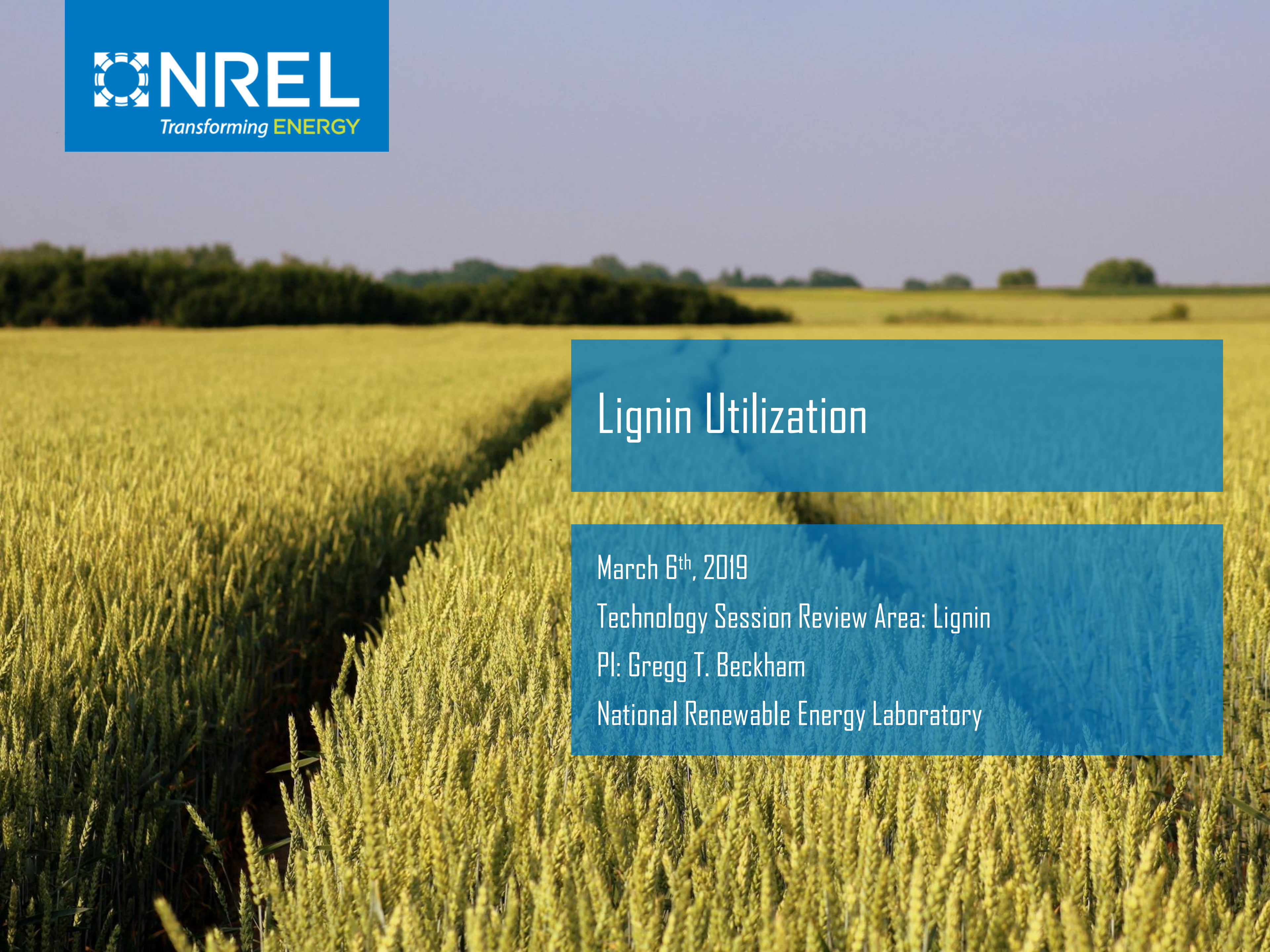


Lignin Utilization

March 6th, 2019

Technology Session Review Area: Lignin

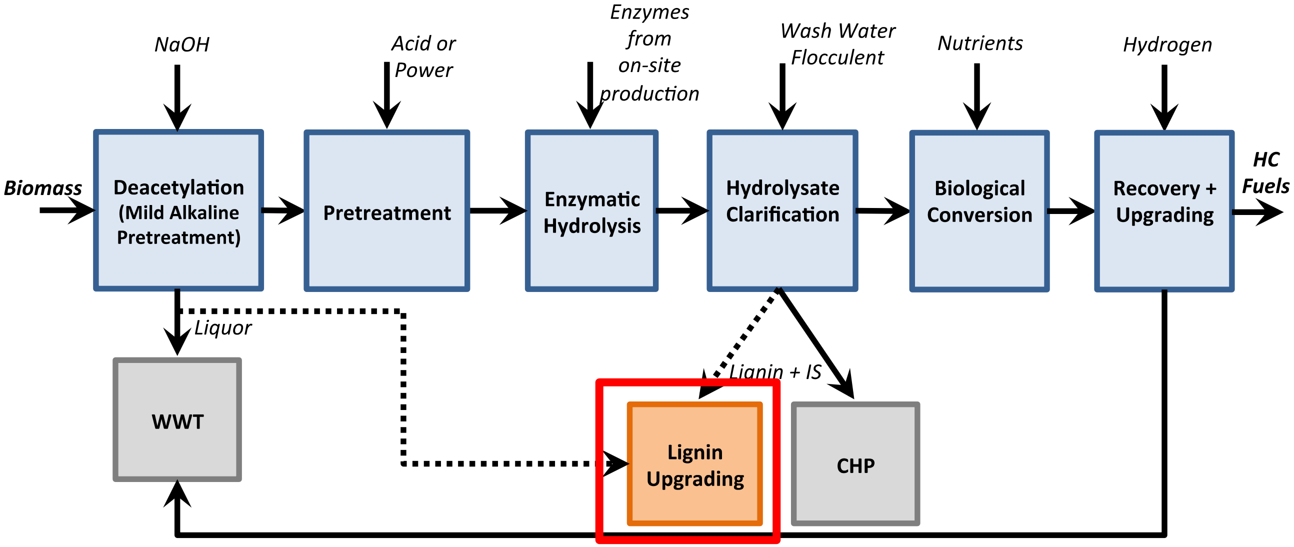
PI: Gregg T. Beckham

National Renewable Energy Laboratory

Goal Statement

Goal: Develop industrially-relevant processes for lignin valorization, focusing on depolymerization catalysis, upgrading catalysis, analytics, and synthesis

- Contribute to $2-3/gge co-product for fuel production
- Work with BETO projects to adapt lignin processing to existing processes
- Support other lignin projects domestically and internationally
- Collaborate with biology and materials projects focused on lignin



Outcome: Catalytic processes to enable lignin valorization

- Catalysis for C-C/C-O bond cleavage to enable higher usable monomer yields (40% target)
- **Industrial relevance**: lignin utilization will be a major benefit to integrated biorefineries

Quad chart overview

Timeline

- Start date: October 2016
- End date: September 2019
- Percent complete: 83%

	Total Costs Pre FY17	FY17 Costs	FY18 Costs	Total Planned Funding (FY19-Project End Date)
DOE funded	--	$1,731k	$1,347k	$1,450k

Partners:

BETO Projects: Biological Lignin Valorization, Lignin-First Biorefinery Biorefinery Development, Metabolic Engineering for Lignin Conversion, Biological Lignin Valorization – SNL, Biological Process Modeling and Simulation, ChemCatBio, Separations Consortium, PABP

Nat'l labs and universities: Oak Ridge National Laboratory, Lawrence Lawrence Berkeley Laboratory, Sandia National Laboratory, University of Portsmouth

Other DOE projects: Center for Bioenergy Innovation (CBI, ORNL), Joint ORNL), Joint Bioenergy Institute (JBEI, LBNL)

Barriers addressed

Ct-C Process development for conversion of lignin

- Catalysis to produce usable monomers from recalcitrant lignin

Ct-F Increasing yield from catalytic processes

- Catalyst design for lignin depolymerization and upgrading to improve monomer/product yields

Objective

Develop catalytic depolymerization and upgrading of lignin to value-added products that integrate with existing BETO polysaccharide processing strategies (e.g., deacetylation/mech. refining (DMR), acid pretreatment, RCF)

End of Project Goal

Demonstrate catalytic processes able to generate >40% yield of <u>usable</u> monomers from lignin. Demonstrate, in collaboration with the Biological Lignin Valorization project, that the monomers can be assimilated by either a native or engineered strain of *P. putida*.

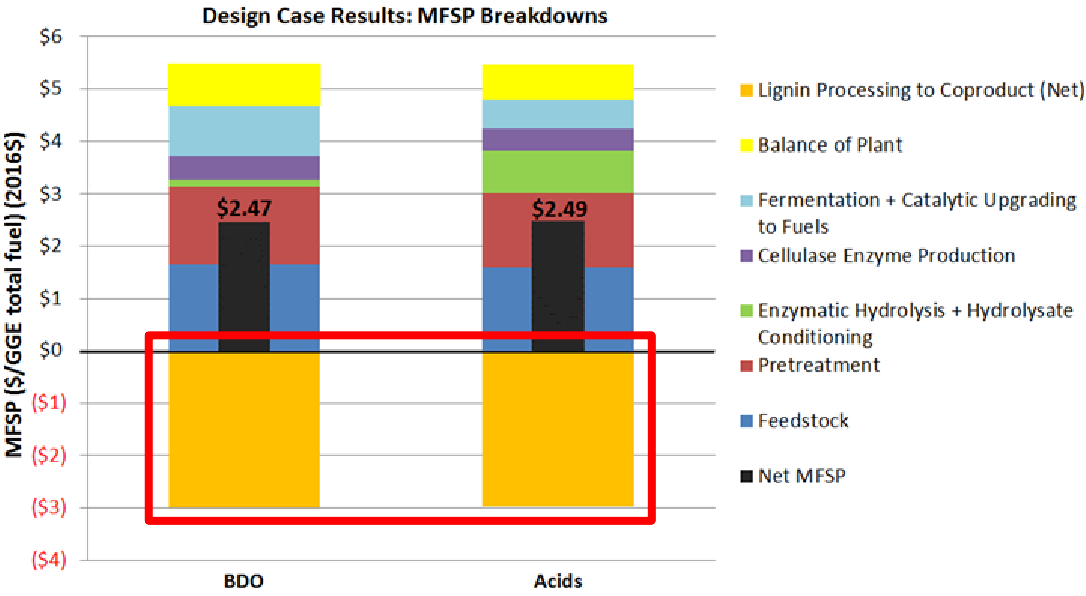
Project overview

History: Project originated in National Advanced Biofuels Consortium (2010-2013)

- **TEA predicts that lignin products can provide ~$2-3/gge, major CO_2 offsets**
- Expanded in FY16 to include oxidation catalysis
- Analytics development/synthesis is a major component

Context: Lignin slated for heat production in modern biorefineries

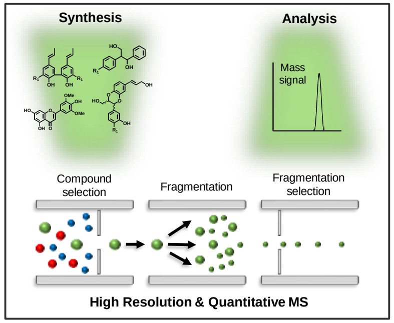
- Can be up to 40% biomass carbon
- C-C bonds limit monomer yields based ether/ester content
- Catalysis of lignin can be combined with funneling and/or with advanced



Goals:

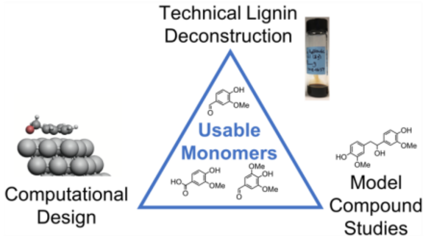
- Develop catalysts to enable higher monomer yields from **lignin depolymerization**
- Develop processes for **lignin upgrading**
- Develop cutting-edge **analytics** and **syntheses**
  - Key for yield calculations, techno-economic analysis (analytics), and catalyst studies (syntheses)
- Work with biological projects to provide streams for conversion

Management approach



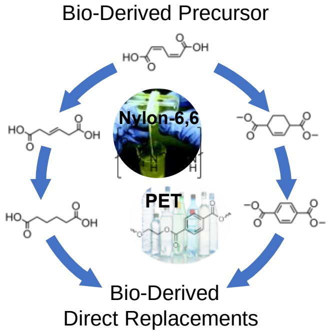
Task 1: Characterization

- Led by Rui Katahira (NMR, synthesis) and Brenna Black (MS)
- Milestones: **lignin characterization, model compound synthesis**
- Collaborate broadly with BETO projects and external partners



Task 2: Deconstruction

- Led by chemical catalysis experts (Jacob Kruger, Allison Robinson)
- Milestones: **usable monomer yield** from catalytic processes
- Includes computational catalyst design



Task 3: Upgrading

- Led by chemical catalysis expert (Derek Vardon)
- Milestones: production of **adipic acid, terephthalic acid**
- Leverage catalyst stability improvements from ChemCatBio et al.

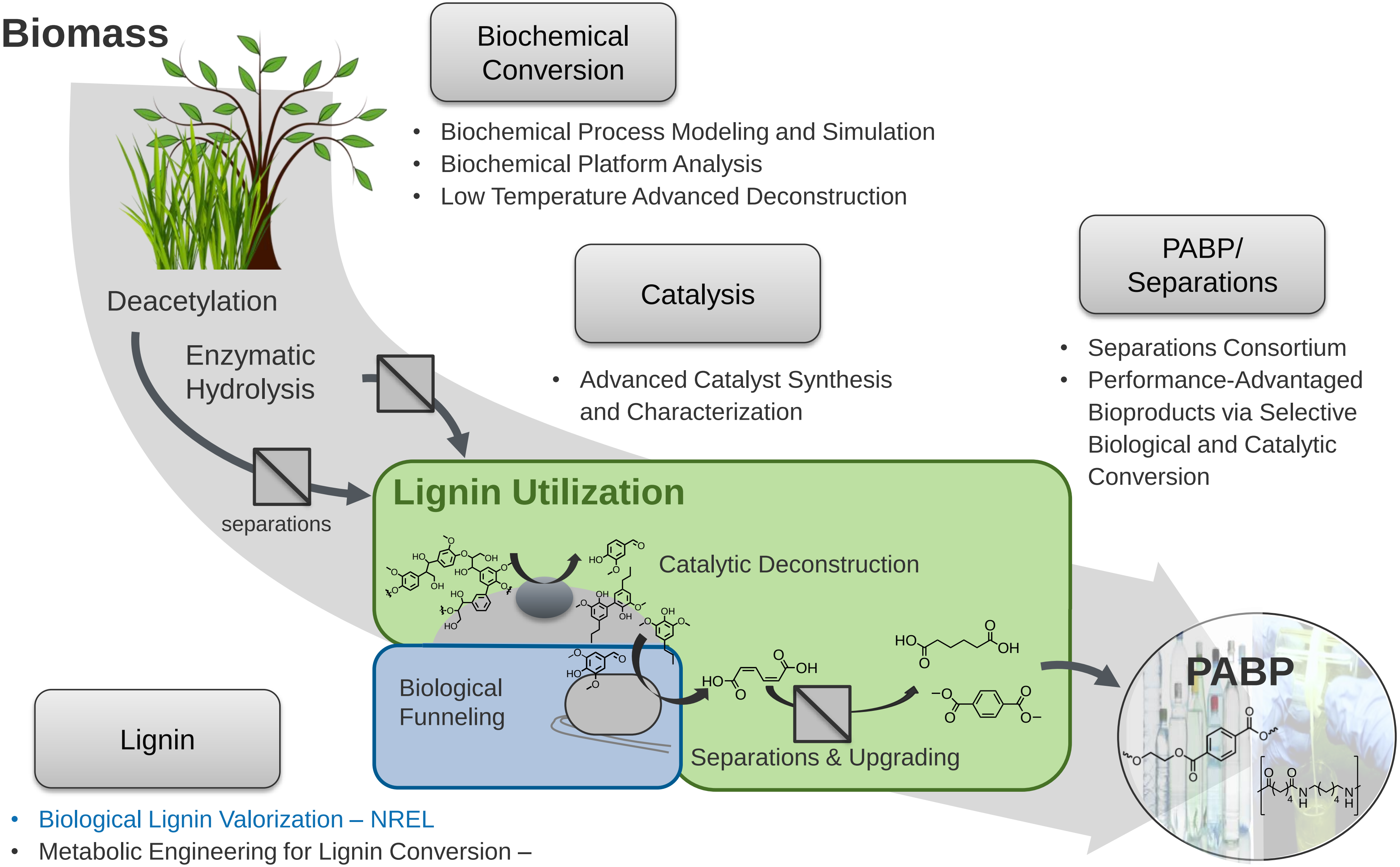
Joint meetings between tasks, among collaborators in BETO lignin portfolio

Substrates from BETO-funded sugar conversion projects

Collaborate with Separations Consortium on lignin-relevant separations

Dedicated project manager to track milestones and budget

Project interactions



Biomass

Deacetylation

Enzymatic
Hydrolysis

separations

Biochemical
Conversion

- Biochemical Process Modeling and Simulation
- Biochemical Platform Analysis
- Low Temperature Advanced Deconstruction

Catalysis

- Advanced Catalyst Synthesis and Characterization

PABP/
Separations

- Separations Consortium
- Performance-Advantaged Bioproducts via Selective Biological and Catalytic Conversion

Lignin Utilization

Catalytic Deconstruction

Biological
Funneling

Separations & Upgrading

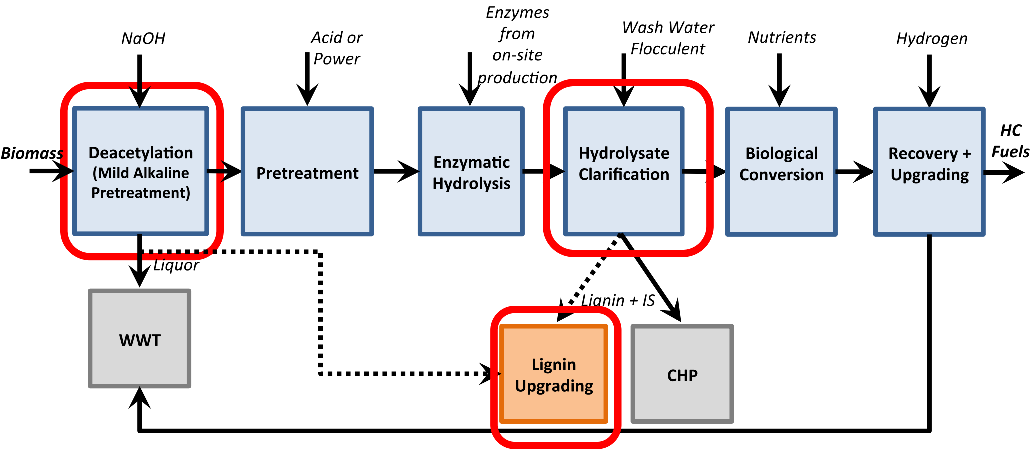
PABP

Lignin

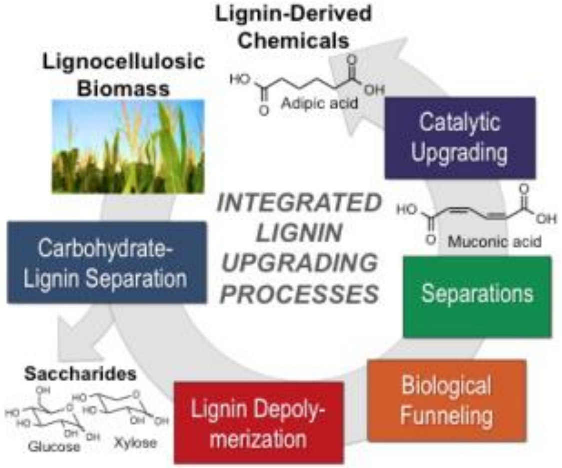
- Biological Lignin Valorization – NREL
- Metabolic Engineering for Lignin Conversion – ORNL
- Lignin-First Biorefinery Development

Technical approach

Aim 1: Develop catalysts to obtain high yields of aromatic monomers


NaOH
Acid or Power
Enzymes from on-site production
Wash Water Flocculent
Nutrients
Hydrogen
Biomass
Deacetylation (Mild Alkaline Pretreatment)
Pretreatment
Enzymatic Hydrolysis
Hydrolysate Clarification
Biological Conversion
Recovery + Upgrading
HC Fuels
Liquor
Lignin + IS
WWT
Lignin Upgrading
CHP

Aim 2: Use biology and catalysis to upgrade lignin monomers


Lignin-Derived Chemicals
Lignocellulosic Biomass
Adipic acid
Catalytic Upgrading
INTEGRATED LIGNIN UPGRADING PROCESSES
Muconic acid
Carbohydrate-Lignin Separation
Separations
Saccharides
Glucose
Xylose
Lignin Depoly-merization
Biological Funneling

Vardon, Franden, Johnson, Karp, *et al.*, *EES* 2015

Critical success factors:

- High yields of stable, liquid, low-MW products

Challenges:

- C-C bond cleavage
- Analysis of substrate and catalytic products

Approach:

- Lignin <u>from pretreatment</u> and/or <u>post-EH solids</u>
- Replace NaOH in pretreatment
- Oxidation catalysts for C-C bond cleavage

Critical success factors:

- High-yielding processes to final products

Challenges:

- Separations of intermediates from lignin streams

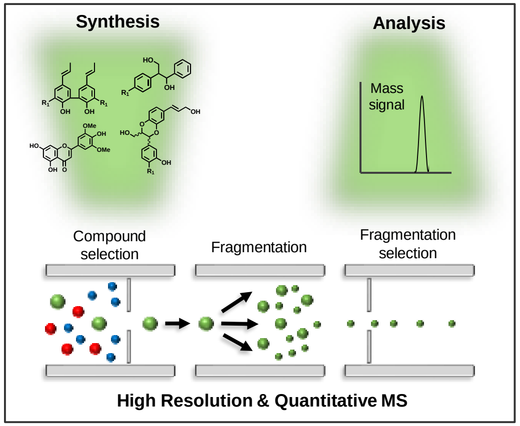
Approach:

- "Biological funneling" to obtain intermediates, **muconic acid with BLV project**
- **Adipic and terephthalic acid** via muconic acid
- Work with SepCon for separations efforts

Outline of technical accomplishments

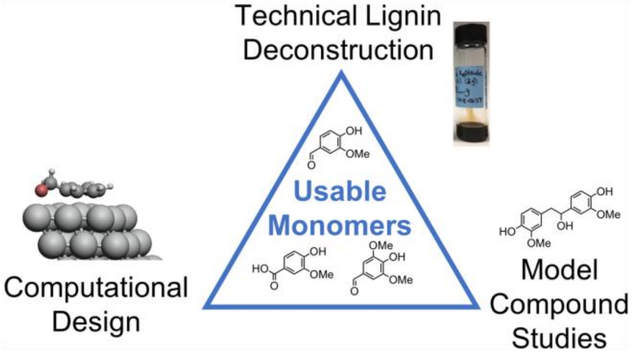
Analytics and model compound syntheses

- Synthesis methods across a wide chemistry range
- Comprehensive portfolio for analytics



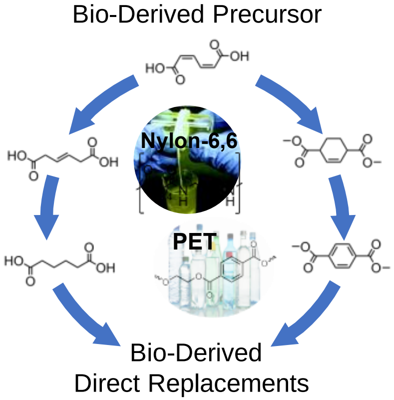
Aim 1: Develop catalysts and processes to obtain high yields of aromatic monomers

- Replacing NaOH in alkaline pretreatment with
- Revisiting alkaline aerobic oxidation
- Vanadium-based catalysts for C–O bond cleavage
- Metal oxides for C–C bond cleavage



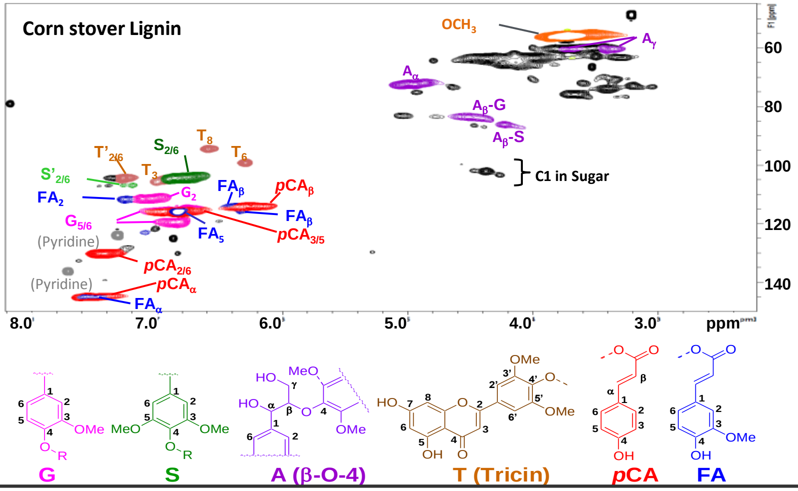
Aim 2: Upgrade bio-derived products from lignin bioconversion

- Adipic acid from muconate
- Terephthalic acid production from muconate

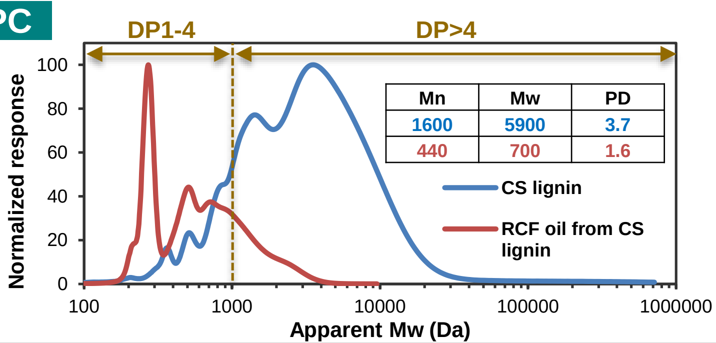


Analytics: Advancing comprehensive lignin characterization

2D HSQC-NMR

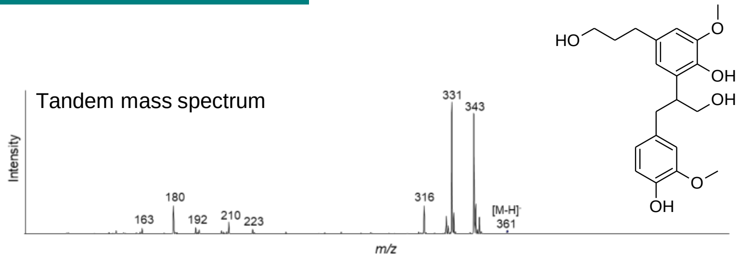


GPC



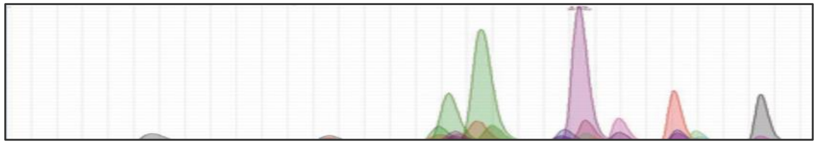
Mn	Mw	PD
1600	5900	3.7
440	700	1.6

LC-MS Identification



- High mass resolution MS – characterizes complex lignin mixtures with four main levels of performance:
  1) 2D chrom. 2) Ion mobility 3) MS 4) MS/MS

LC-MS Quantitation

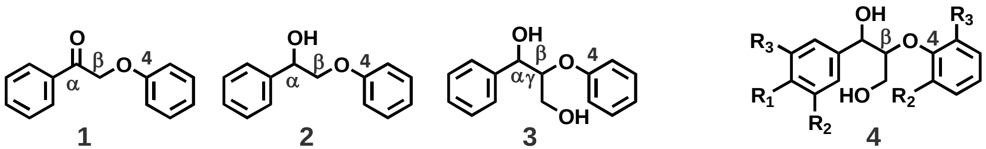


- Low mass resolution MS - sensitive, specific, rapid, quantitation of complex mixtures using authentic standards
- No derivatization required
- Chromatographic resolution not necessary for accuracy

- Lignin inter-unit linkages and MW distribution before/after catalytic conversion from 2D-NMR and GPC
- ID and quantification of monomers/dimers in catalytic breakdown by advanced LC-MS
- **Outcome: comprehensive suite of methods (including new development) for characterizing lignin in solid and liquid in solid and liquid forms**

Analytics: Developing lignin model compound syntheses

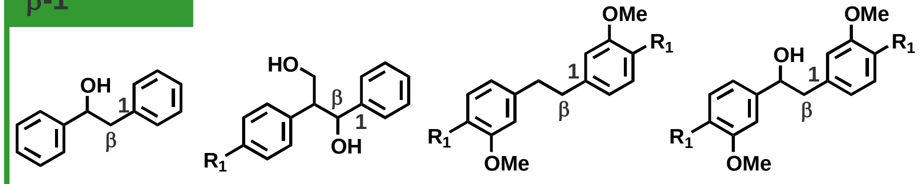
β-O-4



1 2 3 4

	Phenolic (R1= OH)			Non-phenolic (R1= OBn)		
	G-G	S-S	H-H	G-G	S-S	H-H
R2	OMe	OMe	H	OMe	OMe	H
R3	H	OMe	H	H	OMe	H

β-1



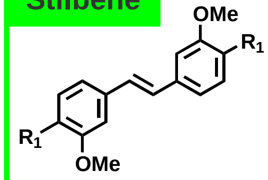
5

6 R1: OH, OBn

7 R1: OH, OMe

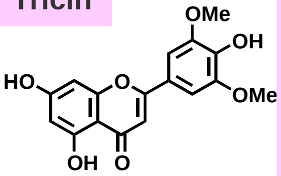
8 R1: OH, OMe

Stilbene



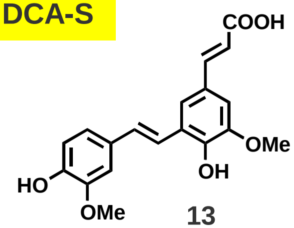
9 R1: OH, OMe

Tricin



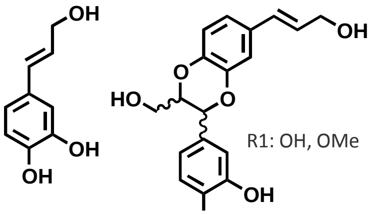
10

DCA-S



13

C-lignin (benzodioxane)

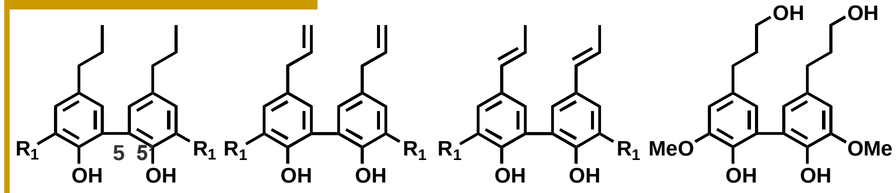


11

R1: OH, OMe

12

5-5’ linked dimers



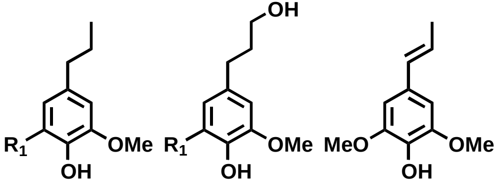
14 R1: H, OMe

15

16

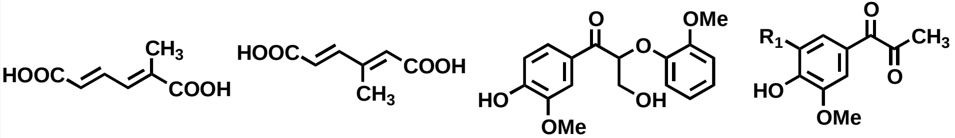
17

Stds for GC in RCF



18 19 20

Stds for HPLC in biological lignin deconstruction



21 (2-methyl Muconate)

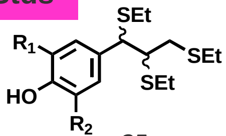
22 (3-methyl Muconate)

23 (MPHPV)

24 R1: OH, OMe

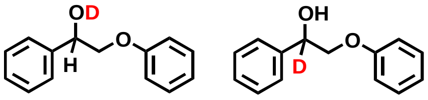
Thioacidolysis Stds

H: $R_1 = R_2 = H$
G: $R_1 = OMe, R_2 = H$
S: $R_1 = R_2 = OMe$



25

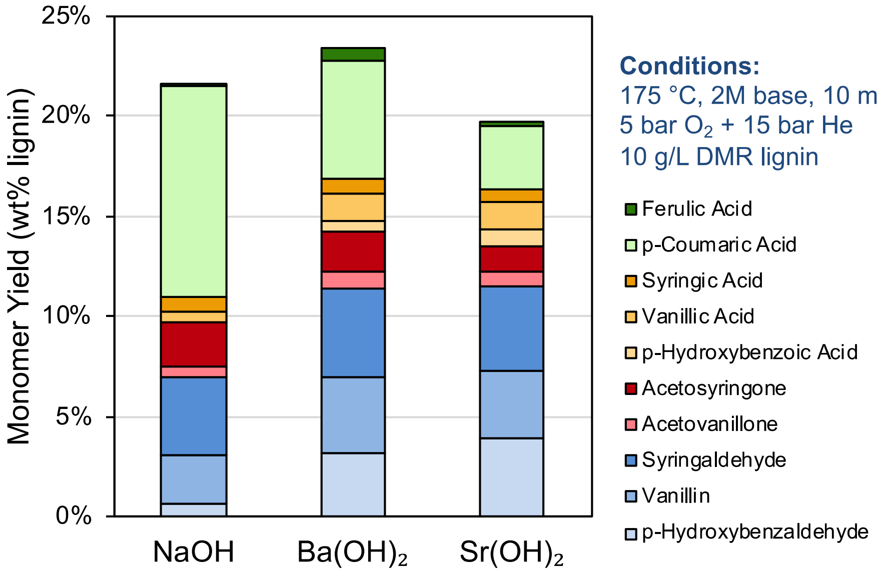
Deuterated compounds



26 27

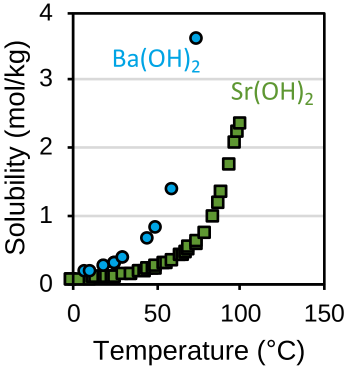
- Synthesized 27 lignin model compounds for analytical, catalysis, and biology efforts
- Preparing standard methods (LAPs) to synthesize lignin model compounds
- **Outcome: enabled multiple biological and catalytic catalytic studies for lignin valorization**

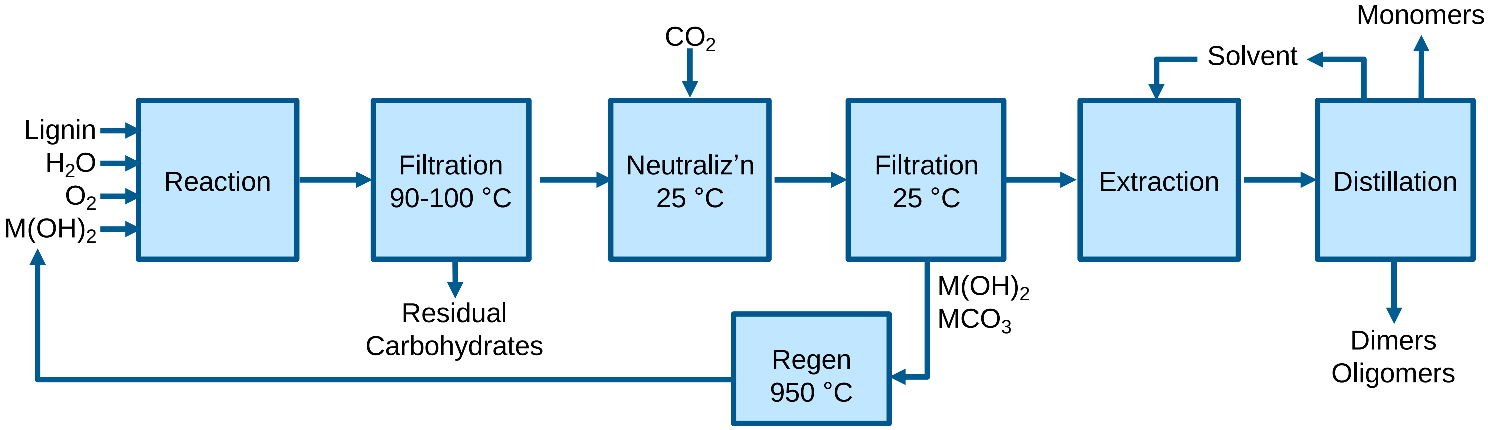
Aim 1: Base-catalyzed depolymerization with recoverable bases



Conditions:
175 °C, 2M base, 10 min
5 bar O_2 + 15 bar He
10 g/L DMR lignin

- Base-catalyzed lignin depolymerization with NaOH has long been studied
- NaOH recovery challenging, exhibits large sustainability footprint
- Hypothesized that reversibly-soluble bases could enable catalyst recovery to replace NaOH
- Can this approach lead to C-C bond cleavage to usable monomers?
- **Outcome: $Ba(OH)_2$ and $Sr(OH)_2$ yield similar monomer yields to base catalysis with NaOH, >99% recoverable**
- TEA/LCA ongoing for this concept



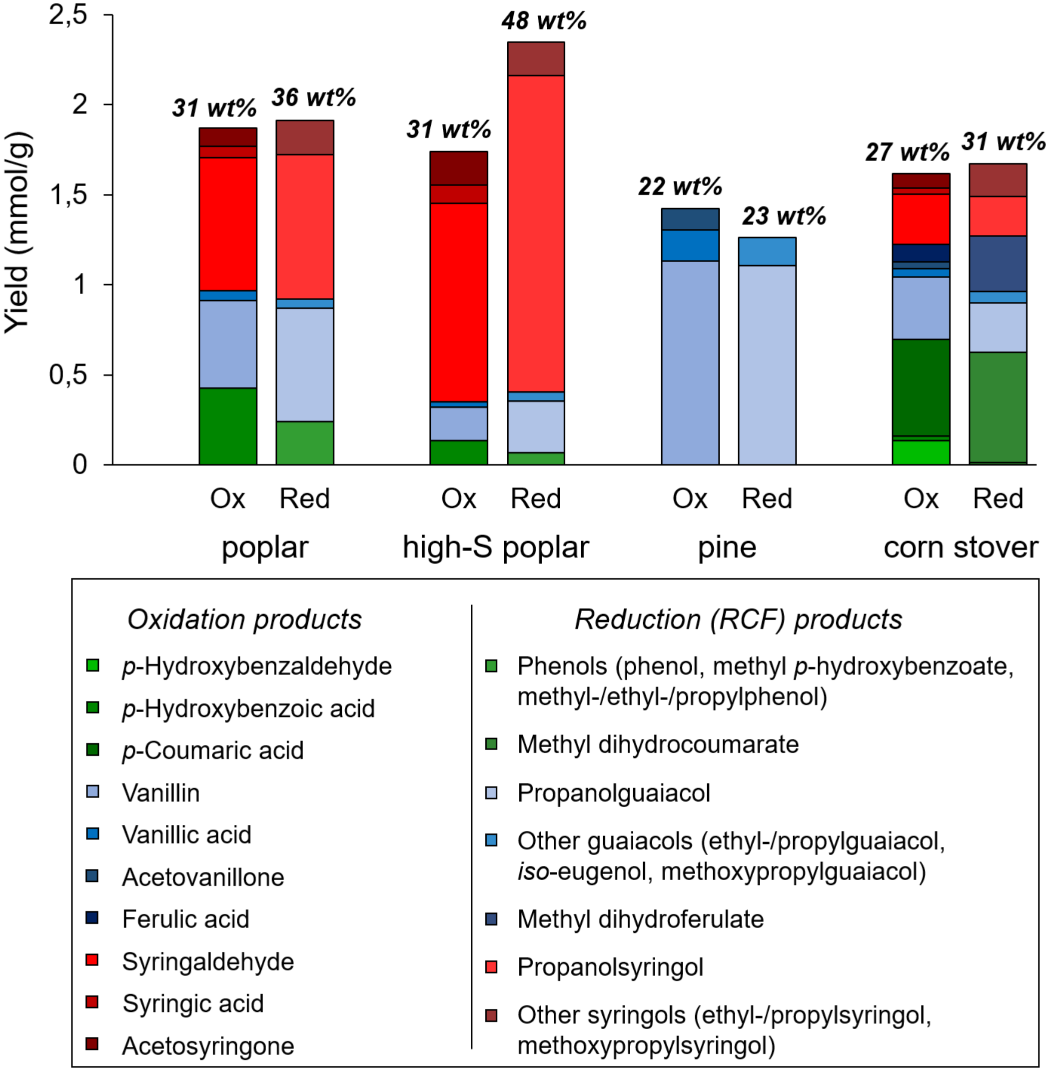


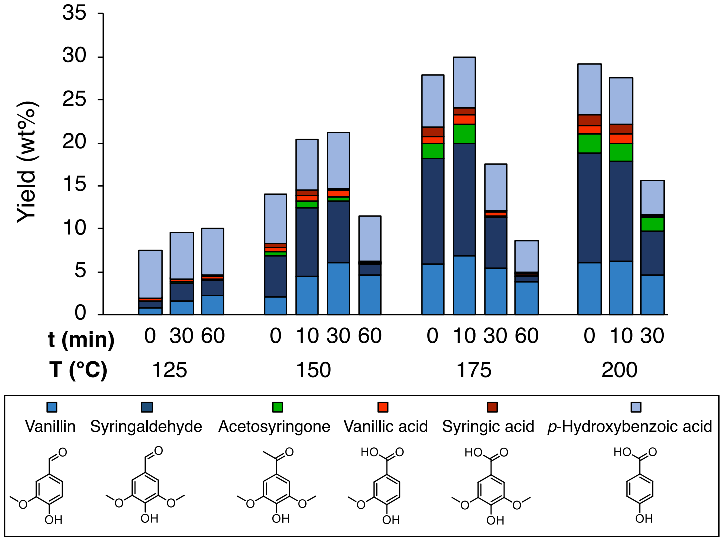
Lambert *et al.* (eds), Alkaline Earth Hydroxides in Water and Aqueous Solutions, *Solubility Data Series*, Vol. 52, **1992**, IUPAC

Kruger *et al.* in preparation

Aim 1: Revisiting alkaline aerobic oxidation

- Alkaline aerobic oxidation long been studied, but little consensus regarding effects of lignin chemistry on yields
- Comprehensive study to evaluate alkaline aerobic oxidation as a function of T, time, $P(O_2)$, [NaOH], catalyst, biomass type
- **Outcome**: Primary monomers from C-O cleavage, cleavage, equivalent monomer yields are similar to reductive processes
- **Alkaline aerobic oxidation likely only cleaves β-O-4 cleaves β-O-4 and ester bonds**



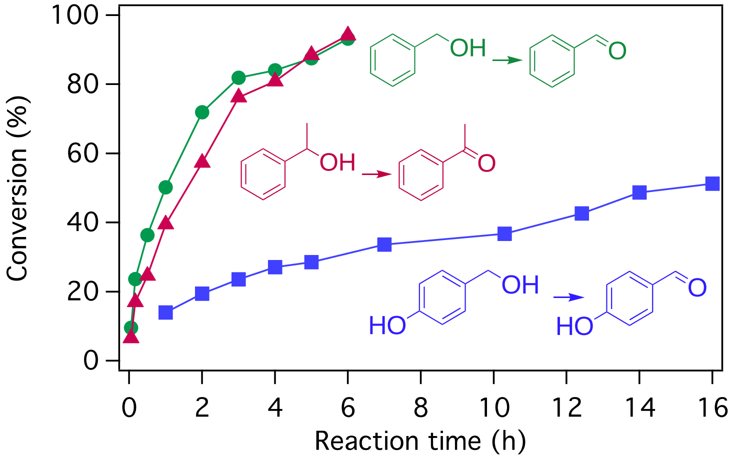


Schutyser *et al. Green Chem.* 2018

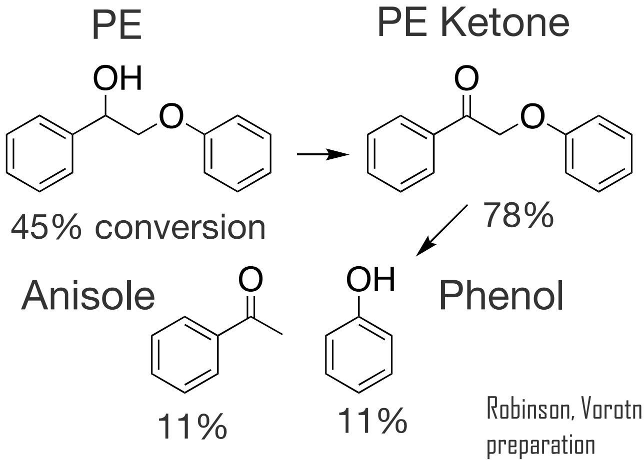
Aim 1: Heterogeneous catalysis for ß-O-4 cleavage

- Oxidation of α-OH promotes ß-O-4 cleavage
- Hypothesized that VO_x on metal oxides could conduct this reaction
- **Outcome**: Heterogeneous VO_x catalysts enable oxidation of α-OH

Alcohol oxidation over VO_x/TiO_2

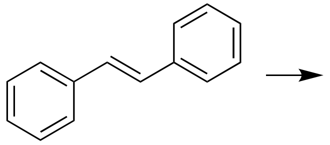


β-O-4 scission over VO_x/TiO_2



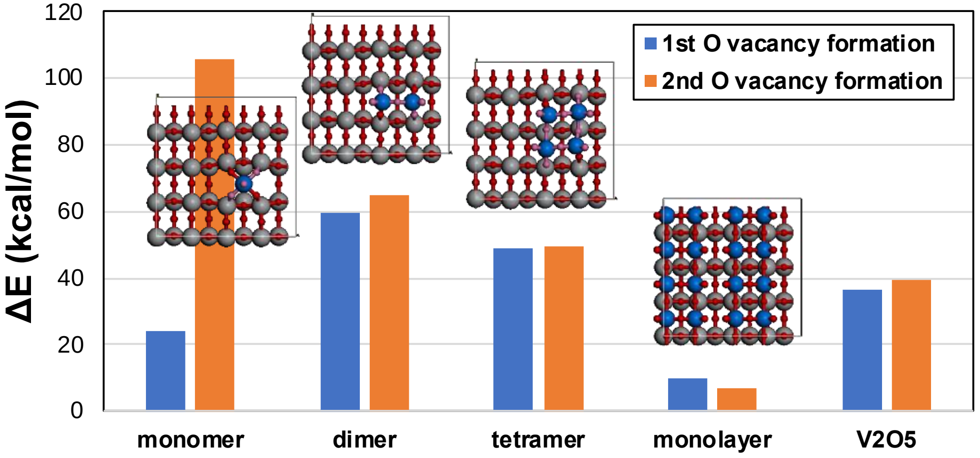
Robinson, Vorotnikov *et al.* in preparation

No C-C scission observed



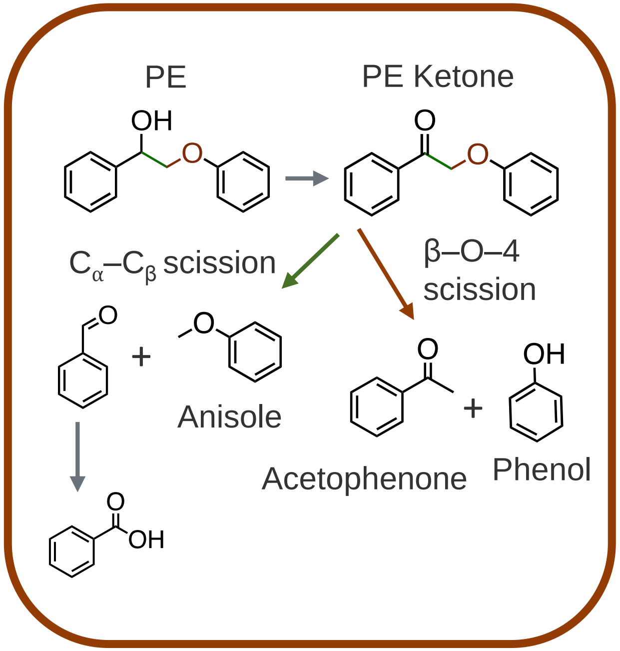
No reaction

O vacancy formation from DFT calculations

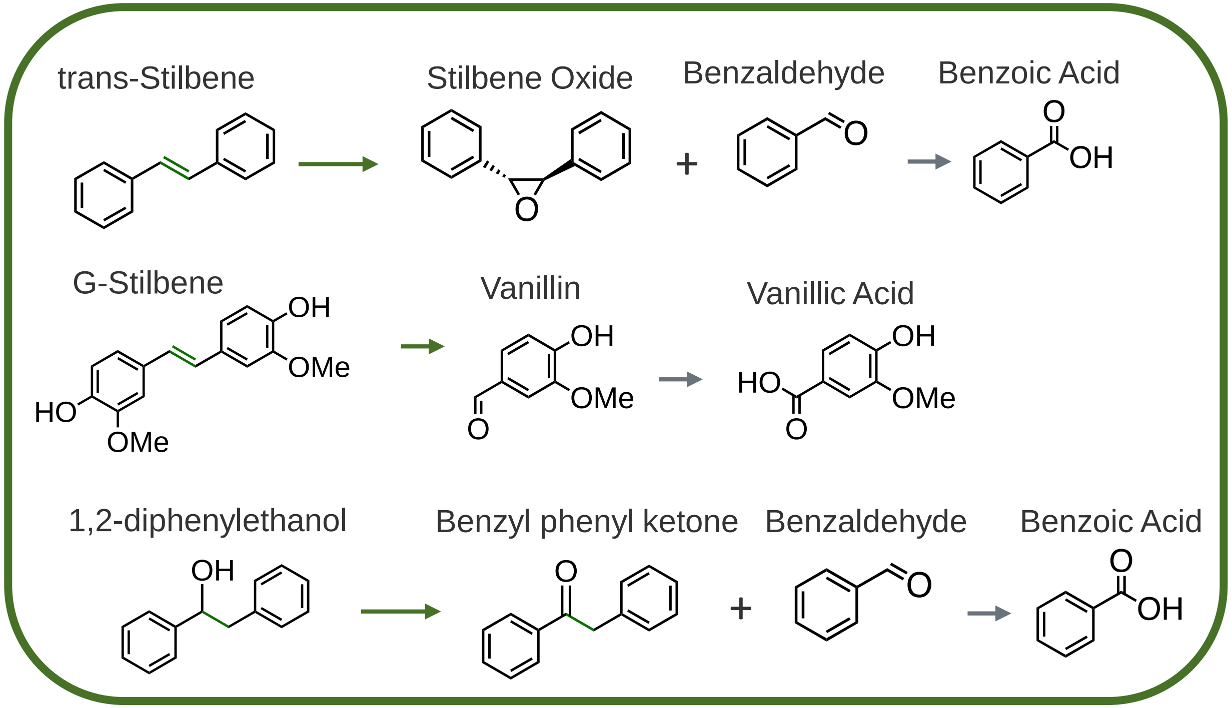


Aim 1: Heterogeneous catalysis for C-C bond cleavage

C-O scission



C-C scission

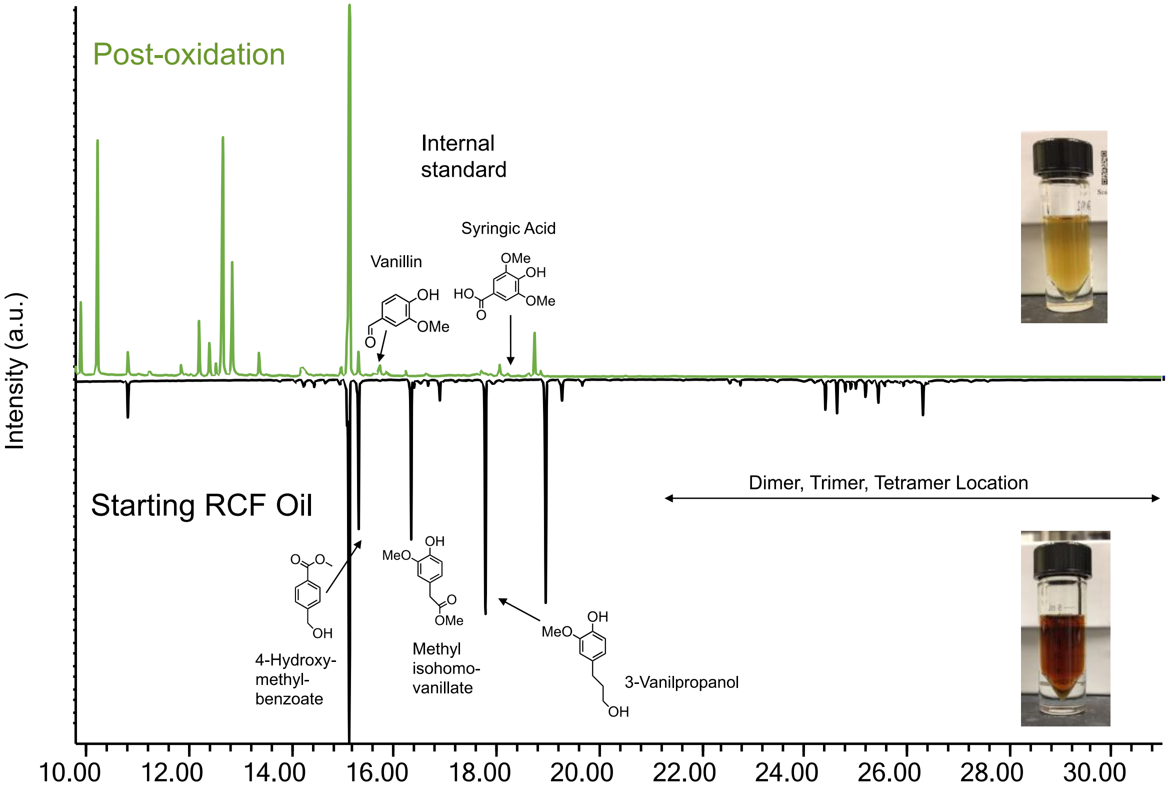


- C-C bond cleavage is still the biggest challenge to increase monomer yields from lignin
- **Outcome:** metal oxide catalyst cleaves C-C and C-O bonds at 150°C in model compounds

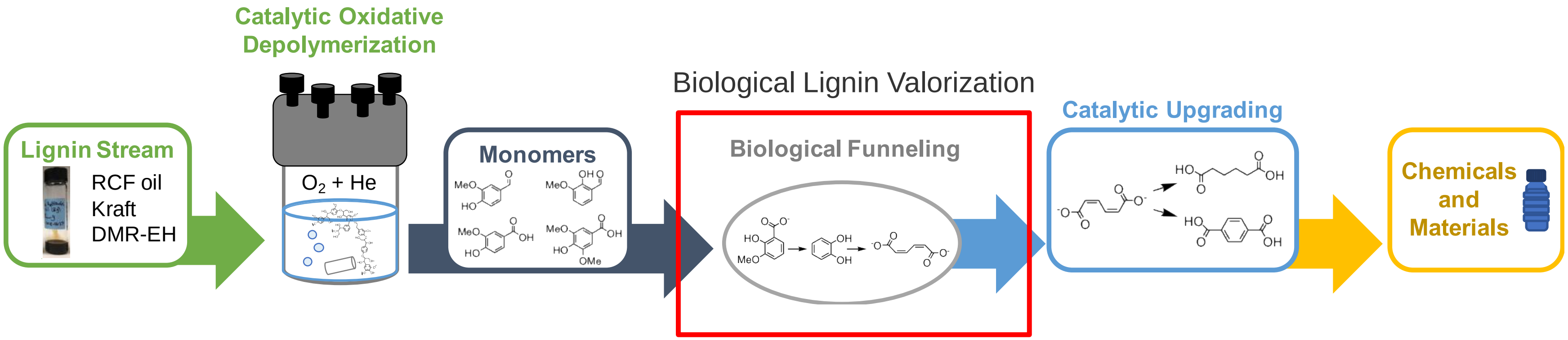
Robinson, Brandner, *et al.* in preparation

Aim 1: Heterogeneous catalysis for C-C bond cleavage

Robinson, Brandner, *et al.* in preparation



- Lignin oil contains C-C dimers+
- Dimers and oligomers gone after oxidation
- **Outcome:** catalytic oxidation increases theoretical monomer yield via C-C bond cleavage
- Ongoing: Reaction mechanism studies, catalyst characterization, bioconversion of products



Lignin Stream

RCF oil
Kraft
DMR-EH

Catalytic Oxidative Depolymerization

O_2 + He

Monomers

Biological Lignin Valorization

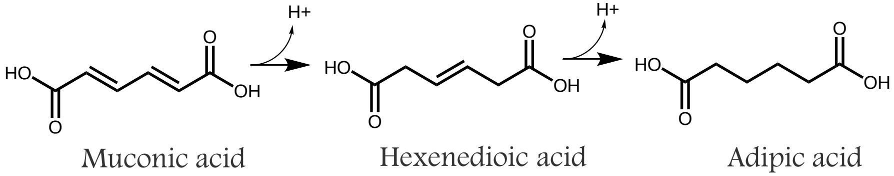
Biological Funneling

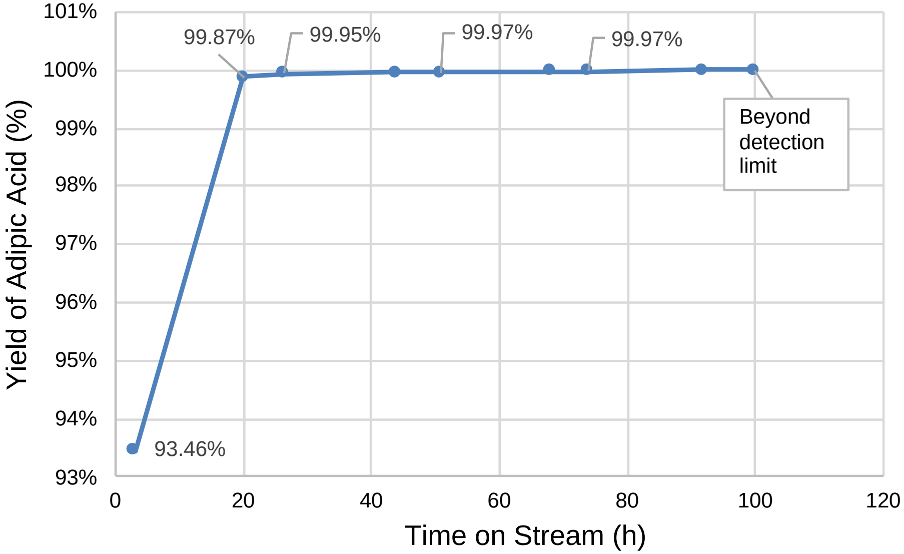
Catalytic Upgrading

Chemicals and Materials

Aim 2: Adipic acid production from muconic acid

- Muconic acid produced from lignin intermediates (**Biological Lignin Valorization**)
- Separable from cultivation broth
- Muconic acid hydrogenation using Pd/C exhibits fouling, switched to TiO_2 support
- Continuous flow: **>99% yield adipic acid at high muconic acid flow rates** (WHSV of 1.2 h^{-1}) at 78°C, 35 bar H_2
- Cat. stability: leaching of 1-2 ppm Pd; addressed via Al_2O_3 coating by ALD in ChemCatBio and TCF projects
- **Outcome**: demonstrated conversion of bio-based muconic to adipic acid





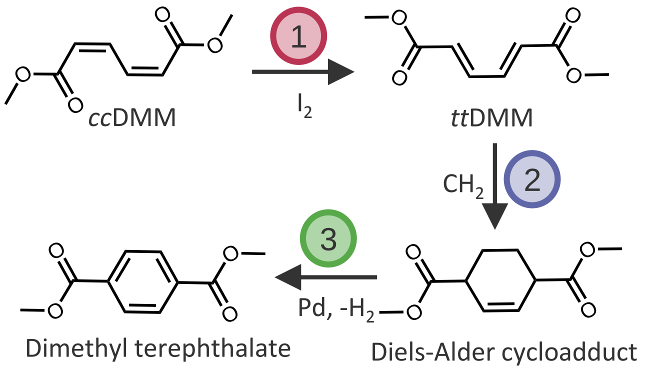
Continuous flow hydrogenation: 78°C, 35 bar H_2, 8 g/L bio-based muconic acid, 0.15 mL/min
Steady state leaching of 1-2 ppm Pd

Vardon, Franden, Johnson, Karp *et al. Energy Env Sci* 2015
Vardon *et al.* Green Chem. 2016
Settle *et al.* in review

Aim 2: Terephthalic acid production from muconic acid

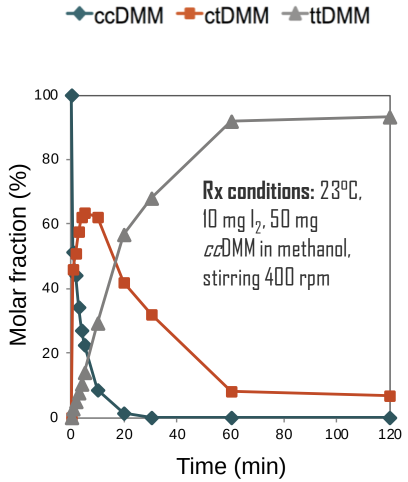
Bio-based *cis,cis*-dimethyl muconate to dimethyl terephthalate:

1. **Isomerization:** Iodine-catalyzed isomerization of *cc*DMM to *tt*DMM to make it Diels-



Isomerization:

>95% yield of *tt*DMM, <30 min

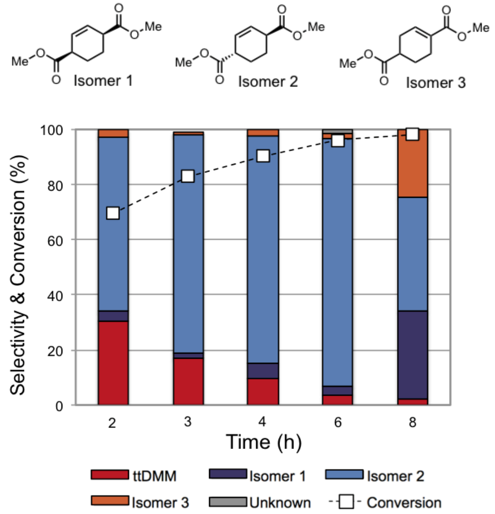


Rx conditions: 23°C, 10 mg I_2, 50 mg *cc*DMM in methanol, stirring 400 rpm

Settle, Vardon, *et al.* *ChemSusChem* 2017

Diels-Alder:

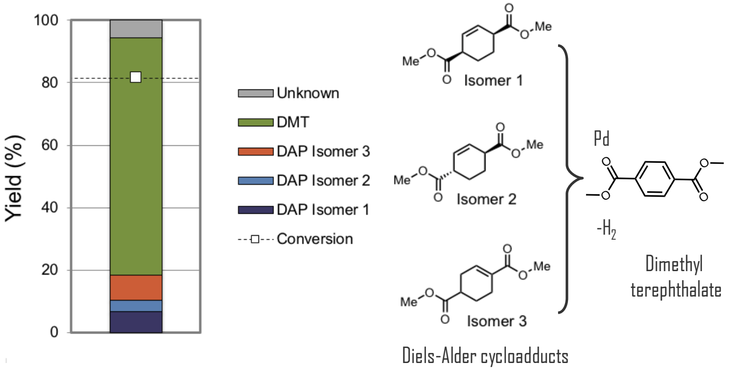
Uncatalyzed; yields 3 isomers: **>97% yield, 8 h**



Settle, Vardon, *et al.* in preparation

Dehydrogenation:

>73% yield of DMT, >70% net process yield from *cc*DMM to DMT



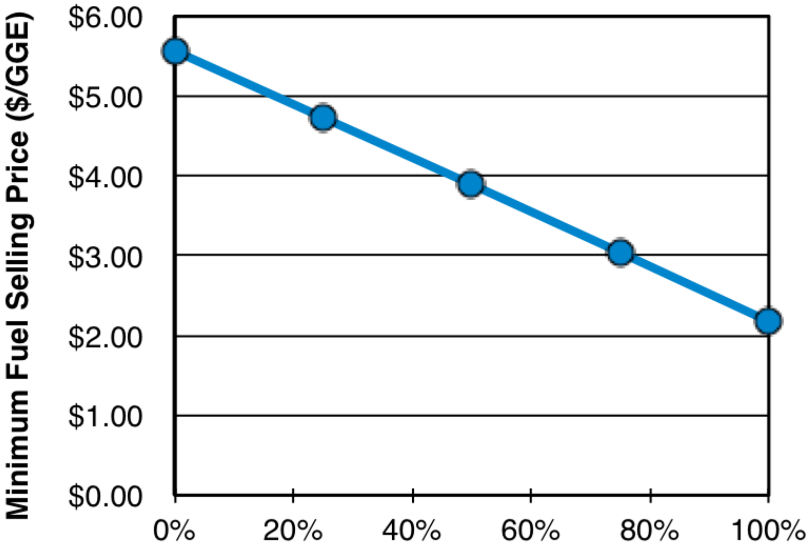
Outcome: Demonstrated TPA production from bio-based muconic acid with catalysis insights along the process

Relevance

Goal: (1) develop catalysts to enable ≥40% monomer yields from lignin, (2) develop processes to upgrade lignin-derived products to commodity chemicals, and (3) conduct comprehensive analyses and syntheses

Why is this project important and what is the relevance to BETO and bioenergy goals?

- Lignin utilization is important to the **cellulosic carbon economy** and to the **BETO cost target goals** for integrated lignocellulosic conversion
- Contribute up to $2-3/gge to MFSP cost targets



Davis *et al.* NREL Design Report 2013

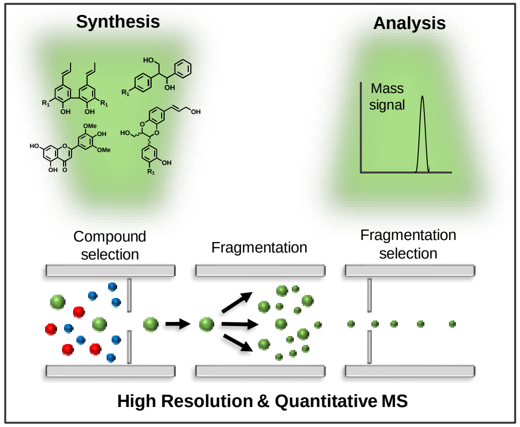
How does this project advance the State of Technology and contribute to biofuels commercialization?

- Catalyst solutions for high-yield lignin monomers *with lignin-agnostic potential*
- Demonstration of commodity-scale products to enable integrated biorefineries
- Enable high atom-to-product efficiency from lignin

Technology transfer activities:

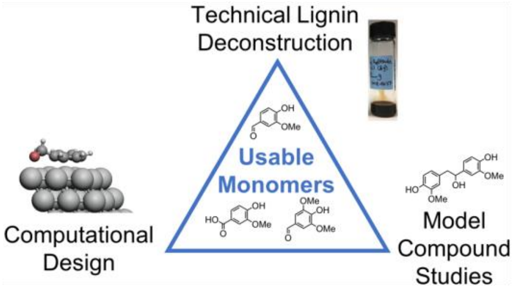
- Patent applications for catalyst formulations and processes
- Peer-reviewed publications
- Laboratory Analytical Procedures for analyses and syntheses

Future work



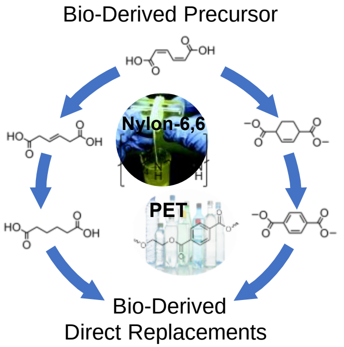
Task 1: Characterization

- Assemble a library of LAPs for lignin model compound syntheses and lignin analyses
- Build libraries of lignin deconstruction products for LC-MS^n efforts
- Work with SepCon to enable separations + analytics of lignin



Task 2: Deconstruction

- Determine mechanism of catalytic C-C bond cleavage catalyst
- **Deploy C-C bond cleavage catalyst to achieve end-of-project goals of >40% monomer yields from lignin in biomass (analytics pending)**
    - **Primary end-of-project goal**
- Optimize catalyst formulation, recyclability, regeneration on real lignin
- Work with SepCon and BLV to enable high product yields from lignin



Task 3: Upgrading

- Develop catalysts for Diels-Alder coupling of ethylene and *tt*-muconate
- Deliver integrated TPA and adipic acid chemistries and processes (**>70% process yield for TPA, >99% process yield for adipic acid**)
- Transition to performance-advantaged products and transformations of additional intermediates from lignin

Summary

Overview

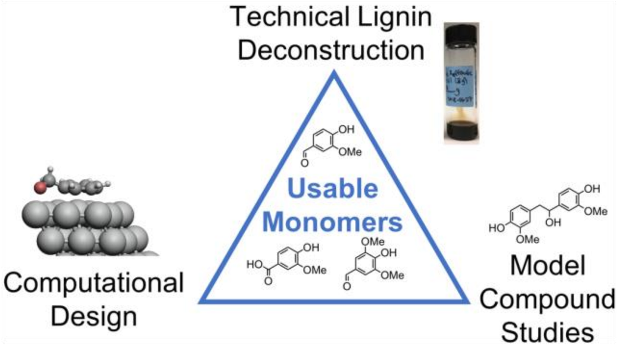
- Comprehensive analytics and chemical synthesis for understanding lignin deconstruction chemistry
- Develop catalysts to enable high theoretical monomer yields from real lignin streams

Approach

- Comprehensive analytics and chemical synthesis for understanding lignin deconstruction chemistry
- Develop catalysts to enable high theoretical monomer yields from real lignin streams
- Develop processes for commodity-scale polymer precursors from lignin
- Collaborate closely with Biological Lignin Valorization project

Technical accomplishments

- New catalyst for selective C-C bond cleavage
- Recoverable bases for replacing NaOH
- Comprehensive analytics and synthesis platforms
- Demonstrated pathways to adipic and terephthalic acids



Relevance

- Contribute $2-3/gge to BETO cost targets for biofuels
- Lignin valorization is essential for a lignocellulose economy

Future work

- **Deploy recoverable bases and oxidation catalysts to enable end-of-project yield targets (40% monomer yields)**

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BETO: **Jay Fitzgerald**

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NREL contributors

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- Amy Settle
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External collaborators

- Adam Guss, Oak Ridge National Laboratory
- Yuriy Roman, MIT

BETO projects:

- Biochemical Platform Analysis
- Separations Consortium
- Performance-Advantaged Bioproducts via Selective Biological and Catalytic Conversion
- Biochemical Process Modeling and Simulation
- Low Temperature Advanced Deconstruction
- Biological Lignin Valorization – NREL and SNL
- Metabolic Engineering for Lignin Conversion – ORNL
- Lignin-First Biorefinery Development
- Advanced Catalyst Synthesis and Characterization

Response to Previous Reviewer Comments

Reviewer Comments

- The project direction looks good. It has the right balance of analysis to understand the chemistry of the depolymerization processes and catalysis and process development. Obviously, it is closely tied to the Targeted Microbial Development project, and those appear to be closely managed. The approach covers a lot of ground in a logical manner and looks to be making good progress. The final determination for the success of the project will perhaps not be whether you can break down lignin chemically, or whether products can be used by a microbial strain (although both of those are great to demonstrate and certainly worthwhile to keep developing), but whether the process is economic in its own right; doesn't interfere with the economics of the sugars process (as is being addressed in this project); and is modeled properly in the TEAs covering both parts of a process scheme. Looking at some of the other TEAs, it can start to look like the lignin process is being used as a way to say "and then we reach $3/gge in 2022 with lignin valorization." It would be good to start making sure the numbers being applied to other TEAs from the lignin-derived co-product have some foundation in a modeled-out, full-on lignin stream/biofuel process.

- Lignin deconstruction and conversion is a critical part of biorefinery development and will be a key contributor to meeting BETO's goals. This project is doing an excellent job of addressing this challenge and has come up with interesting potential solutions to (1) converting lignin into a mixture of more-tractable low-molecular-weight compounds for eventual conversion, and (2) demonstrating high-yield conversion of lignin models (coumarate, ferulate) to muconate, an adipic acid precursor. Although the focus has been on NREL's current alkaline pretreatment, the project plans to make catalytic systems that work with lignin from any pretreatment process...however, this seems like a very large challenge, so it might be wise to test depolymerization and catalytic conversion with lignins from a range of known pretreatments. While all the pieces are not yet in place, the PI has done an excellent job of breaking the project down into manageable parts and addressing each part in turn. As a result, the project has a good chance for success.

- The Lignin Utilization program is essential to reaching the $3/gge objective, as lignin valorization is a key assumption of all the TEA performed. Nonetheless, this work is extremely challenging, and the team has done an amazing amount of work to de-risk both lignin depolymerization and upgrading. The team has also put together two steps that require very different scientific disciplines and, in addition, the need for complex analytical chemistry. The project has been very well-managed so that these groups all work well together, united toward the same overarching goals.

Response to Previous Reviewer Comments

- It is commonly accepted now that lignin valorization will be the key to the success of near-term biorefineries. This is a well-designed approach to a difficult problem. The proof of concept for each of the pieces of a process has been demonstrated (lignin extraction, depolymerization, and bioconversion to muconate). The challenge ahead is to integrate these pieces into a relevant process (could be pulp and paper first) with bioconversion of complex lignin aromatics. A number of new unit operations are being proposed, so keep an eye on the TEA and good luck! This project has the possibility to change the biorefinery equation. • Overall, this is a very good project and a great example of how to connect things from end to end. This should be, in the future broken, down to lignin de-polymerization group (pretreatment, analytic, separation etc.) and upgrading group (i.e., Agile BioFoundry, Targeted Microbial Development, etc.).

Responses:

- We thank the Review Panel for the positive feedback. As noted, we are conducting TEA with detailed models for the lignin valorization process trains. These TEAs are now being incorporated in the BETO MYPP to outline strategies and key process metrics to meet the out-year $3/gge cost goal through lignin utilization. We agree that this will be a key component of lignin valorization process economics.

- We agree that the catalytic challenges here are considerable. Namely, the primary challenge going forward is developing catalytic systems that can cleave both C-O bonds and C-C bonds, the latter of which is especially challenging to do selectively at moderate temperatures. Fortunately, many groups are now working on C-C bond cleavage from a mechanistic standpoint, so we can leverage work from the scientific community in this vein to develop improved oxidation catalysts in a rational manner, which is a key aim going forward in the Lignin Utilization project.

- We thank the reviewers for the positive comments on the integration and multidisciplinary aspects of the project. In terms of the way that this project is managed, we have tasks focused on analytics, lignin depolymerization (including pretreatment), and conversion to value-added compounds (both catalytically and biologically). In addition, the Lignin Utilization project works closely with other projects to leverage expertise and capabilities, including the Targeted Microbial Development project (for strain development), the Separations Consortium and the Separations Development and Application projects, and the various catalyst projects being funded by BETO at present, including the Computational Chemistry and Physics Consortium and the Advanced Catalyst Synthesis and Characterization Project.

Milestone Table

FY17		
Q1	QPM	Finalize development of a GCxGC/TOF-MS method to characterize and quantify lignin-derived species in complex depolymerization streams.
Q2	QPM	Demonstrate a bench-scale process for ammonia pretreatment with alkaline extraction, including mass balances, digestibility of resulting polysaccharides, and lignin characterization from the alkaline extracts.
Q3	Annual	Production of Aromatic Monomers and Aliphatic Carboxylic Acids by Alkaline Catalytic Oxidation of Lignin
Q4	QPM	Convert bio-muconic acid to adipic acid in a flow reactor for a continuous 100 hours of time on stream at >99% conversion and >99% selectivity at mild conditions (< 100°C and < 50 bar H_2). Deliver TEA to identify cost drivers for muconic acid catalytic upgrading. [SMART milestone]

Milestone Table

FY18		
Q1	QPM	Evaluate three model compounds for oxidation of aromatic alcohols (with and without ring functionalization) for production of aldehydes with high selectivity using a heterogeneous catalyst.
Q2	G/NG	Demonstrate >30% upgradeable products from a relevant lignin stream (DMR-EH) via at least one catalytic process (e.g., an alkaline or oxidative process).
Q3	Annual	Demonstrate the production of dimethyl terephthalate from bio-derived muconic acid in yields >70% and final purity >95%. Report target yields and major side products for the sequential reaction steps of catalytic isomerization, Diels-Alder ring formation, and dehydrogenation.
Q4	QPM	Explore quantitative kinetics and molecular weight distributions of batch-mode lignocellulosic biomass solvolysis for representative hardwood, softwood and herbaceous whole feedstocks at single-minute reaction timescales.

Milestone Table

FY19		
Q1	QPM	Identify at least 10 model compounds representative of BETO-relevant lignin streams, including relevant monomers and dimers containing linkages found in important feedstocks (such as whole biomass and DMR-EH lignin). Screen the oxidation of these model compounds in batch reactions in organic solvents using a metal oxide catalyst. Use these results to down-select three model compounds to use in Q3 for both DFT modeling and more in-depth reaction studies.
Q2	QPM	Demonstrate at least 10% yield of monomers from catalytic oxidative upgrading of biomass-derived dimer and/or oligomer mixtures accessed from Lignin First co-product streams. Streams will be produced in the Lignin First Biorefinery Development Project.
Q3	QPM	Determine morphology, oxidation state, and electronic structure of a solid metal oxide and (2) examine its reactivity towards oxidative C-C bond scission of model compounds representative of lignin streams down-selected from FY19 Q1. XPS, TEM, XAS, TPR, and DFT calculations will be used to characterize the material; batch reactors and DFT calculations will be used to assess its catalytic performance and reaction thermochemistry.
Q4	Annual	Demonstrate catalytic processes able to generate >40% yield of usable monomers from lignin in biomass, either biologically convertible or separable. Demonstrate, in collaboration with the Biological Lignin Valorization project, that the monomers can be assimilated by either a native or engineered strain of Pseudomonas putida KT2440 (joint with the Biological Lignin Valorization project).

Publications

1. Josh V. Vermaas, Lauren D. Dellon, Linda J. Broadbelt, Gregg T. Beckham*, Michael F. Crowley*, “Automated transformation of lignin topologies into atomic structures with LigninBuilder”, in press at ***ACS Sust. Chem. Eng.***
2. Josh V. Vermaas, Loukas Petridis, Michael F. Crowley*, Gregg T. Beckham*, “Systematic parameterization of lignin for the CHARMM force field”, ***Green Chem***. (2019) 21, 109-122.
3. Davinia Salvachúa*, Christopher W. Johnson, Christine A. Singer, Holly Rohrer, Darren J. Peterson, Brenna A. Black, Anna Knapp, Gregg T. Beckham*, “Bioprocess development for muconic acid production from aromatic compounds and lignin”, ***Green Chem***. (2018) 20, 5007-5019.
4. Michael L. Stone, Eric M. Anderson, Kelly M. Meek, Michelle Reed, Rui Katahira, Fang Chen, Richard A. Dixon, Gregg T. Beckham*, Yuriy Román-Leshkov*, “Reductive catalytic fractionation of C-lignin”, in press at ***ACS Sus. Chem. Eng.***
5. Andrea Corona, Mary J. Biddy, Derek R. Vardon, Morten Birkved, Michael Hauschild, and Gregg T. Beckham*, “Life cycle assessment of adipic acid production from lignin”, ***Green Chem***. (2018) 20, 3857-3866.
6. Wouter Schutyser, Jacob S. Kruger, Allison M. Robinson, Rui Katahira, David G. Brandner, Nicholas S. Cleveland, Ashutosh Mittal, Darren J. Peterson, Richard Meilan, Yuriy Román-Leshkov*, and Gregg T. Beckham*, “Revisiting alkaline aerobic lignin oxidation”, ***Green Chem**.* (2018) 20, 3828-3844.
7. Amy E. Settle, Laura Berstis, Shuting Zhang, Nicholas A. Rorrer, Haiming Hu, Ryan M. Richards, Gregg T. Beckham, Michael F. Crowley*, Derek R. Vardon*, “Iodine-catalyzed isomerization of dimethyl muconate”, ***ChemSusChem*** (2018) 11, 1768-1780.
8. Wouter Schutyser, Tom Renders, Sander Vanden Bosch, Stef Koelewijn, Gregg T. Beckham, Bert Sels*, “Chemicals from lignin: an interplay of lignocellulose fractionation, depolymerisation, and upgrading”, ***Chem. Soc. Rev**.* (2018) 47, 10-20.
9. Eric M. Anderson, Michael L. Stone, Rui Katahira, Michelle Reed, Gregg T. Beckham*, Yuriy Román-Leshkov*, “Flowthrough reductive catalytic fractionation of biomass”, ***Joule***. (2017) 1, pp. 613-622.
10. Alberto Rodriguez‡, Davinia Salvachúa‡, Rui Katahira‡, Brenna A. Black, Nicholas S. Cleveland, Michelle Reed, Holly Smith, Edward E.K. Baidoo, Jay D. Keasling, Blake A. Simmons, Gregg T. Beckham*, John M. Gladden*, “Low-temperature base-catalyzed depolymerization of solid biorefinery enriched-lignin streams enables effective microbial conversion”, ***ACS Sust. Chem. Eng***. (2017) 5, 8171-8180.
11. Ashutosh Mittal*, Rui Katahira, Bryon S. Donohoe, Sivakumar Pattathil, Jack M. Stringer, Gregg T. Beckham*, “Alkaline peroxide delignification of corn stover”, ***ACS Sust. Chem. Eng***. (2017) 5, 6310-6321.
12. Amy E. Settle, Laura Berstis, Nicholas A. Rorrer, Yuriy Roman-Leshkov, Gregg T. Beckham, Ryan M. Richards, Derek R. Vardon*, “Heterogeneous Diels-Alder catalysis for biomass-derived aromatic compounds”, ***Green Chem**.* (2017) 19, 3468-3492.
13. Ashutosh Mittal*, Rui Katahira, Bryon S. Donohoe, Sivakumar Pattathil, S. Kandemkavil, Mary J. Biddy, Gregg T. Beckham*, “Ammonia pretreatment of corn stover enables facile lignin extraction”, ***ACS Sust. Chem. Eng***. (2017) 5, 2544-2561.

Presentations

1. Oxidation of Lignin-Rich Residue from DMR-EH Refining of Lignocellulose, AIChE Annual Meeting, Oct 31st, 2018
2. Catalytic valorization of lignin in the biorefinery, 4th Ibero-American Congress on Biorefineries, **Plenary** Invited Lecture, October 24, 2018
3. Oxidation of Lignin-Rich Residue from DMR-EH Refining of Lignocellulose, ACS Fall Meeting, Aug 13th, 2018
4. Lignin depolymerization and fractionation in flow-through systems, 14th International Conference on Renewable Resources and Biorefineries, May 31st, 2018
5. Developing new processes to valorize lignin and sugars to building-block chemicals and materials, RWTH Aachen University, May 28th, 2018
6. Recent adventures in the deconstruction of cellulose and lignin, LBNet3 Meeting (UK), May 16th, 2018
7. Lignin conversion by biological funneling and chemical catalysis, COST FP1306 Workshop, **Plenary** Invited Lecture, March 12th, 2018
8. Hybrid biological and catalytic processes to produce chemicals and materials from biomass, University of Delaware, October 5, 2017
9. Lignin valorization to chemicals, Bioeconomy 2017, July 12, 2017
10. Hybrid biological and catalytic processes to produce chemicals and materials from biomass, USDA-ARS Western Regional Research Center, June 14, 2017
11. Hybrid biological and catalytic processes to produce chemicals and materials from biomass, University of Minnesota, March 27, 2017
12. Hybrid biological and catalytic processes to produce chemicals and materials from biomass, École polytechnique fédérale de Lausanne, March 24, 2017
13. Hybrid biological and catalytic processes to produce chemicals and materials from biomass, Michigan State University, February 2, 2017
14. Lignin valorization via biological funneling, January 23, 2017, NMBU Norway