Impact of acetylation on xylan-cellulose interactions: a QCM-D and molecular dynamic study

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[1]Unité de recherche sur les Biopolymères, Interactions Assemblages – Institut National de la Recherche Agronomique : UR1268 – France

[2]Centre de Recherches sur les Macromolécules Végétales – Centre National de la Recherche Scientifique : UPR5301, Université Grenoble Alpes – France

Abstract

Xylan is a ubiquitous hemicellulose in plant cell wall and its interaction with cellulose plays an important role in plant crop and biomass development and uses. The hemicellulose structure is substituted by various groups whose roles are poorly understood with regard to the polysaccharide functional properties. Among these decorations, the effect of acetyl esters in xylan adsorption on cellulose was assessed by QCM-D and molecular dynamics studies. Acetylated and mild alkali de-acetylated xylans from apple pomace formed different organization and hydration complexes with model cellulose nanocrystals surfaces. The two xylans had distinct kinetics of adsorption on cellulose indicating that acetyl esters favor xylan coverage of cellulose. Acetylated xylans chains have a conformation with two residues per helical turn and produced a dense and poorly hydrated layer on cellulose. In contrast, de-acetylated xylan chains have three residues per turn and formed a swollen and more viscous layer in which only the xylan chains in direct contact with cellulose surface displayed the two residues per helical turn conformation. These results open new views on biomass recalcitrance to biotransformation and means of regulating xylan interactions in plant cell walls.

*Speaker