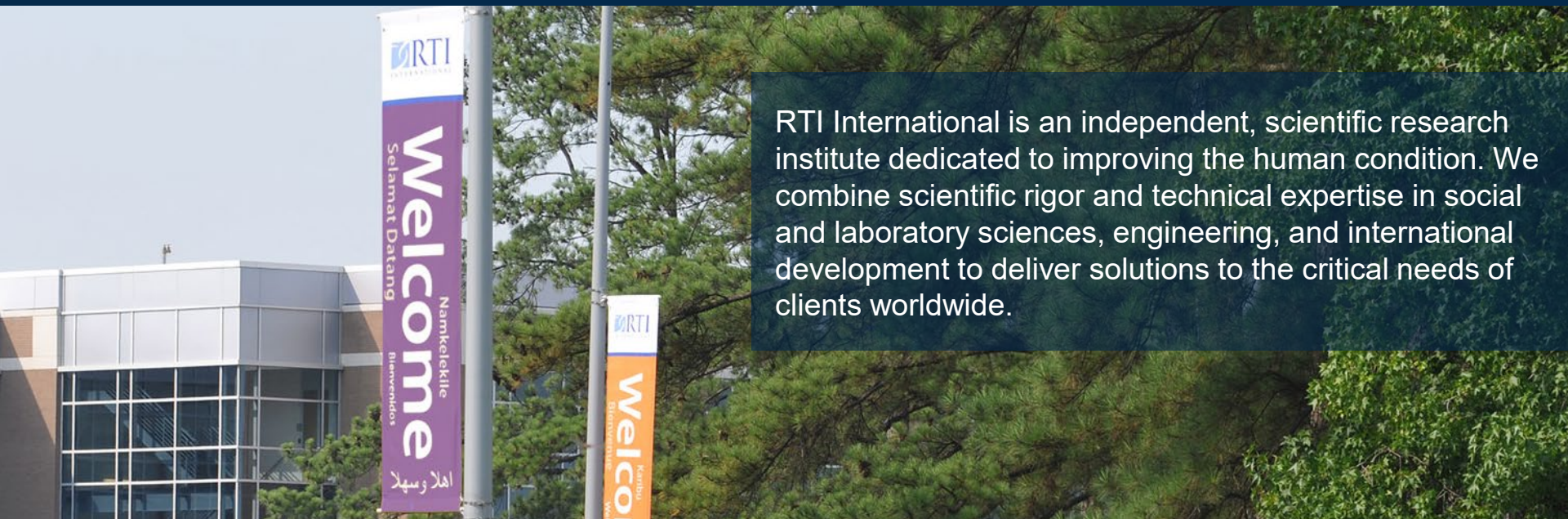


Advanced Analytical Methods to Support Biofuels Technology Development

tcbi mass⁺2026

David C. Dayton, Ph. D.
RTI Senior Fellow and Biofuels Director
August 27, 2025



RTI International is an independent, scientific research institute dedicated to improving the human condition. We combine scientific rigor and technical expertise in social and laboratory sciences, engineering, and international development to deliver solutions to the critical needs of clients worldwide.

RTI Catalytic Biomass Pyrolysis Technology Development

Feedstock



Biomass, MSW, Plastics

Catalytic Fast Pyrolysis



Fast Catalytic
Pyrolysis Lab at RTI

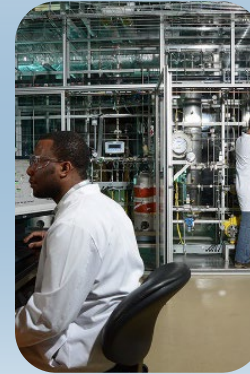


1 Ton / Day Pilot Scale
Process Unit at RTI

Separation / Refining



Lab-scale
Separation Unit



Hydrotreatment
Process Unit at RTI

Products

Advanced Biofuel
*Stable, tunable, high
value biocrude*

Bio-Chemicals
*Flavors and fragrances,
flame retardants, Bio-BPA*

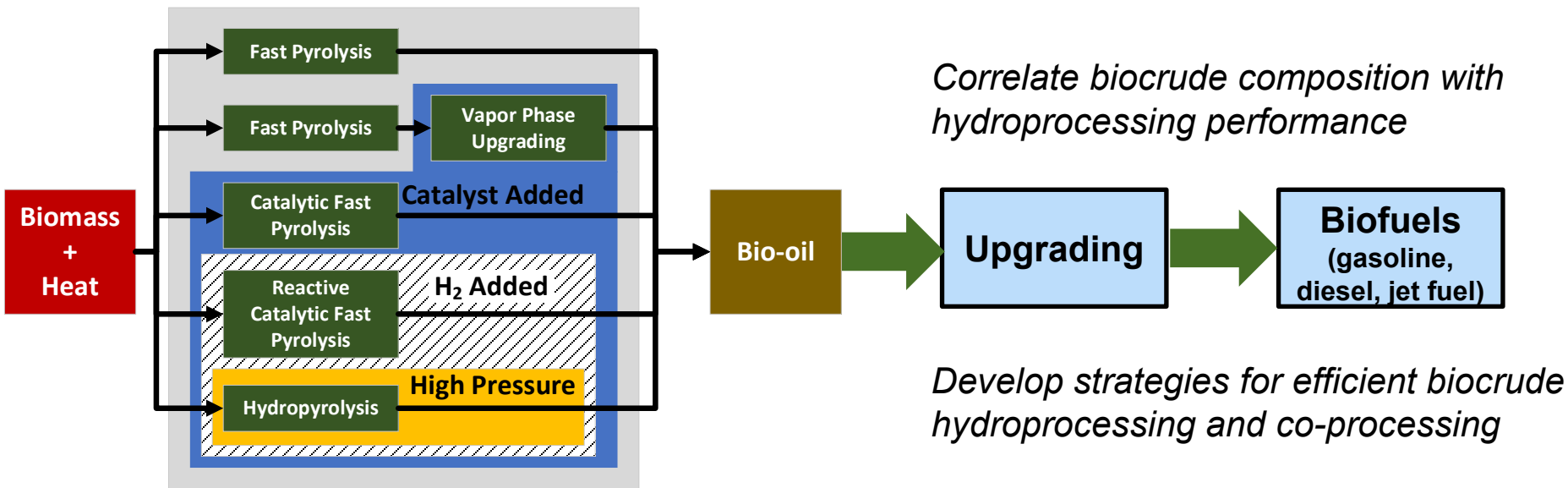
**Monomers and Plastics
Upcycling**

***Analytical methods applied for process monitoring and sample
characterization to support technology development and scaleup***

In-house capabilities for full value-chain assessment

Biomass Pyrolysis Pathways for Advanced Biofuels

Apply catalysts and reagents to maximize yields and improve biocrude **quality** (oxygen content, chemical composition, thermal stability) for upgrading



- Mante, O. D., Dayton, D. C., Carpenter, J. R., Wang, K., & Peters, J. E. (2018), Pilot-scale catalytic fast pyrolysis of loblolly pine over γ -Al₂O₃ catalyst. *Fuel*, 214, 569–579.
- Cross, P.; Wang, K. G.; Weiner, J.; Reid, E.; Peters, J.; Mante, O.; Dayton, D. C., Reactive Catalytic Fast Pyrolysis of Biomass Over Molybdenum Oxide Catalysts: A Parametric Study. *Energy & Fuels* 2020, 34 (4), 4678-4684.

The Challenge of Biocrude Analysis

Physical and chemical properties of biomass direct biomass liquefaction liquids

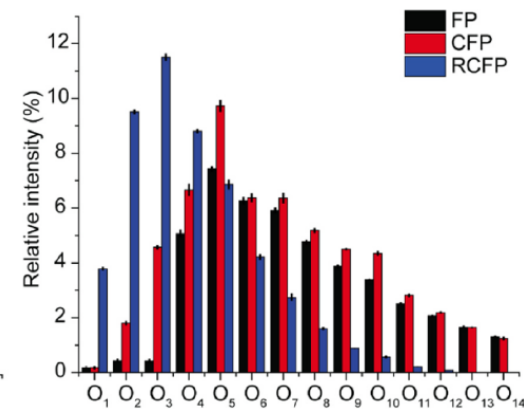
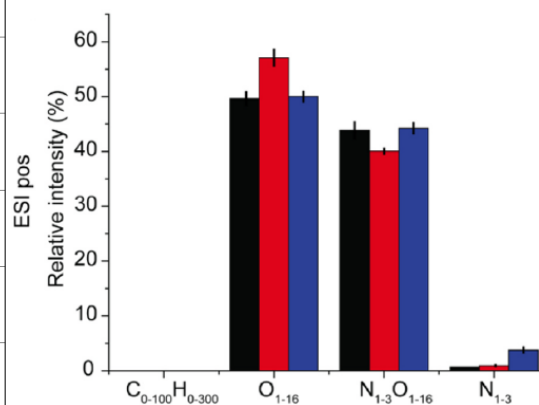
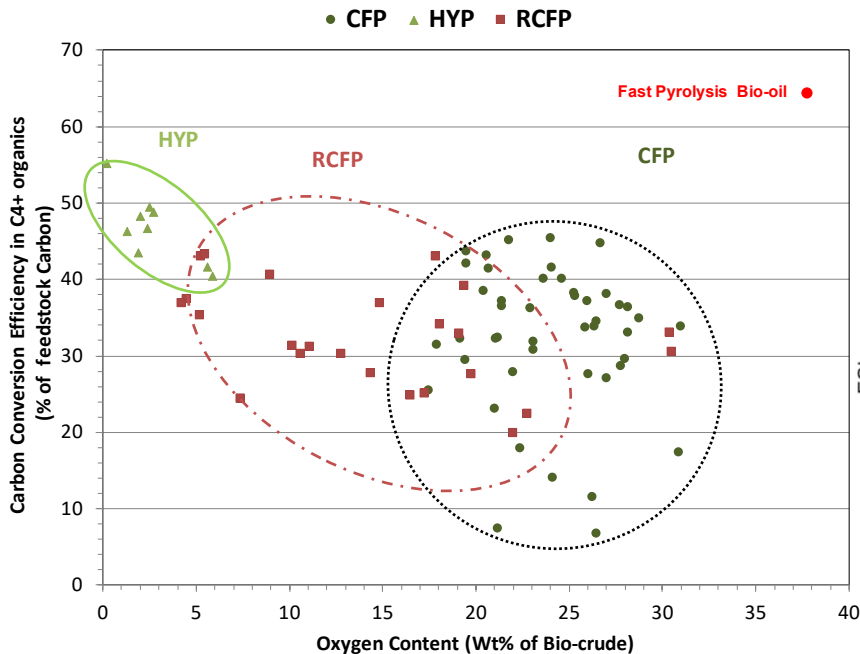
- Complex, multicomponent mixtures
 - Broad molecular weight distribution
 - Wide boiling range (low volatility)
 - Poor thermal stability
 - Partially water soluble
 - Acidic
- Multiple complementary analyses required for comprehensive, molecular level characterization to understand physical and chemical properties
 - Understanding the limitations of the measurements is critical to avoid over- or under-interpreting the results
 - Access to advanced techniques should not be a deterrent for not using them or an excuse to use them
 - Measure what you should, not what you can



Tuesday August 25th Conversion 1 3:00pm – M. Barron “Impact of Feedstock Preprocessing on Biocrude Yield”

Wednesday August 26th Upgrading II 3:30pm – A. Starace “Impact of Feedstock on CFP Biocrude Stability for Upgrading”

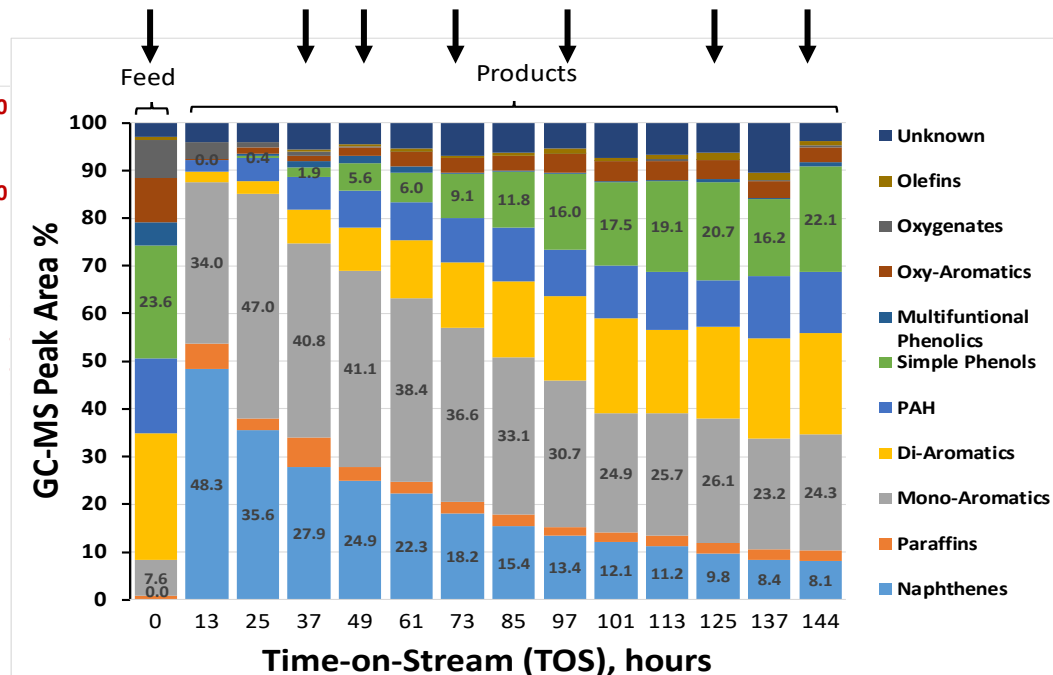
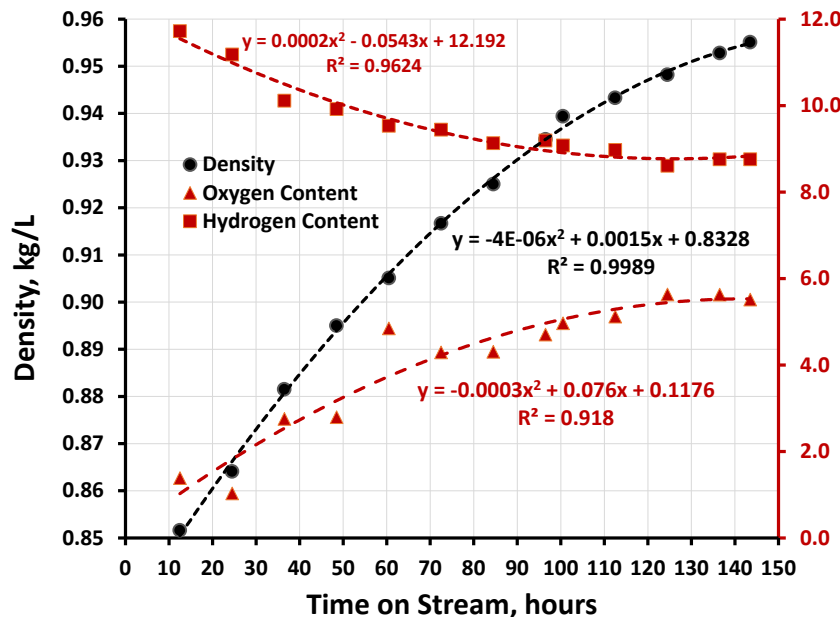
Effect of Pyrolysis Process on Biocrude Composition



- Dayton, D.C., Wang, K., Peters, J.E. and Mante, O.D. Chapter 5 - Catalytic Biomass Pyrolysis with Reactive Gases, in Fast Pyrolysis of Biomass: Advances in Science and Technology. 2017, The Royal Society of Chemistry. p. 78-95.
- Mase, C., R. Moulian, E. Lazzari, C. Garnier, M. Piparo, M. Hubert-Roux, C. Afonso, D. C. Dayton, C. Barrère-Mangote and P. Giusti (2024). "Comparison of lignocellulosic-based biomass pyrolysis processes by multi-scale molecular characterization." Journal of Analytical and Applied Pyrolysis 177: 106354.

RCFP Biocrude Upgrading

No increase in pressure drop

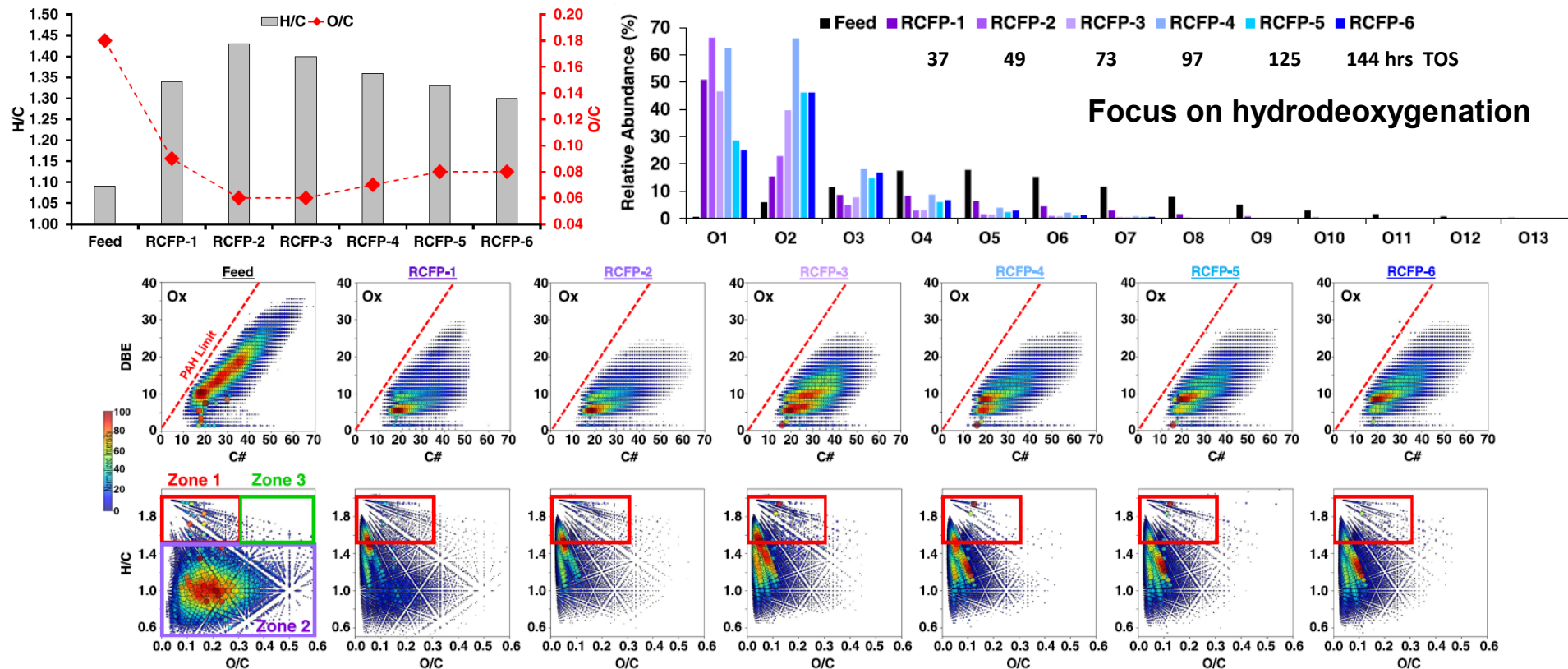


Focus on hydrodeoxygenation

Dayton, D. C.; Mante, O. D.; Weiner, J.; Komnaris, C.; Verdier, S.; Gabrielsen, J., Integrated Reactive Catalytic Fast Pyrolysis: Biocrude Production, Upgrading, and Coprocessing. *Energy&Fuels* **2022**, 36 (16), 9147-9157

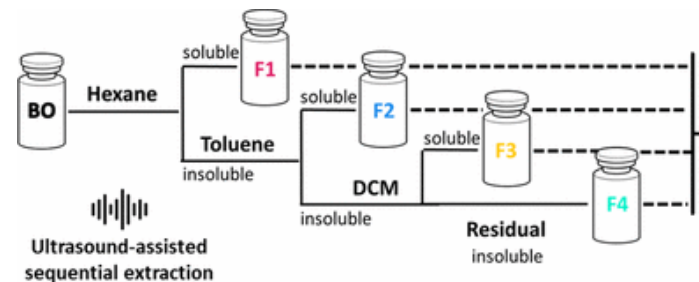
Advanced Analytical (FT-ICR-MS) Sample Analysis

Molecular composition of the bio-oil feed and hydrotreated effluents (RCFP-1–6) obtained via –ESI 21 T FT-ICR MS.

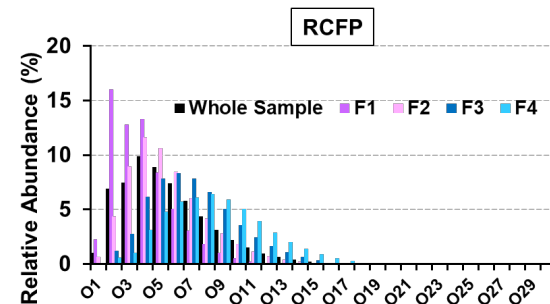
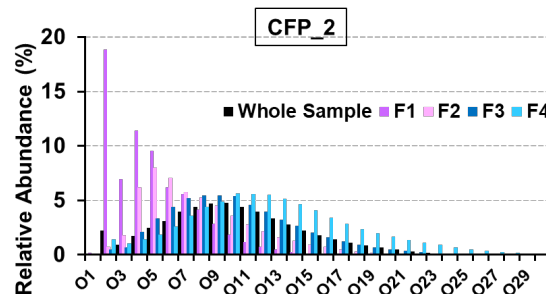
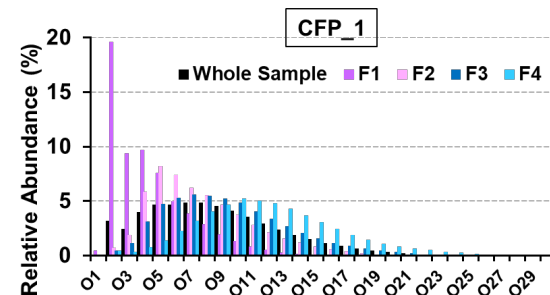
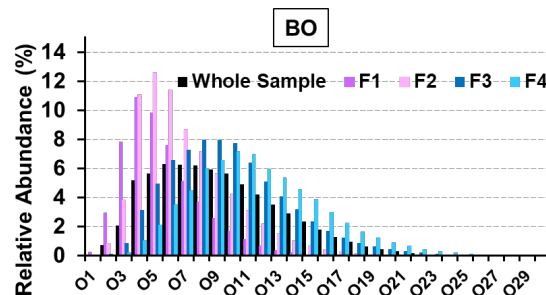
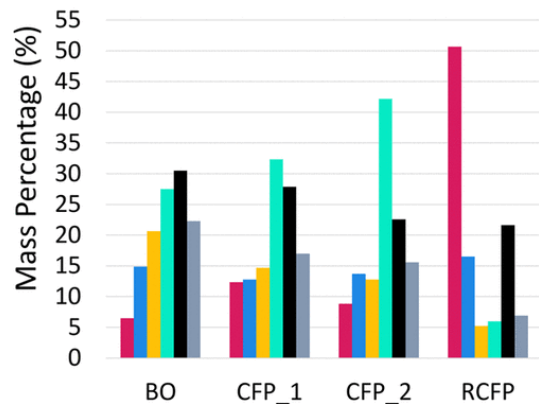


Chacón-Patiño, M. L.; Mase, C.; Maillard, J. F.; Barrère-Mangote, C.; Dayton, D. C.; Afonso, C.; Giusti, P.; Rodgers, R. P., *Petroleomics Approach to Investigate the Composition of Upgrading Products from Pyrolysis Bio-Oils as Determined by High-Field FT-ICR MS. Energy & Fuels* **2023**.

Analytical Biocrude Separations

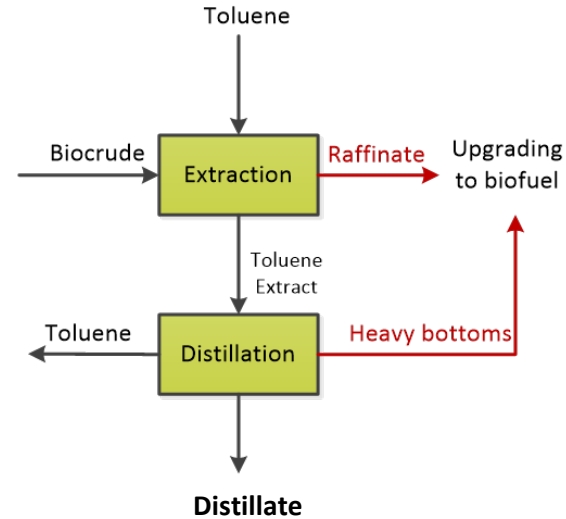


■ F1 ■ F2 ■ F3 ■ F4 ■ Lost Fraction ■ Water



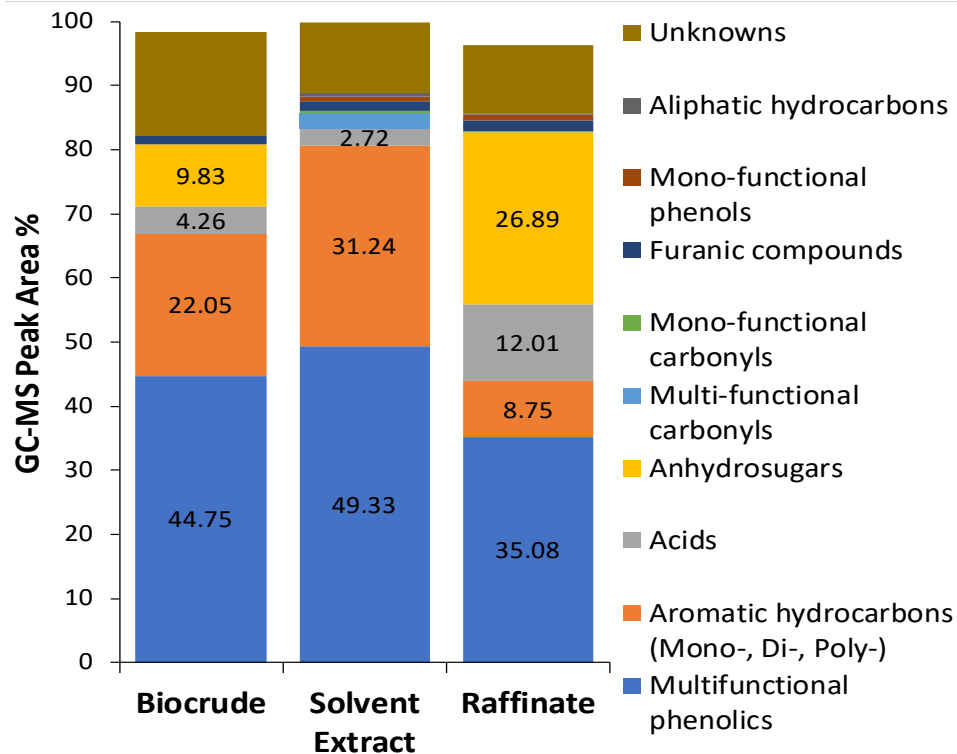
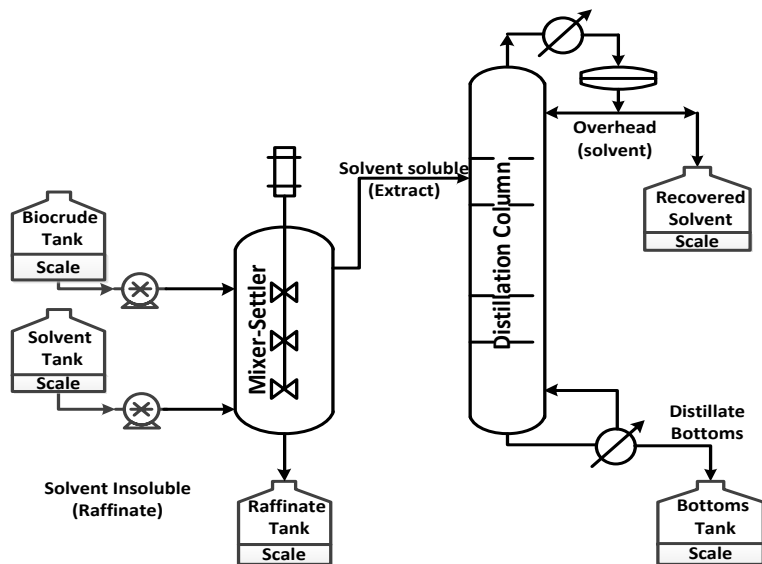
Wladimir Ruiz, German Gascon, Ryan P. Rodgers, David C. Dayton, Caroline Barrère-Mangote, Pierre Giusti, Brice Bouyssiere, and Martha L. Chacón-Patiño. *Ultrasound-Assisted Sequential Extraction for Lignocellulose Pyrolysis Bio-oil Fractionation. Part II: Comparative Application. Energy & Fuels* **2024** 38 (18), 17697-17705 DOI: 10.1021/acs.energyfuels.4c02496

Separations Process Development



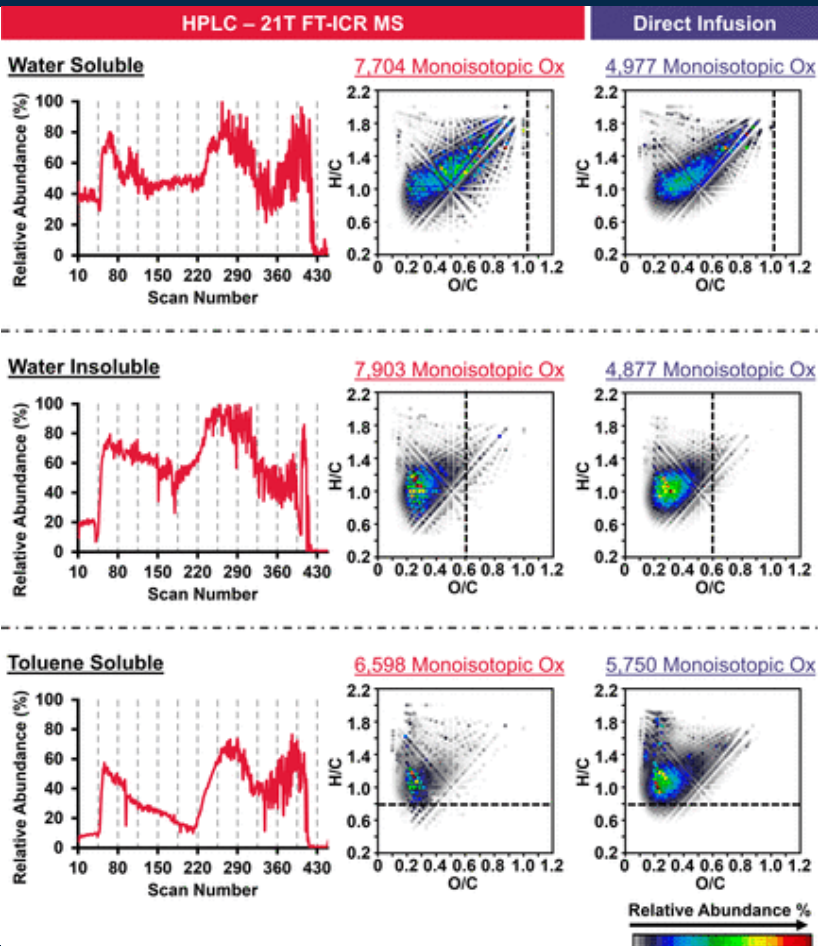
Solvent extraction	
Toluene Soluble Fraction, wt%	47.5 ± 3.2
Raffinate, wt%	52.5 ± 3.2
Distillation of Toluene Soluble Fraction	
Distillate, wt%	19.3 ± 1.9
Bottoms, wt%	28.9 ± 2.3
Solid Residue, wt%	0.0

Bench-scale Biocrude Separations



- Solvent extraction separates out acids and anhydrosugars that reduce thermal stability
- Although not detected with GC-MS, oligomers likely end up in the raffinate

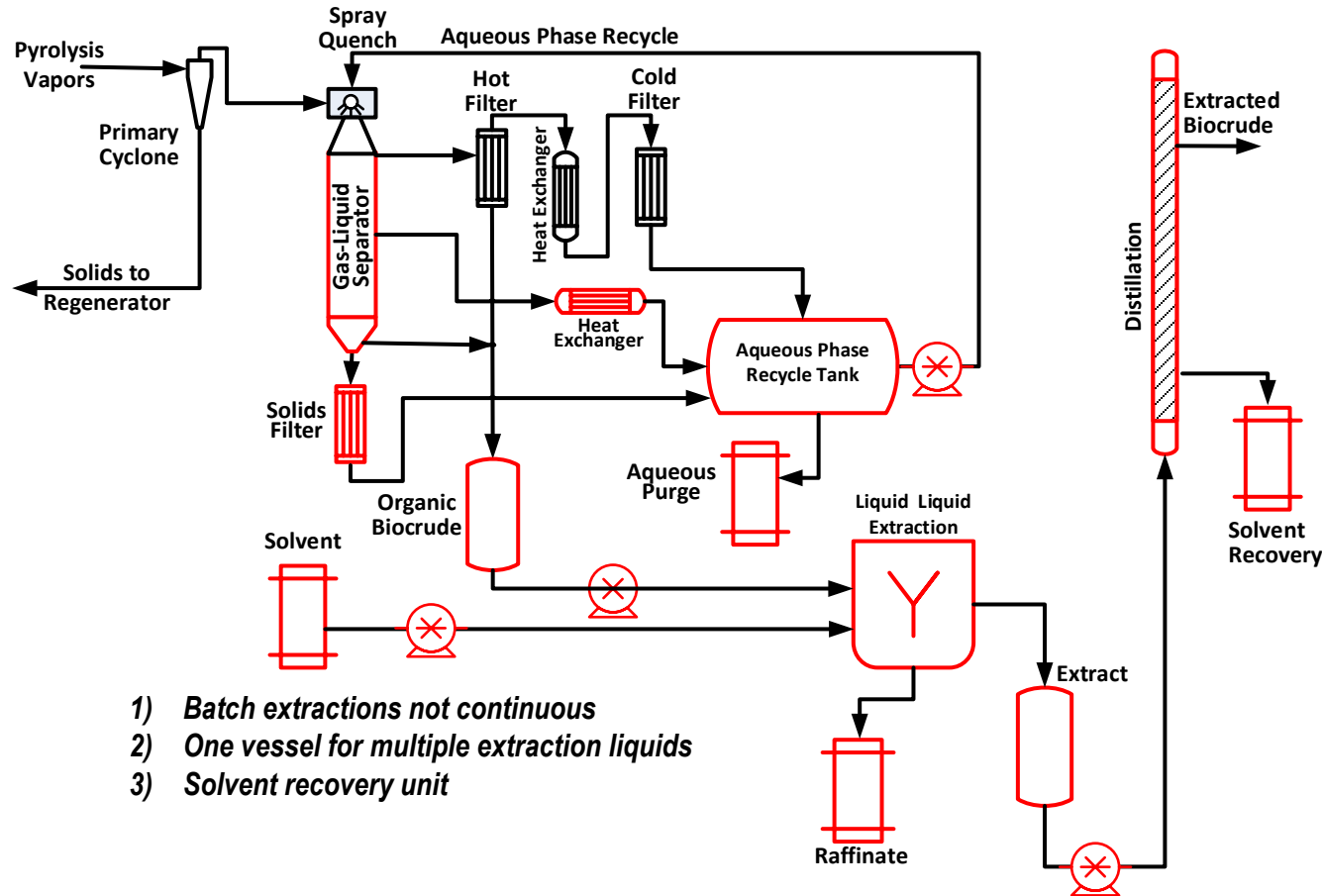
A more detailed view.....



- Total ion chromatograms (TIC) obtained via (-)ESI 21T FT-ICR MS for the water-soluble, water-insoluble, and toluene-soluble biocrude fractions.
- Van Krevelen diagrams show unique, nonrepeated monoisotopic O_x molecular formulas from combined HPLC-MS scans (left) and direct infusion MS (right).
- Number of detected compositions is highlighted in red for HPLC-MS and purple for direct infusion MS.
- HPLC-MS reveals an extended number of molecular formulas and compositional trends across the fractions compared to direct infusion.
- Black dashed lines are included to facilitate visual comparison across van Krevelen diagram pairs for the different bio-oil fractions.

Chacón-Patiño, M. L., J. W. Frye-Jones, L. C. Anderson, W. K. Robbins, G. Salvato Vallverdu, Á. J. Tello-Rodríguez, W. Ruiz, G. Gascon, C. P. Rüger, D. C. Dayton, P. Giusti, C. Mase, C. Barrère-Mangote, C. Afonso, B. Bouyssiere and R. P. Rodgers (2025). "Detailed Molecular Composition of Wood Pyrolysis Bio-Oils Revealed by HPLC-FT-ICR MS." *Energy & Fuels* 39(7): 3575-3588.

Pilot Separations in RTI 1TPD Biomass Unit



Final Thoughts

The integrated biomass pyrolysis/biocrude hydrotreating process is a pathway to infrastructure compatible, hydrocarbon biofuels

- Very high hydrogen demand compared to petroleum processing
 - Biomass is ~45 wt% oxygen and biocrude intermediates contain 10-30 wt% oxygen & ~50% aromatics

Maximize biofuel yields for attractive process economics

- Factors effecting biocrude yield and quality
 - Biomass feedstock
 - Biomass (catalytic) pyrolysis process and process conditions

Biocrude thermal stability, oxygen content, and type of oxygenates are quality metrics

- Mitigate HDT catalyst deactivation and reactor plugging by removing or eliminating reactive biocrude components
 - Maximize HDO in pyrolysis process
 - Pretreatment/Mild hydroprocessing for stabilization
 - Fractionation to segregate reactive components
 - Co-processing to delay catalyst deactivation

GC/MS analysis of biocrude and upgraded products highlights gross differences but advanced analytical methods can provide comprehensive molecular-level species identification

Inform advanced biofuel process development by correlating process conditions with intermediate compositions to support downstream applications

Contributors

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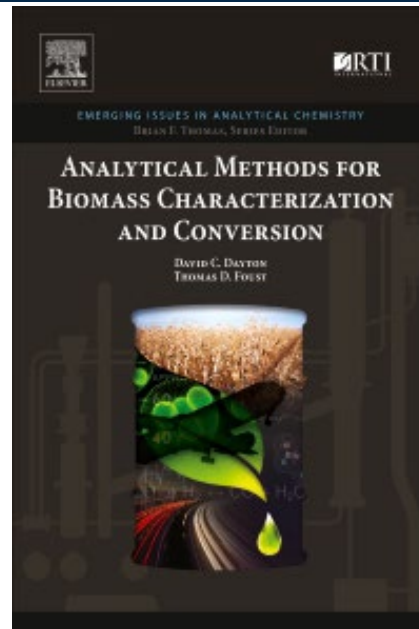


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