

# Solvent Selection in Liquid-Liquid Reactive Extraction of HMF

## Scientific Achievement

Cellulose → Glucose → Fructose → HMF → Byproducts

An improved predictive solvation thermodynamic model (COSMO-SAC) was developed and its validity for screening extractant solvents for HMF production in biphasic systems has been demonstrated.

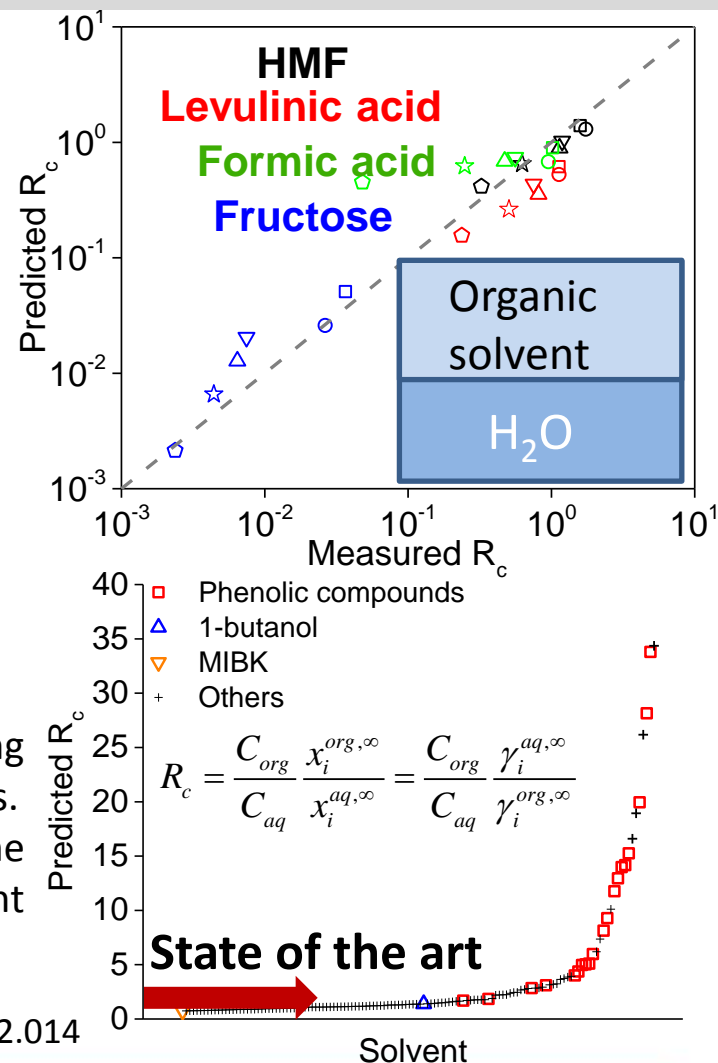
## Significance and Impact

- Solvent selection has remained elusive.
- Our work is the first demonstration of the predictive ability of the COSMO-SAC model for biomass compounds.
- The method could potentially impact the HMF production by optimizing the extractant solvent selection.

## Research Details

- The predictive accuracy of the model was validated using biomass-derived compounds in biphasic alcohol-water systems.
- Initial screening of 420 organic extractants reveals that the phenolic compounds could be “best” potential extractant candidates; experimental validation looks very promising.

Xiong *et al.* *Chem. Eng. Sci.* **2015**, 126, 169-176, doi:10.1016/j.ces.2014.12.014



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Work was performed at the University of Delaware by the group of Sandler and Nikolakis

