THF-Water solvation influences xylan hydrolysis rate and subsequent furfural product formation

**Objective:**
- Elucidate xylan behavior under THF-Water cosolvent used during co-solvent enhanced lignocellulosic fractionation (CELF).

**Approach:**
- We paired molecular simulation and experimental evidence, and revealed how the solvation of xylan in an water–tetrahydrofuran (THF) pretreatment can lead to single-pot conversion of biomass xylose to furfural and cellulose to 5-hydroxymethylfurfural.

**Results:**
- Xylan is solvated by both THF and water at CELF pretreatment temperatures.
- Partial solvation by THF was found to slow down xylan solubilization.

**Significance:**
- In aqueous solution, xylan is depolymerized faster than cellulose is, making it difficult to convert both biopolymers to fuel precursors at the same time.
- We showed that solvation by THF:water (CELF) slows the rate of xylan hydrolysis, allowing an economically desirable “single-pot” conversion of both xylan and cellulose to fuels and products.

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*(Dynamic Visualization of Lignocellulose degradation …)*