant cellulose
- Generated in pure form – *i.e.*, without hemicellulose and lignin
- Deuterium (^2H) incorporated in cellulose at high levels of substitution enabling neutron studies for molecular structure, water dynamics and chain conformation

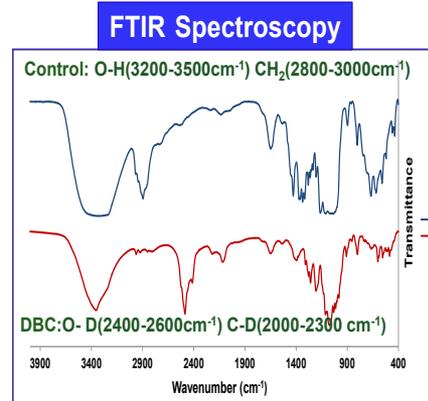
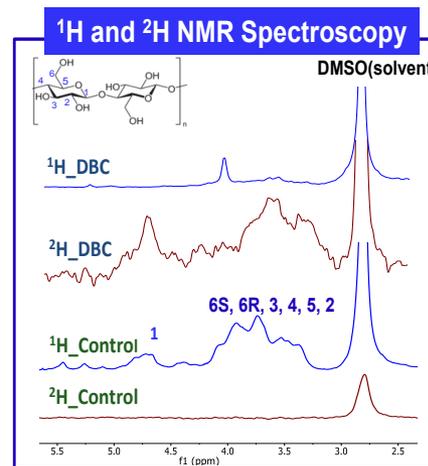
Deuteration of biopolymers: an important tool for contrast variation studies using neutron scattering, but predicts that the deuterated polymer is otherwise comparable in its physiochemical properties to its protio counterpart (control)

Objective: Direct measurement of deuterium incorporation in bacterial cellulose (BC) and its complete structural characterization

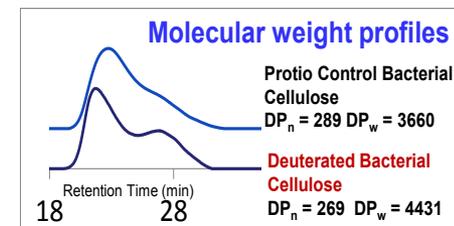
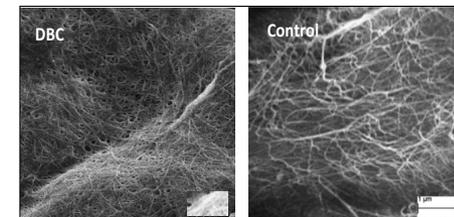
Results:

- NMR analysis demonstrated ~85% of deuterium incorporation in cellulose from *Acetobacter xylinus* subsp. *Sucrofermentans* grown in a D_2O medium.
- Acetylation of bacterial cellulose showed site-specific deuteration.
- No significant alterations in bacterial cellulose physiochemical properties due to deuteration.
- Similar proportions of I_α and I_β in DBC and protio control showed that the structural heterogeneity of native cellulose I was preserved upon deuteration.

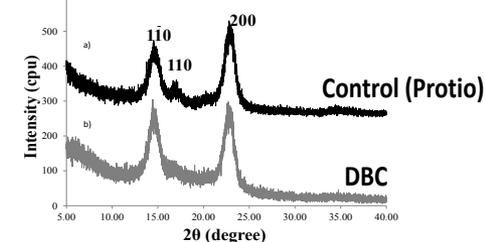
Significance: The findings clearly demonstrated the possible use of deuterated bacterial cellulose (DBC) in small angle neutron scattering (SANS) as well as a model substrate to understand the role of cellulose structure in enzymatic hydrolysis or other complex conversion processes.



Scanning electron micrographs



X-ray diffraction spectra of bacterial cellulose films



Citation: Bali G., Foston M. B., O'Neill, H. M., Evans B. R., He J., Ragauskas A. J., "The effect of deuteration on the structure of bacterial cellulose" *Carbohydrate Research* (2013) in press. Contact: Art.Ragauskas@chemistry.gatech.edu