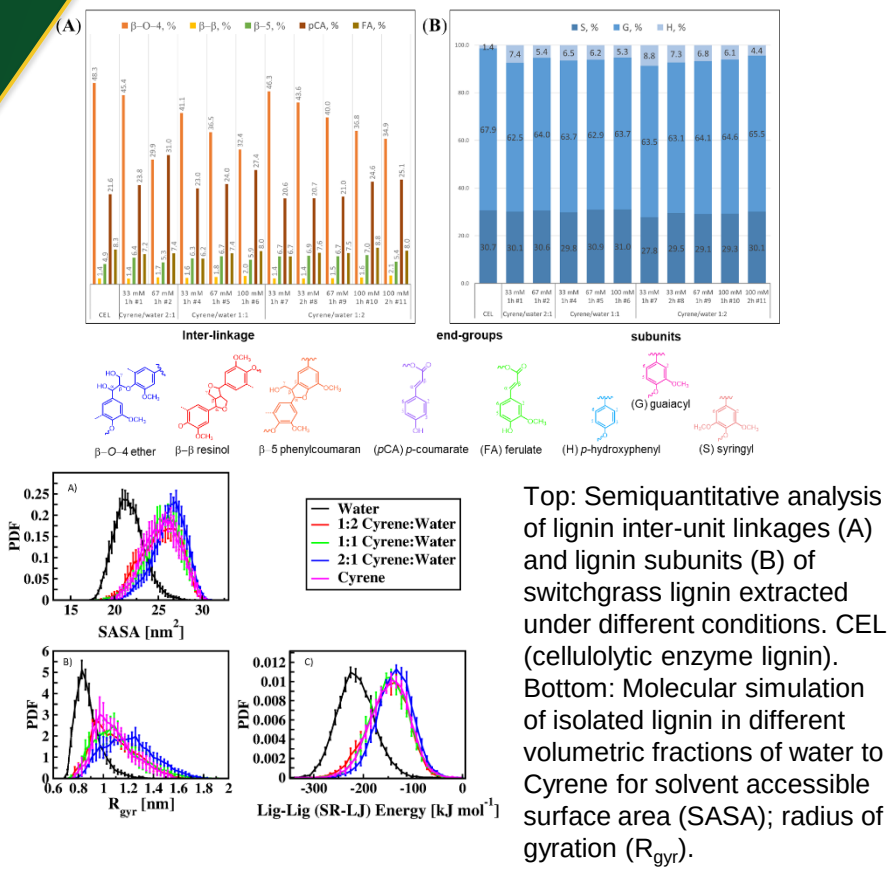
Characterization and Molecular Simulation of Lignin in Cyrene Pretreatment of Switchgrass Explains Effective Delignification



Top: Semiquantitative analysis of lignin inter-unit linkages (A) and lignin subunits (B) of switchgrass lignin extracted under different conditions. CEL (cellulolytic enzyme lignin). Bottom: Molecular simulation of isolated lignin in different volumetric fractions of water to Cyrene for solvent accessible surface area (SASA); radius of gyration (R_{gyr}).

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Scientific Achievement

We characterized lignin isolated after pretreatments with Cyrene co-solvent under various Cyrene/water compositions, acid loading, and reaction time; we correlated the experimental results with molecular simulations – revealing interactions between lignin and the cosolvent.

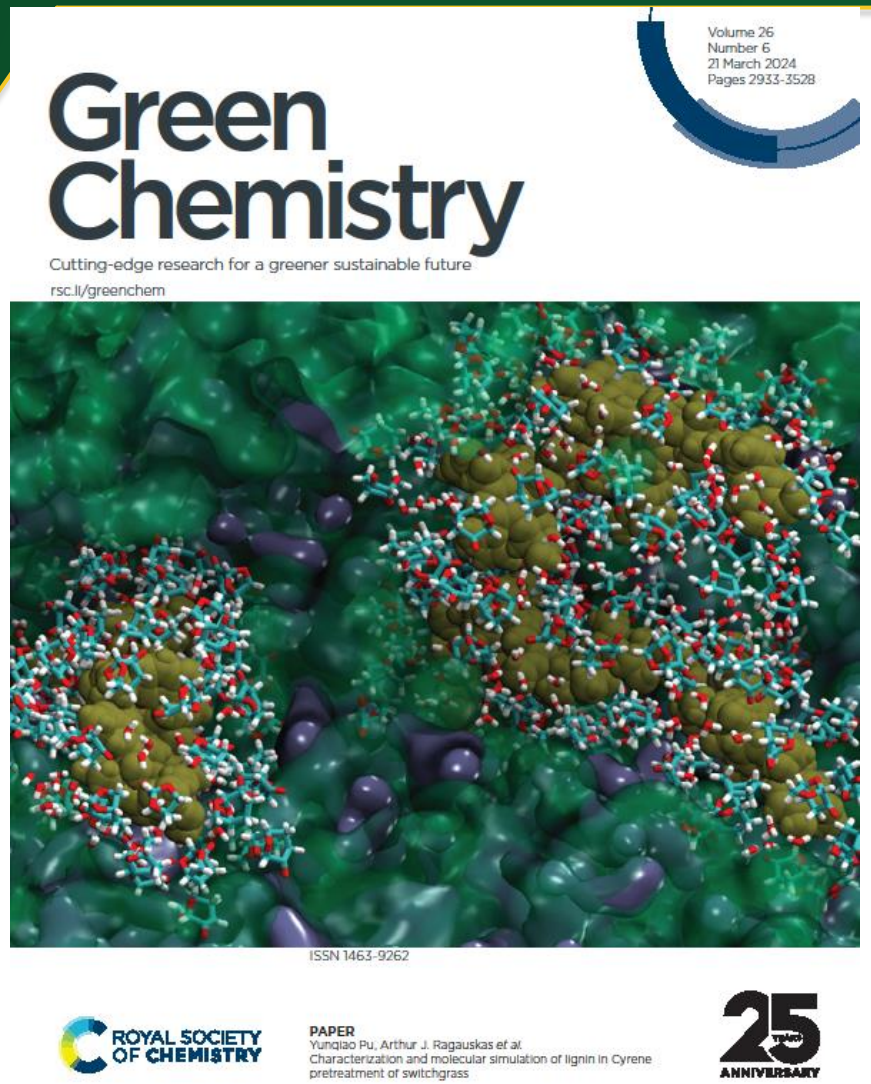
Significance and Impact

Solvent effect plays important roles in organosolv pretreatment. This work integrates biomass pretreatment, characterization with molecular simulation for in-depth understanding of the effect of Cyrene cosolvent on lignin. Cyrene pretreatment was effective at lignin fractionation and retains key lignin bonds for further valorization due to a preferential interaction of lignin with Cyrene.

Research Details

- Cyrene cosolvent showed high delignification efficiency, extracting up to 73% of lignin from switchgrass at a mild temperature of 120 ℃.
- Lignin structural integrity is inversely correlated to delignification, especially for β-O-4 linkage retention.
- Molecular simulation shows that lignin chains adopt expanded, open-chain conformations and its aggregation is disrupted in this cosolvent.
- The optimal Cyrene volumetric fraction from simulation correlated with experiments and explained these observations. Cyrene retards the diffusion and localization of acidic species.

SFA publication by Wang et al. has cover



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About the Cover:
Cyrene is an effective co-solvent to solubilize biomass and lignin. Cyrene (the small molecule in blue, white and red) accomplishes this by interacting with the lignin (brown) and preventing lignin self-aggregation.

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