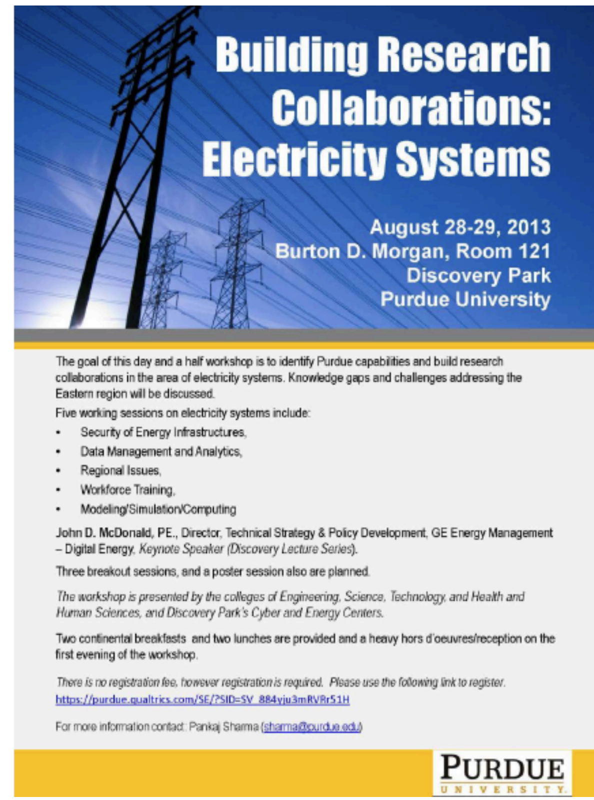
Purdue Energy Center: *We engage researchers and students in a community that delivers new discoveries and develops disruptive technologies with national and global impact.*

- Over 150 faculty engaged in interdisciplinary energy science and engineering
- Research strengths in transportation (biofuels, aviation engine testing, electric vehicles, ground vehicle power, transportation systems)
- Power generation and transmission (solar, wind, nuclear, smart grid, energy efficiency, state utility forecasting)

PURDUE UNIVERSITY
Discovery Park Energy Center

Maureen McCann, Director
Pankaj Sharma, Managing Director

Facilitate emerging research communities at Purdue



Discovery Park

PURDUE UNIVERSITY

The Burton D. Morgan Center for Entrepreneurship

Initiated in 2001, opened 2004; Lilly Endowment grant of $2.3M funded new programs; building funded by the Burton D. Morgan Foundation with $7M.

Business Plan Competition for undergraduate and graduate students (since 1987)

Life Sciences Business Plan Competition (since 2006)

Student Managed Venture Fund (since 2011)

Certificate in Entrepreneurship & Innovation (since 2005)

Only **one of six biology PhDs** in the United States lands a **tenure-track faculty position** within five years of graduation.

1 of 6

PhDs BECOME FACULTY

Energy Biosciences Research Community (EBRC)

Feedstock Improvement	Sustainable Cropping Systems	Harvesting Logistics and Pre-processing	Biofuels Engineering	Economics and Policy

80 Purdue faculty from 4 colleges and 23 departments

Collaborating Laboratories

Air Transport Institute for Environmental Sustainability
Biofeedstock and Water Quality Project
Center for direct catalytic conversion of biomass to biofuels
EFRI-HyBi: Maximizing Conversion of Biomass Carbon to Liquid Fuel
Laboratory for Renewable Resource Engineering
National Test Facility for Fuels and Propulsion
Purdue Center for Research on Energy Systems and Policy
Purdue Extension Bioenergy Series

U.S. DEPARTMENT OF ENERGY | Office of Science
AFOSR
GCEP
USDA United States Department of Agriculture
National Institute of Food and Agriculture
NSF

Basic and Applied Research Integration

How Nature Works ··· Design and Control ··· Technologies for the 21st Century

Grand Challenges *How nature works*	Discovery and Use-Inspired Basic Research *Materials properties and chemical functionalities by design*		Applied Research	Technology Maturation & Deployment
▪ Controlling materials processes at the level of quantum behavior of electrons ▪ Atom- and energy-efficient syntheses of new forms of matter with tailored properties ▪ Emergent properties from complex correlations of atomic and electronic constituents ▪ Man-made nanoscale objects with capabilities rivaling those of living things ▪ Controlling matter very far away from equilibrium	▪ Basic research for fundamental new understanding on materials or systems that may revolutionize or transform today's energy technologies ▪ Development of new tools, techniques, and facilities, including those for the scattering sciences and for advanced modeling and computation	▪ Basic research, often with the goal of addressing showstoppers on real-world applications in the energy technologies	▪ Research with the goal of meeting *technical milestones*, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes ▪ Proof of technology concepts	▪ Scale-up research ▪ At-scale demonstration ▪ Cost reduction ▪ Prototyping ▪ Manufacturing R&D ▪ Deployment support

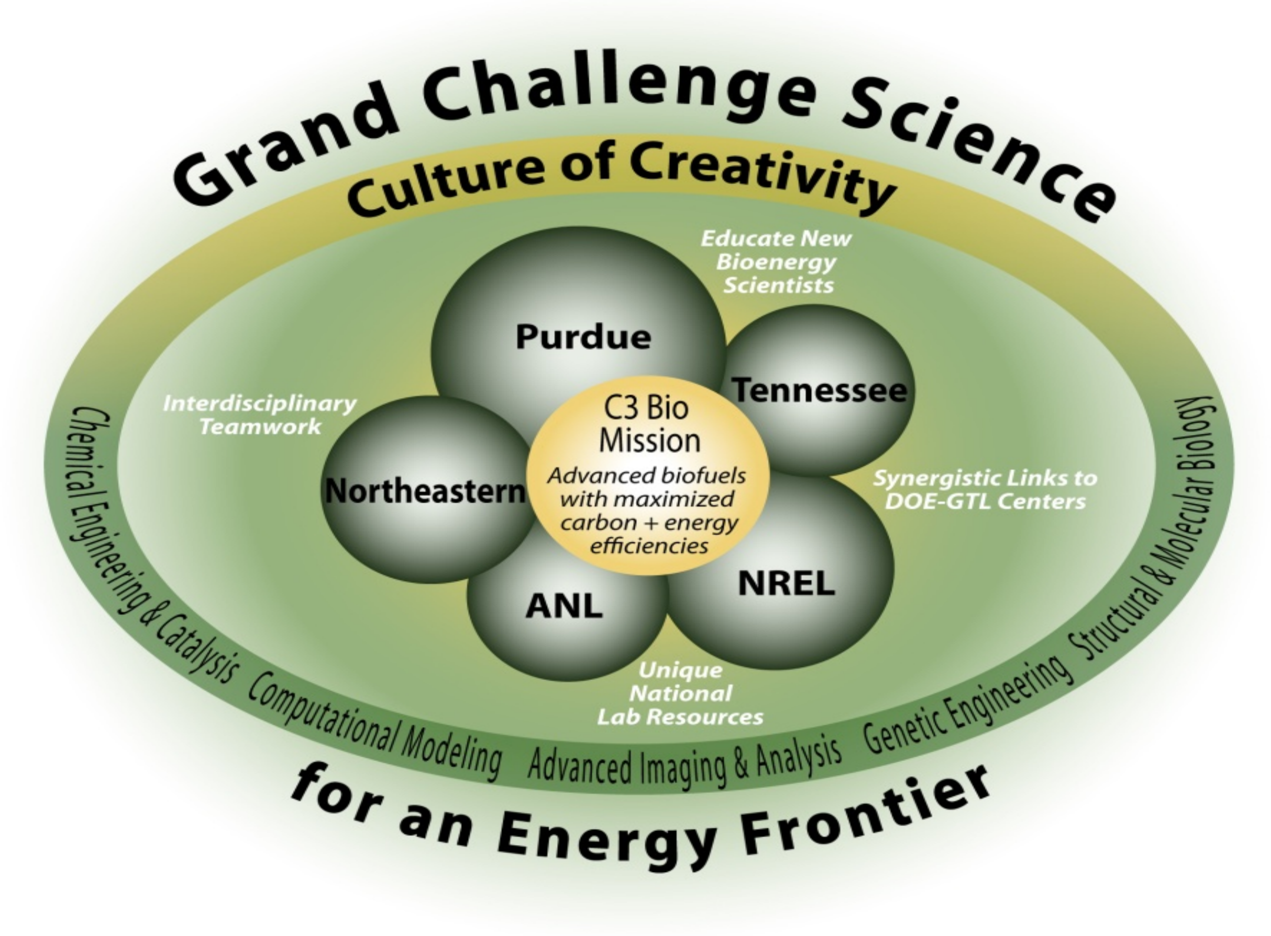
BESAC & BES Basic Research Needs Workshops

BESAC Grand Challenges Panel

DOE Technology Office/Industry Roadmaps

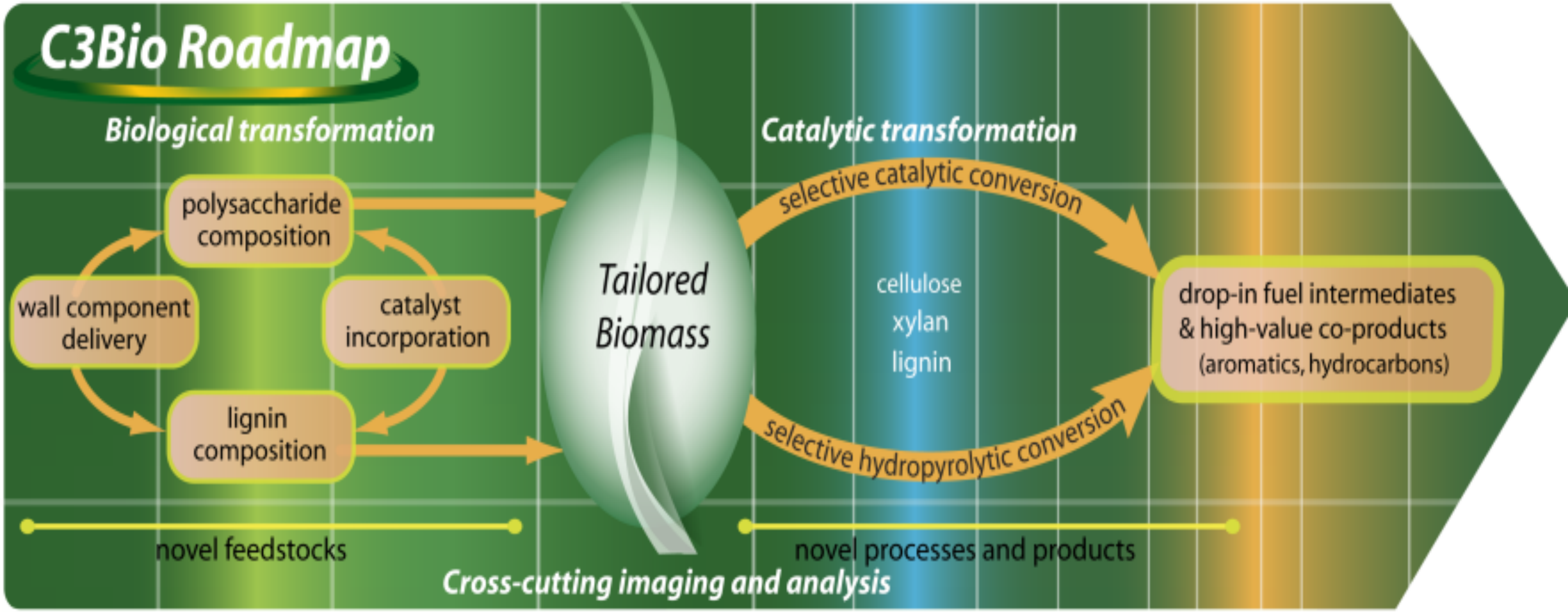
EFRC

No carbon left behind: A new paradigm in the conversion of biomass to biofuels and high-value products



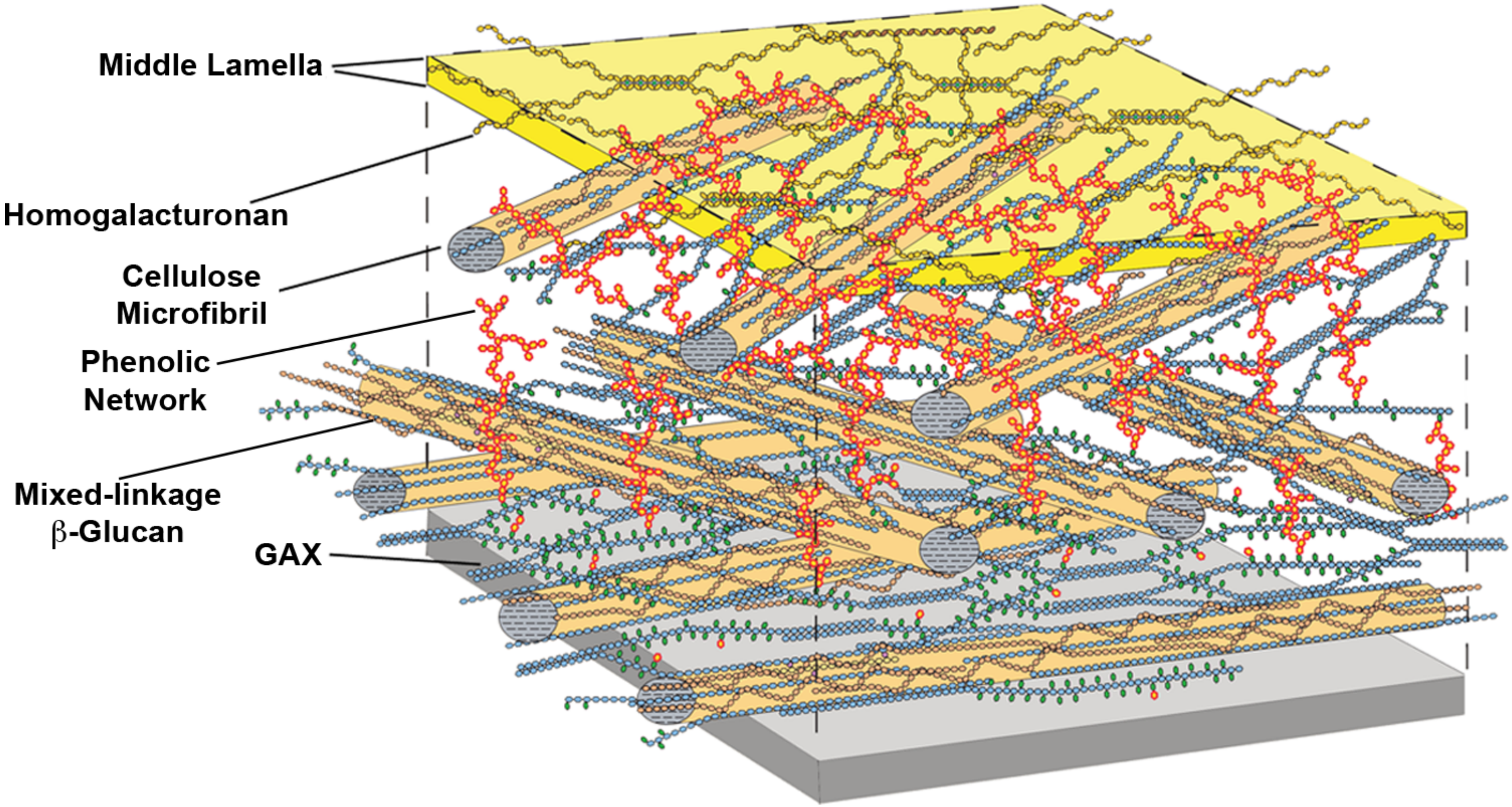
A strategy to genetically tailor biomass for producing advanced biofuels and bioproducts

Roadmap for selective deconstruction of lignocellulosic biomass to useful products



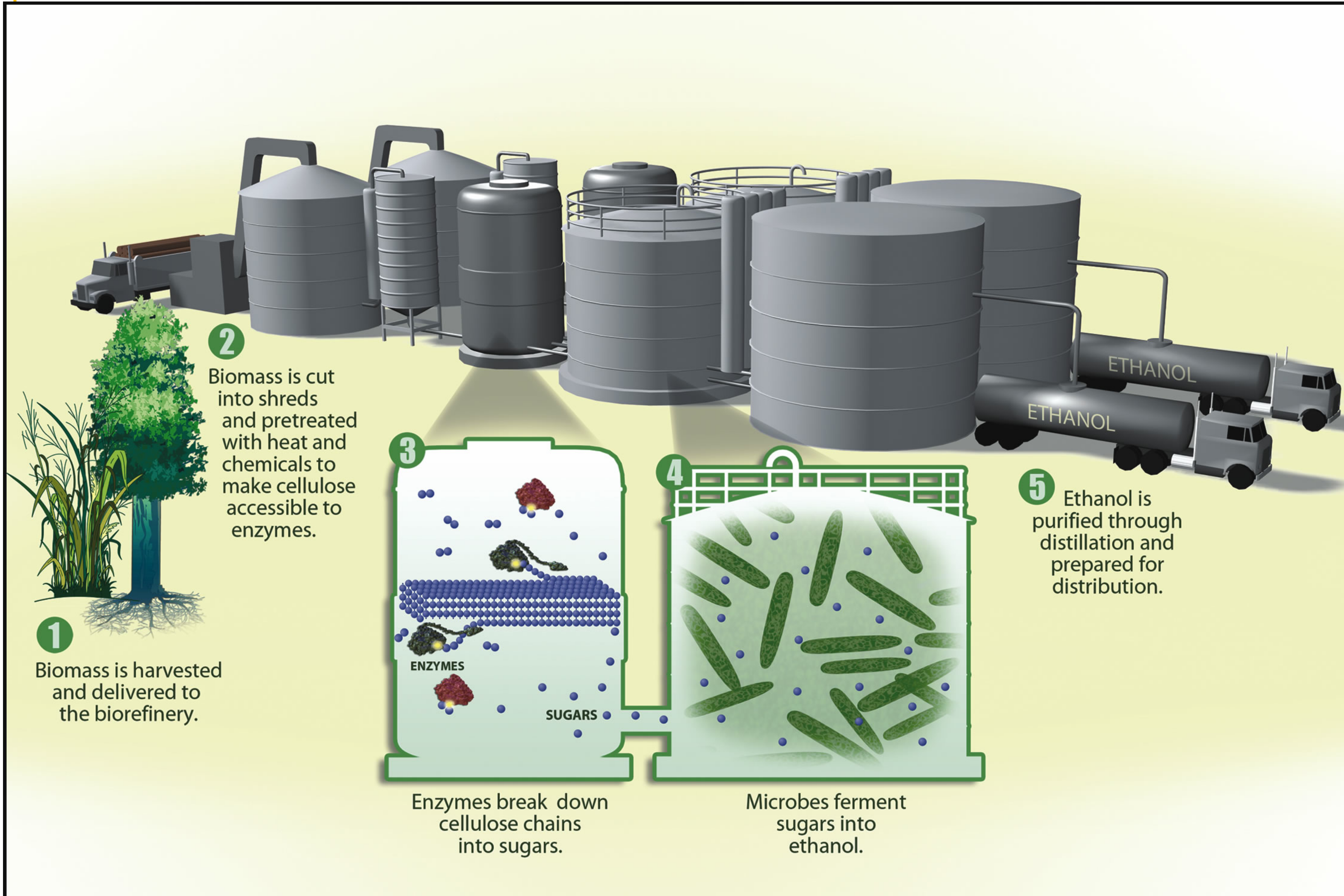
Tailored biomass is the result of recognition of new traits arising from understanding catalytic conversion of 'biomass' to useful products and then determining the genetic basis of them

A challenging set of substrates



Carpita and McCann (2008)

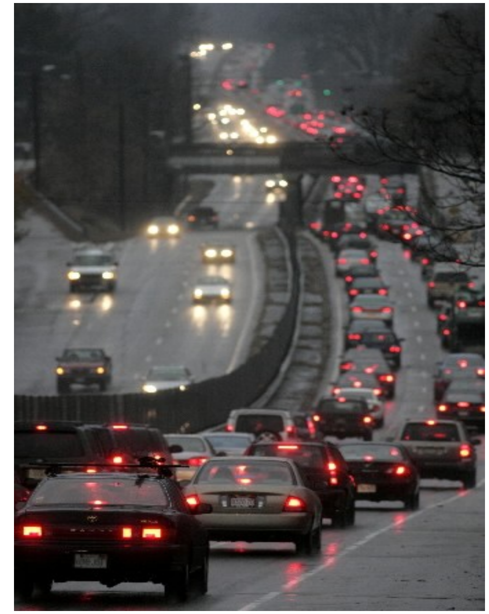
Biological conversion route for biomass to biofuel



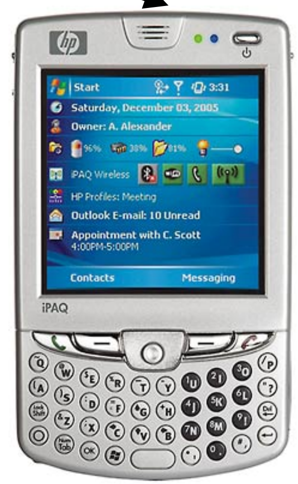
DOE-GTL *Research Roadmap to Breaking the Biological Barriers to Cellulosic Ethanol* 2005

The petrochemical industry: a 20th century success story built on chemical catalysis

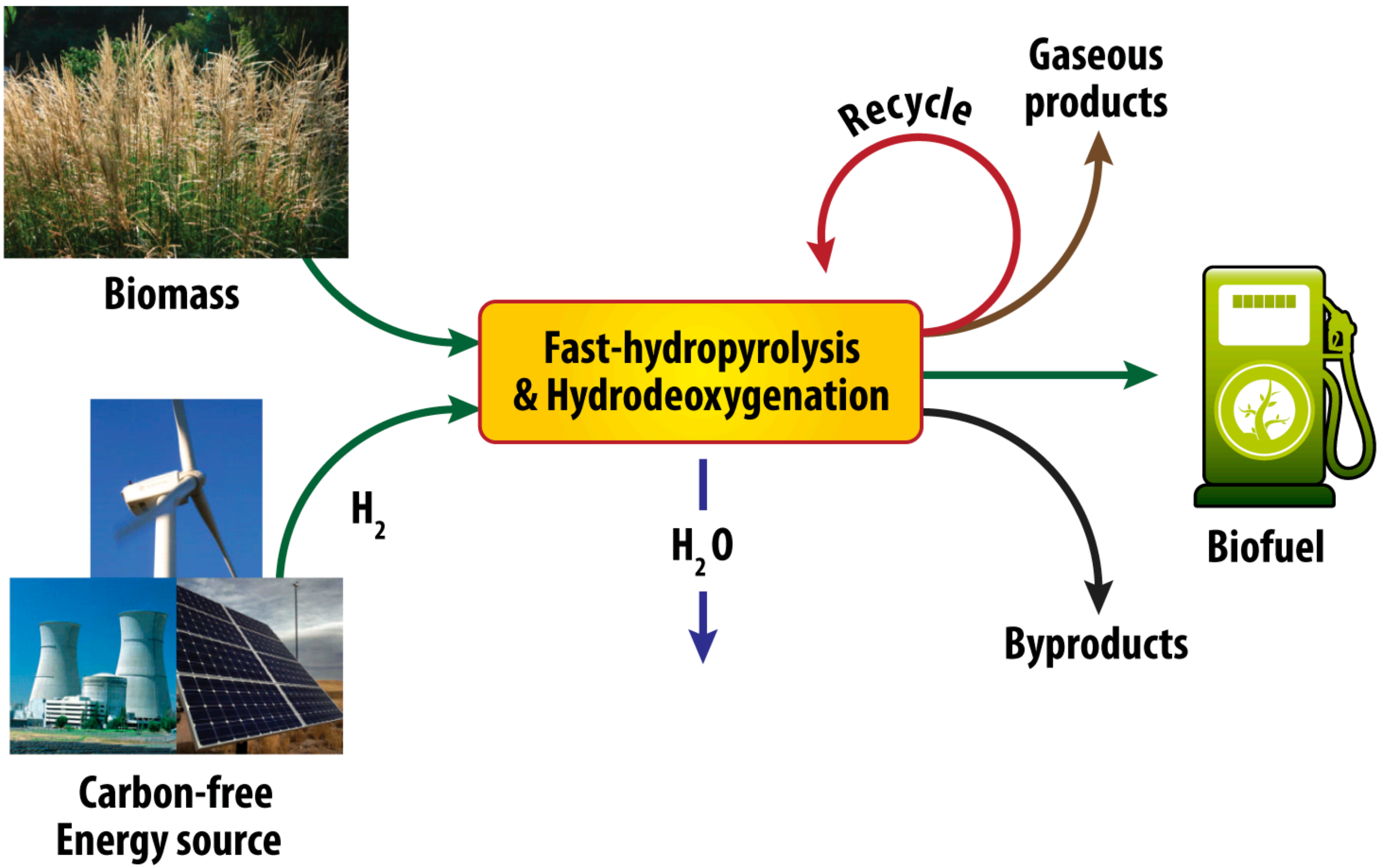
drop-in biofuel



Interesting Materials

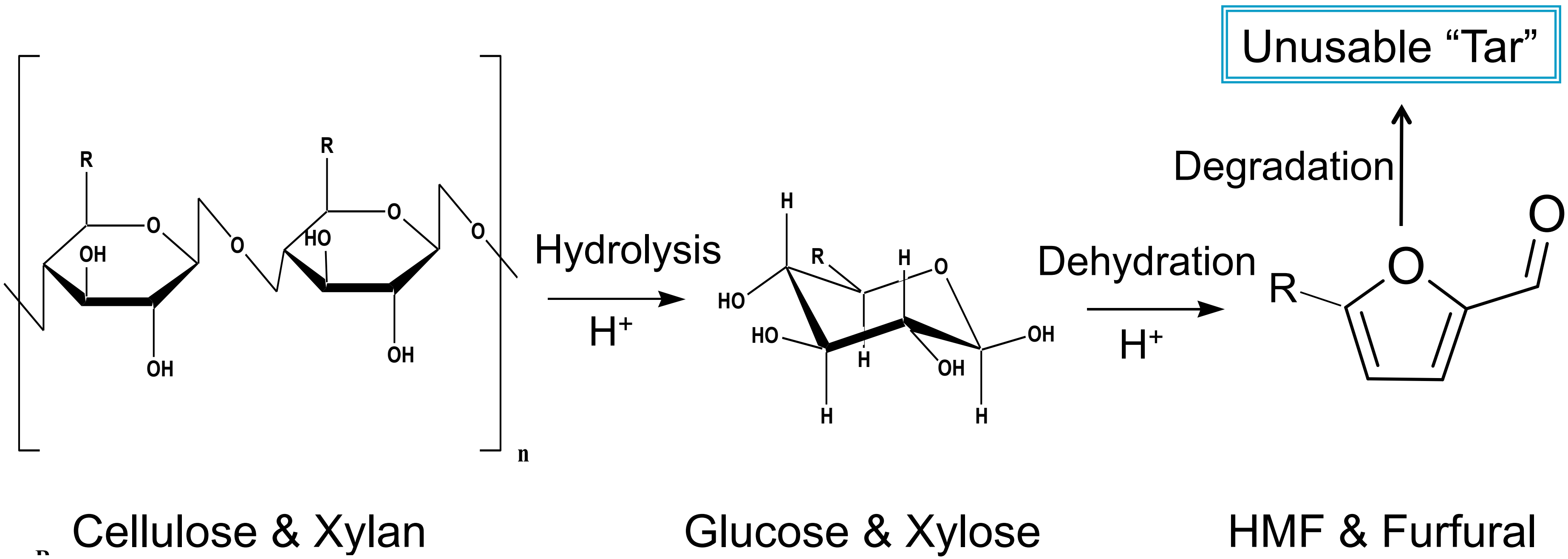


A paradigm for carbon-free reduction to biofuels and bioproducts



High-temperature treatments may produce a bio-crude oil for biorefinery fractionation

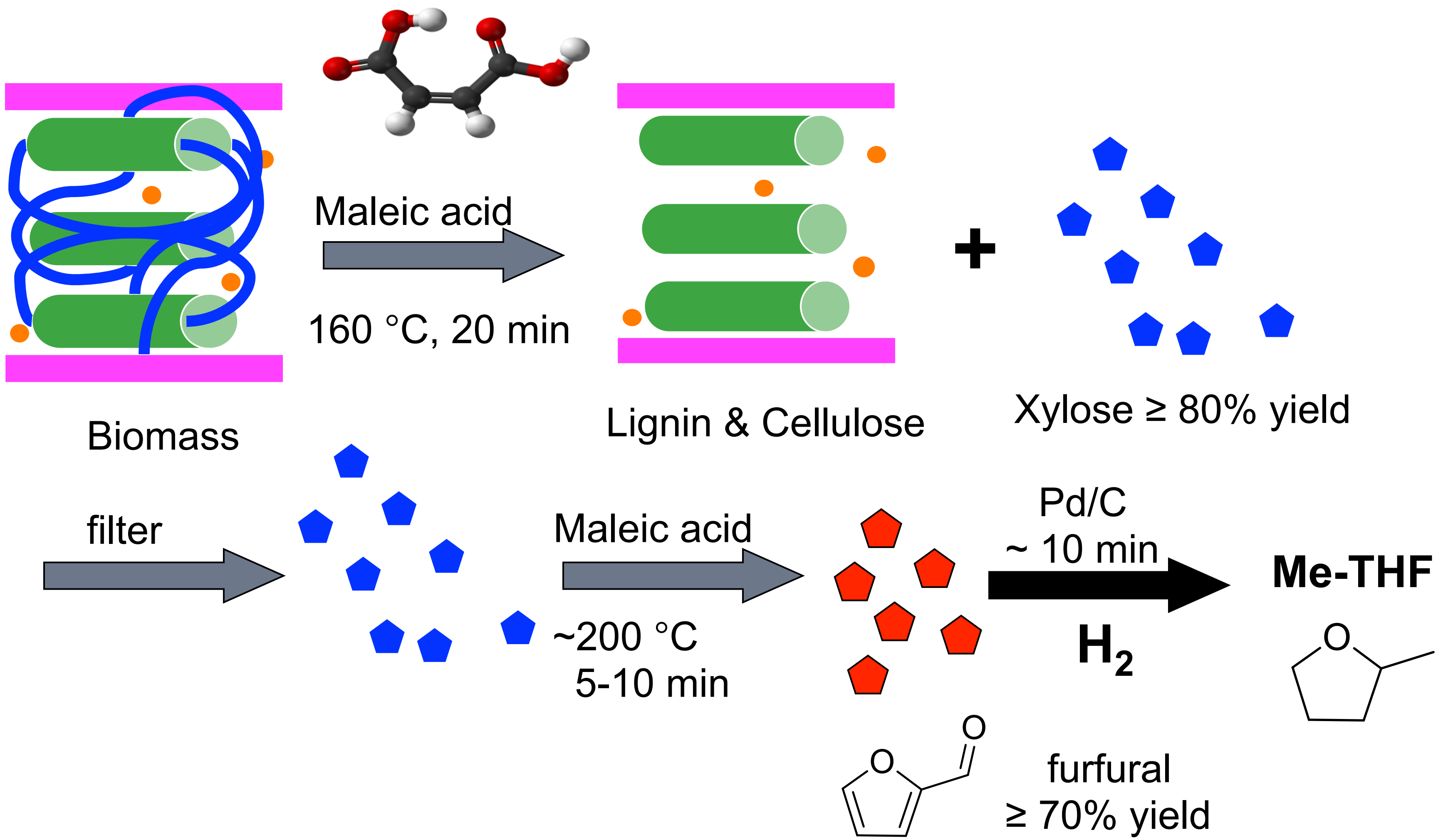
The acid problem: need selectivity toward reaction products that are not degraded but dehydrated



building blocks for fuels, plastics and household chemicals

Abu-Omar, Kim, Liu, Mosier (Purdue)

Catalysis using maleic acid enables selective fractionation of biomass to access carbohydrates for conversion to furfurals



Kim ES, Liu S, Abu-Omar MM, Mosier NS (2012)

Fast Pyrolysis

- A relatively simple and scalable process
- However, the low quality and instability of the resulting bio-oil limit its utility
- Upgrading is hindered by bio-oil’s enormous complexity
- This arises from a multitude of unknown primary, secondary and later reactions

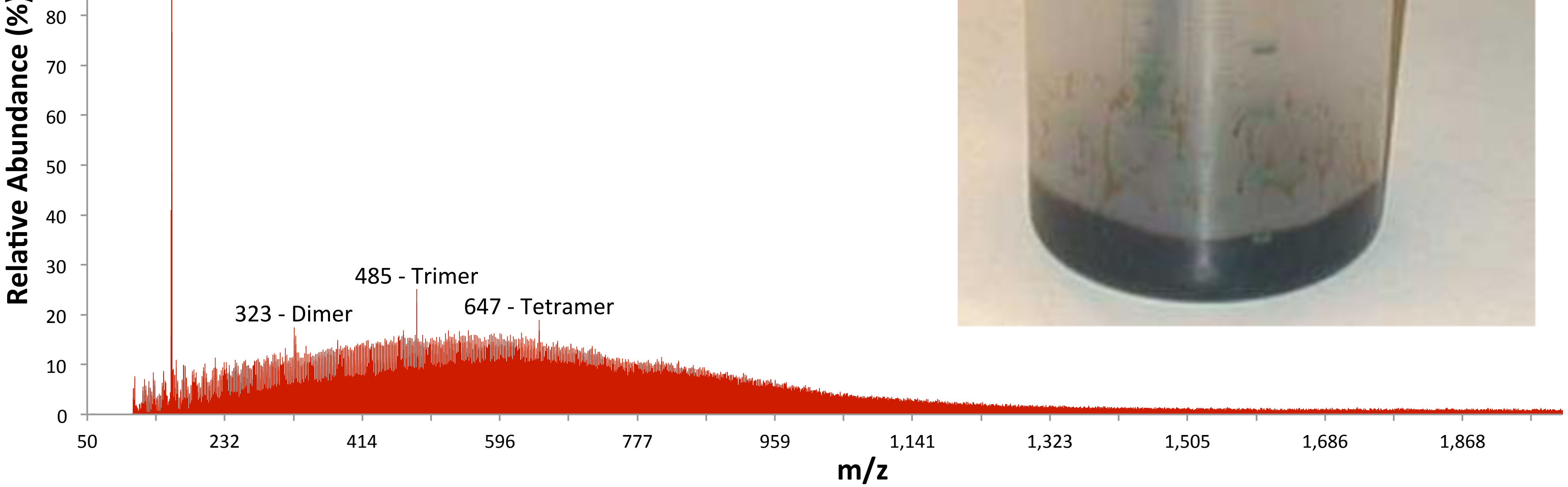
C3Bio

- Obtain fundamental knowledge that allows control over the products

Radlein et al. (1987)

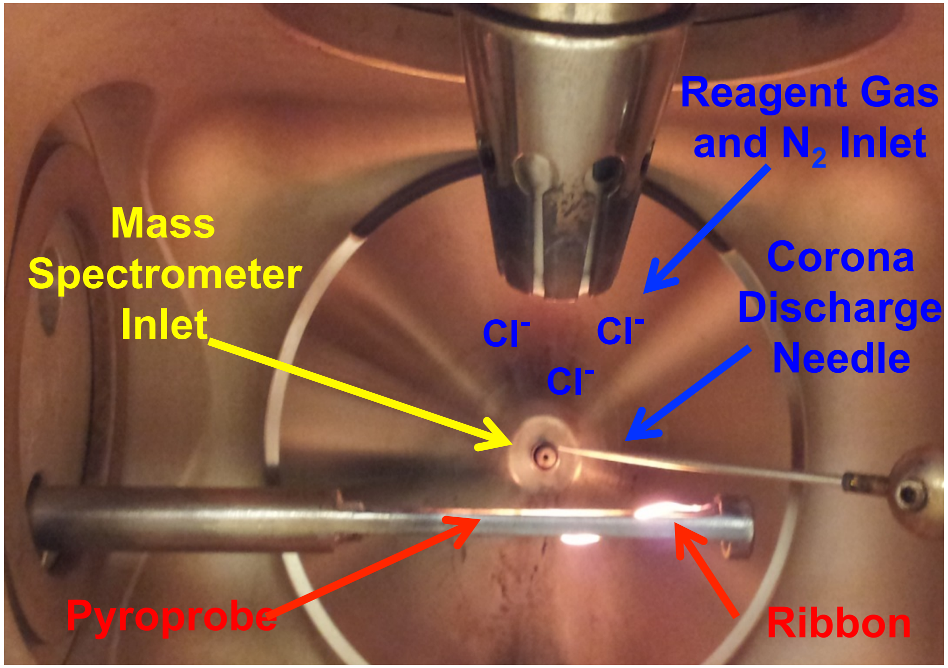
Traditional bio-oil comprises thousands of compounds

Cellulose pyrolyzed in an ablative reactor with ~30s residence time; bio-oil collected



Ribeiro, Delgass, Agrawal, Kentämaa (Purdue)

Pyroprobe/High Resolution Ion Trap Tandem Mass Spectrometer

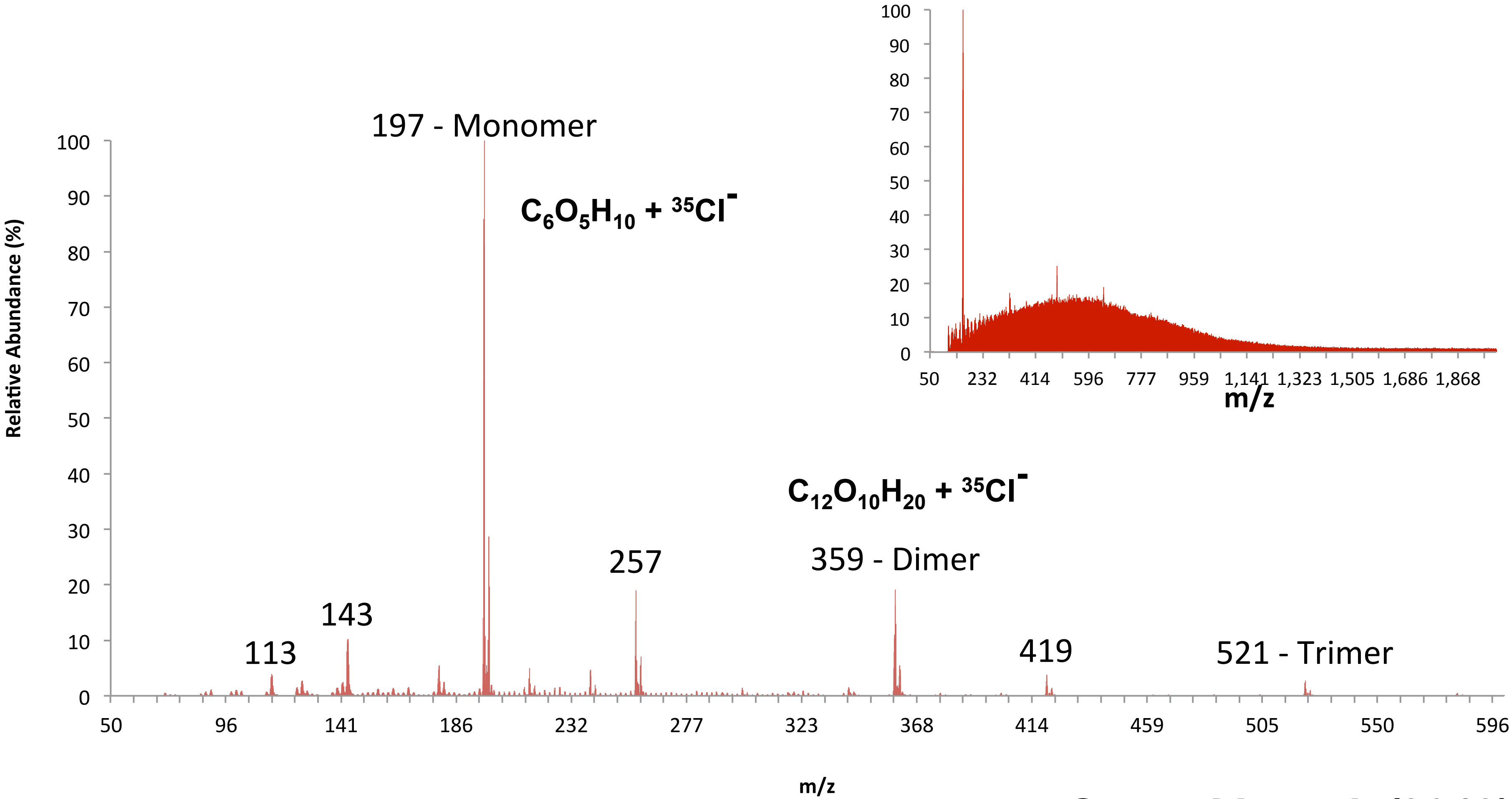


- **Heating rate** 1000°C/s; final temperature 600°C
- Product **quenching** upon evaporation into 100°C N_2
- **Instant** ionization (APCI) and **analysis** with **no size limitations** as opposed to commonly used gas chromatography/mass spectrometry (GC/MS)
- **Elemental compositions** of products via high resolution measurements; **structures** via multi-stage tandem mass spectrometry (MS^n)
- Probing **mechanisms** via partially ^{13}C-labeled compounds

High-level Quantum Chemical Calculations

Agrawal, Delgass, Kenttämaa, Ribeiro

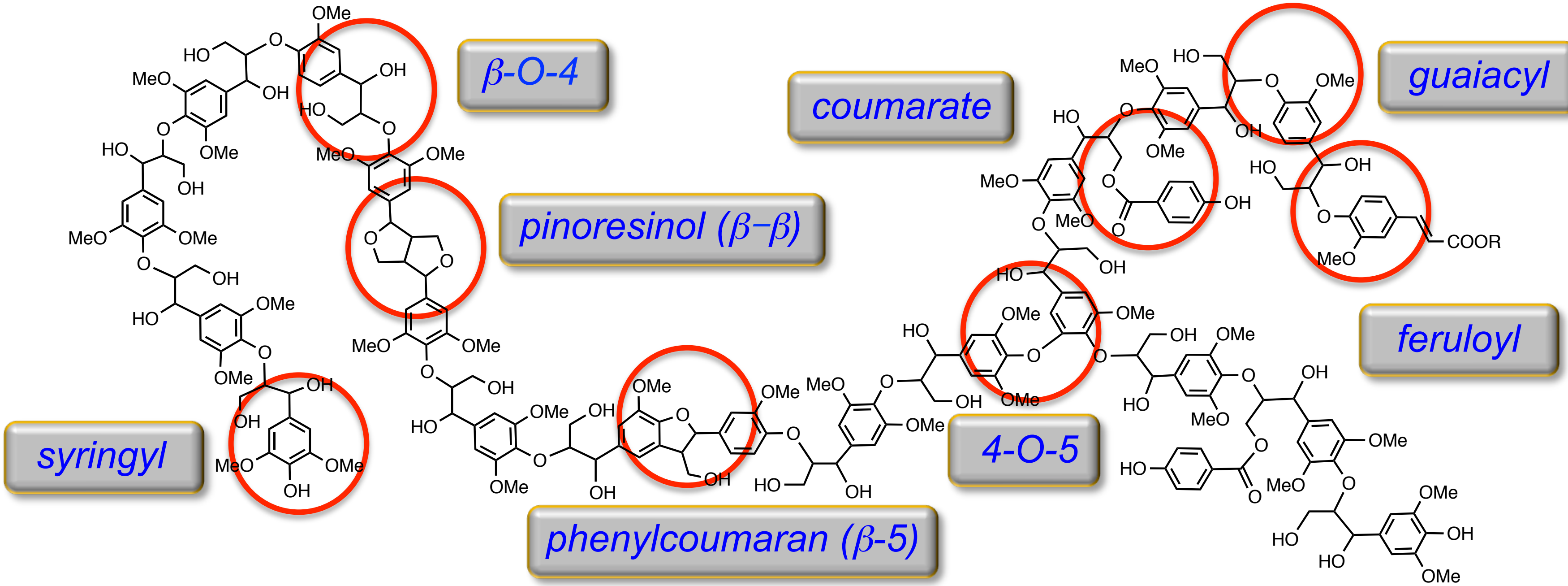
During pyrolysis of cellulose, the glucan chains are converted to small, dehydrated levoglucosans



Gawecki et al. (2012)

Unlike what is seen in bio-oil, primary products are recognizable molecules

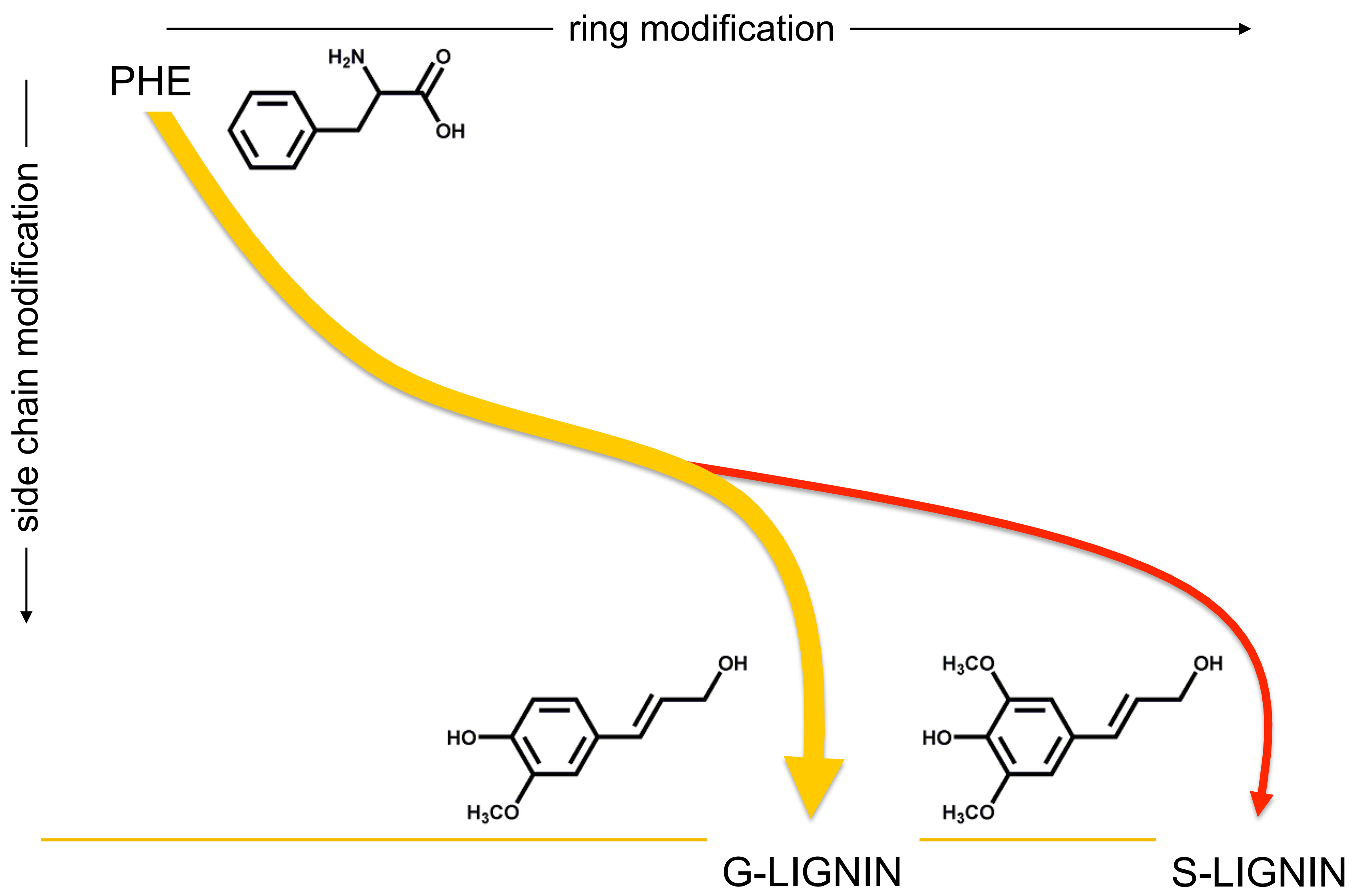
Lignin is 15-25% of biomass but contains ca. 40% of the energy



Plants require the phenylpropanoid pathway for:

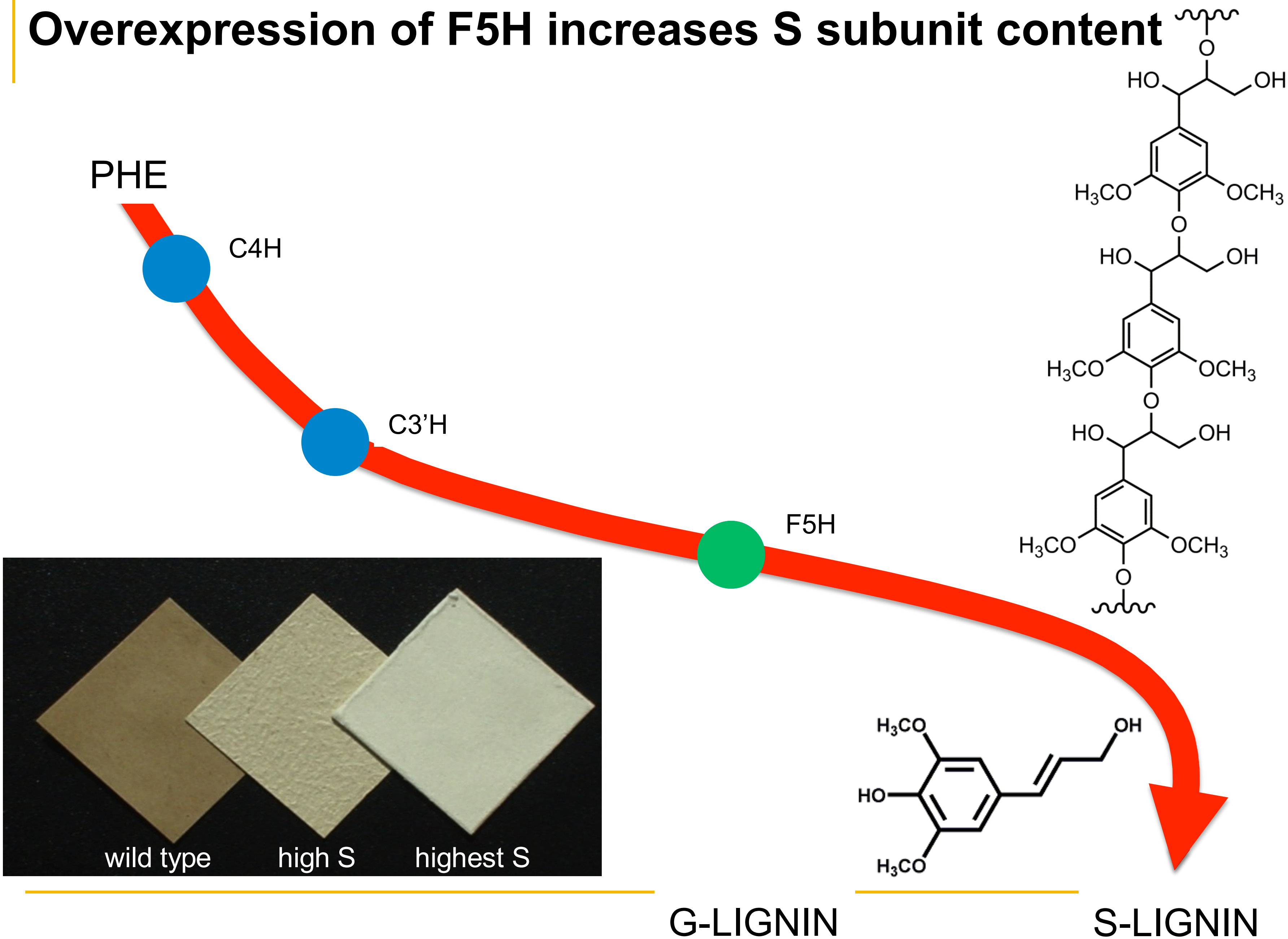
- **UV resistance**
- **structural support**
- **water transport**

The lignin biosynthetic pathway



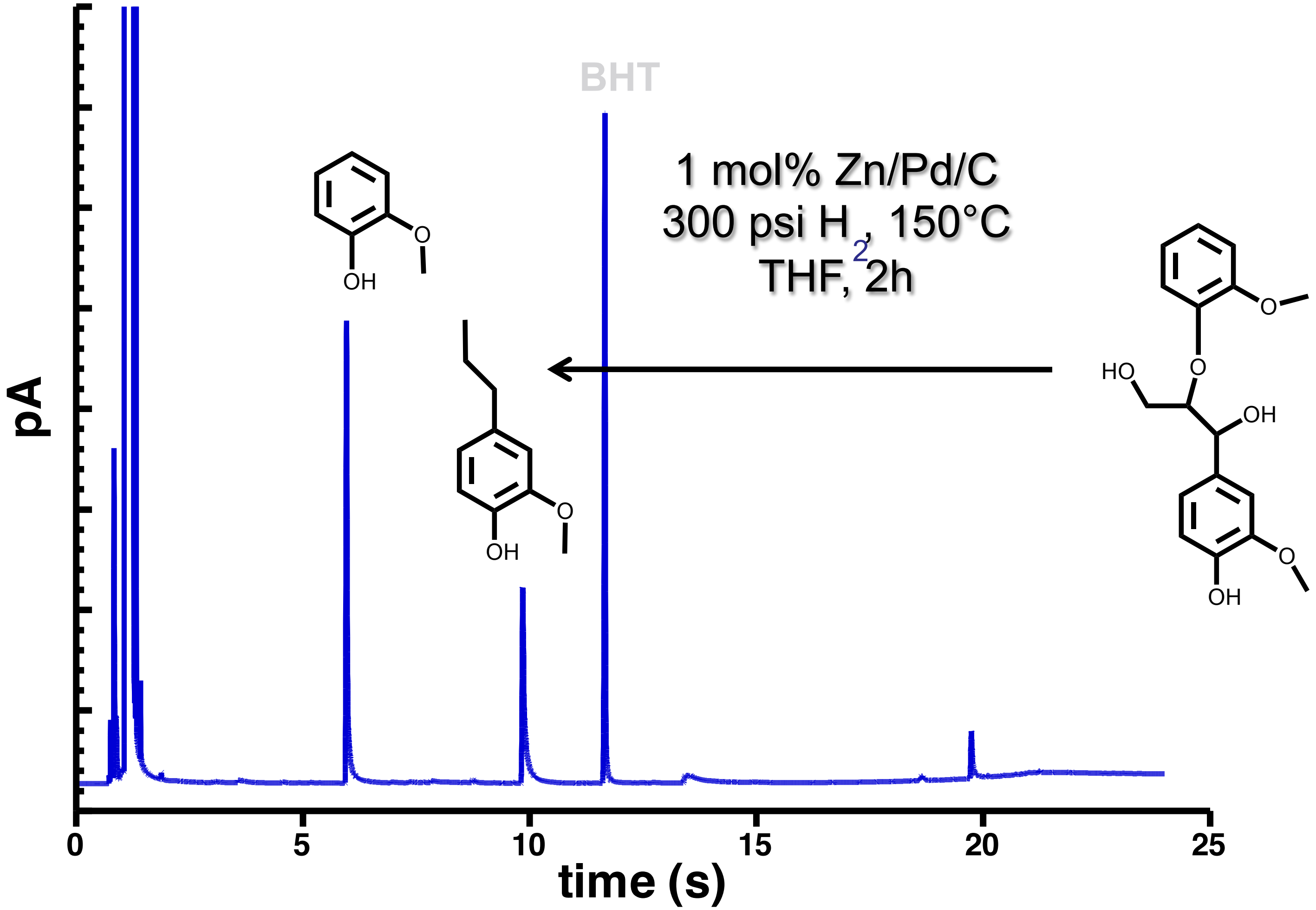
Clint Chapple

Overexpression of F5H increases S subunit content



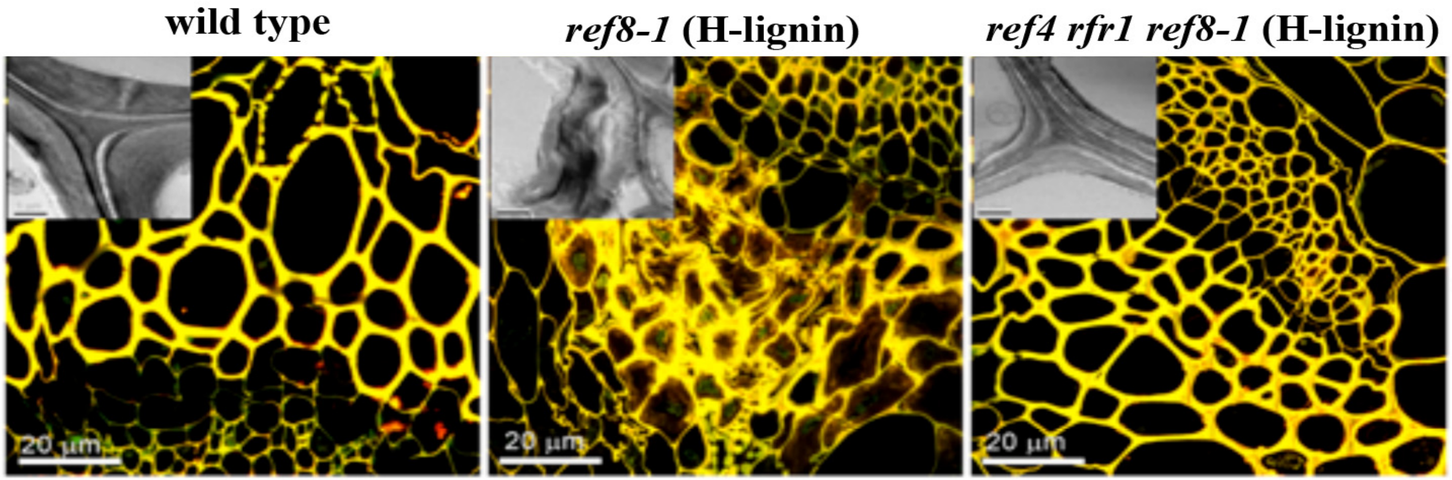
Huntley et al. (2003)

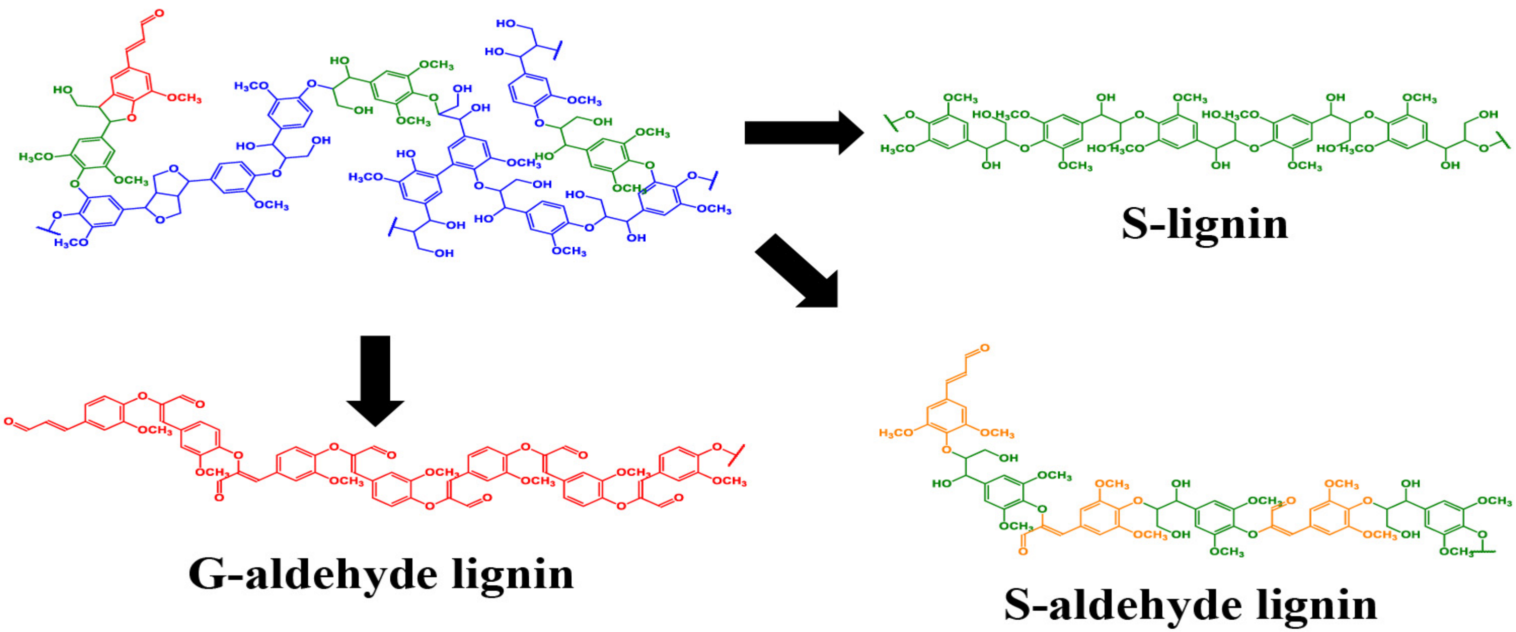
A Zn/Pd/C catalyst that cleaves the ether bond in a synthesized model dimer



Mahdi Abu-Omar, Shuo Liu: Purdue

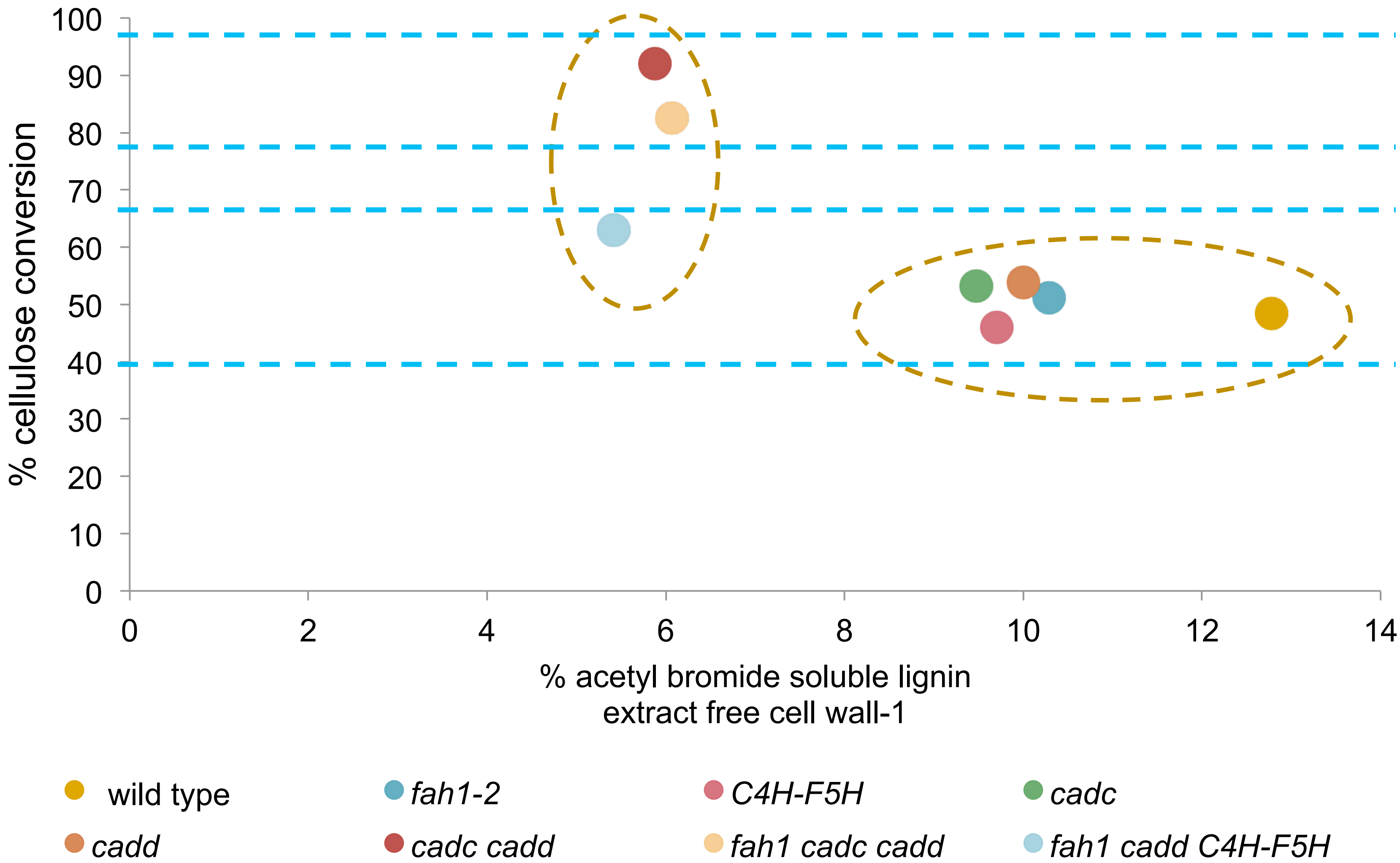
Sclerenchyma cell walls in vascular tissue with H-lignin



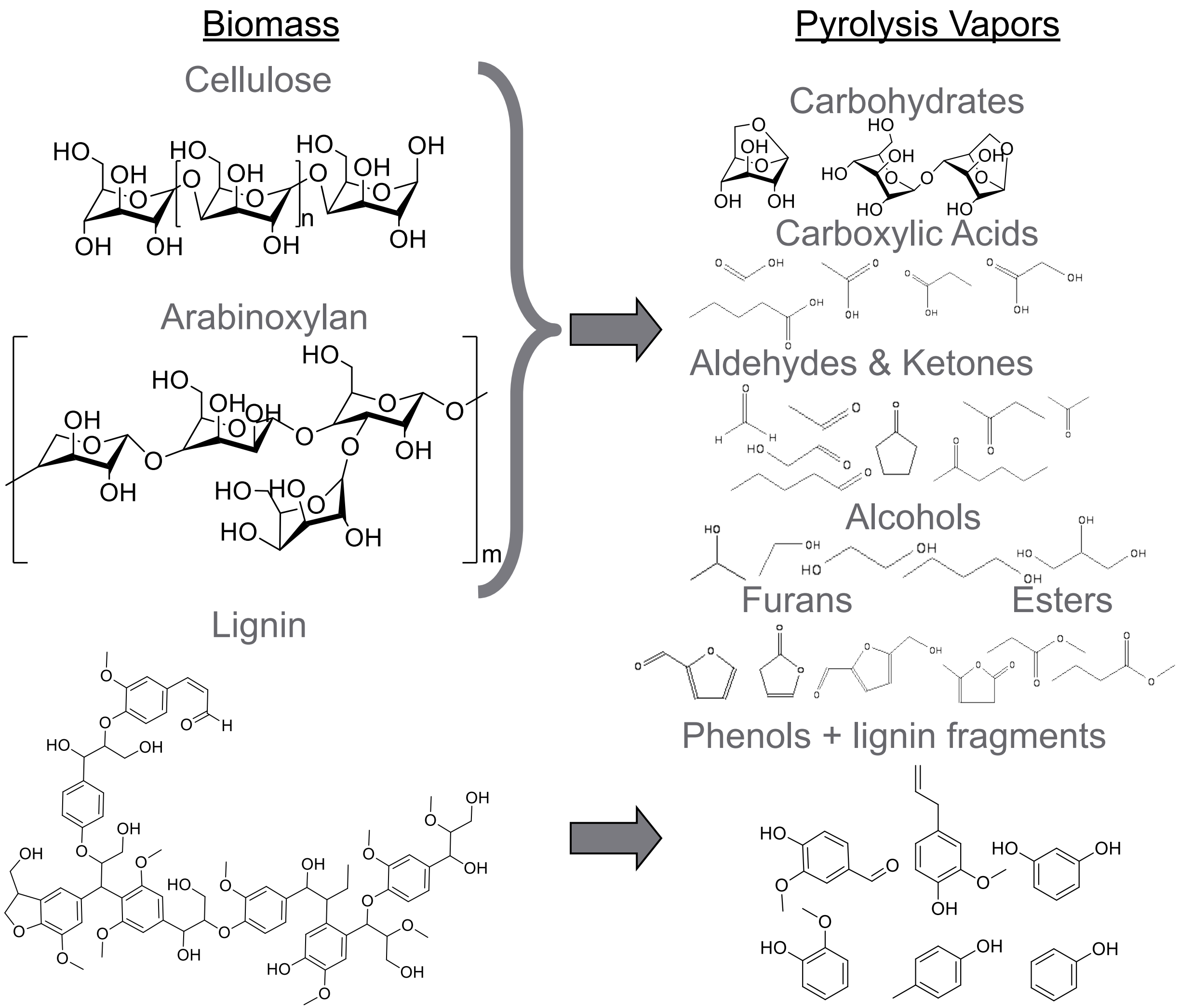


Clint Chapple

Aldehyde enrichment in lignin increases cell wall digestibility

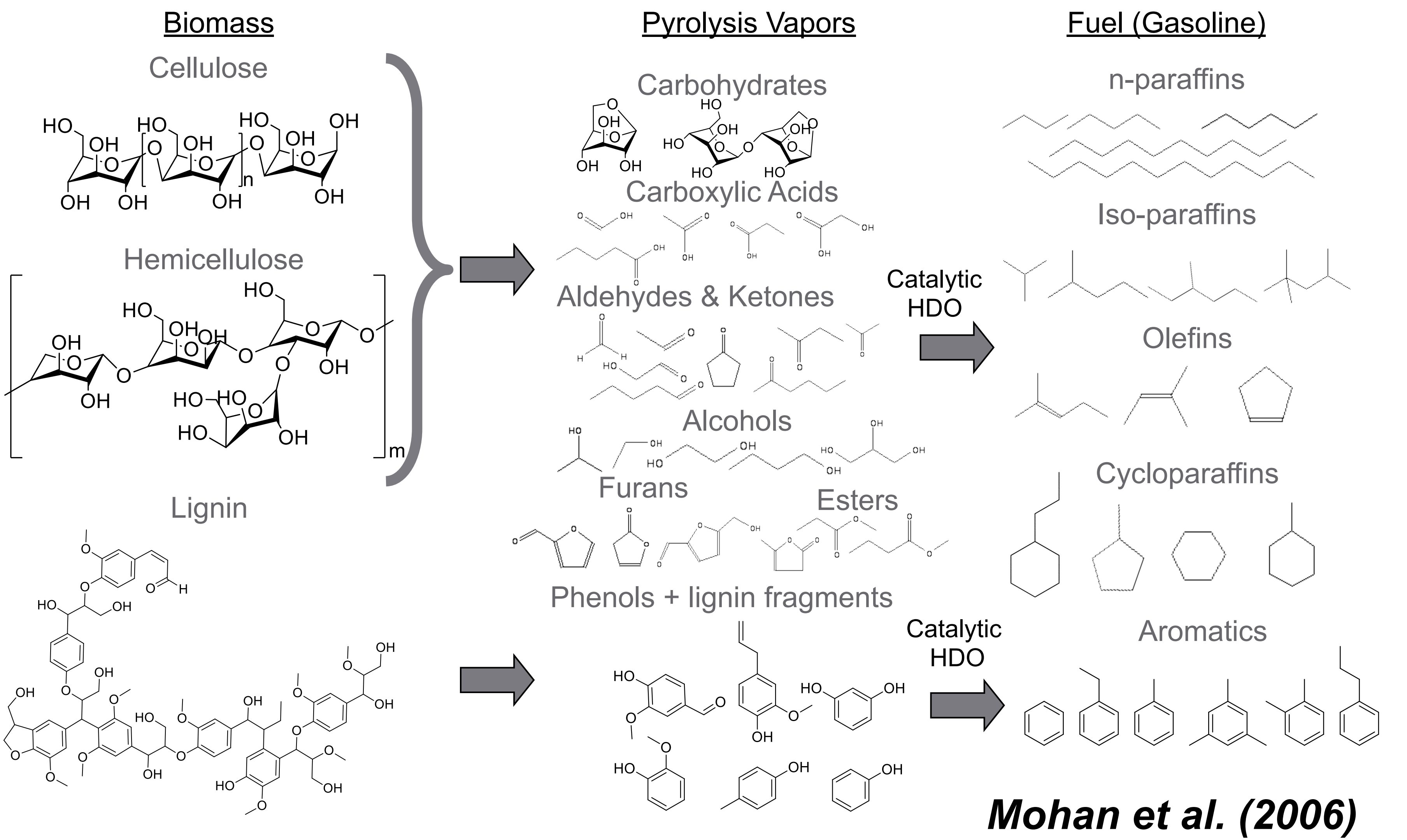


Pyrolysis fragments *biomass* into oxygenated vapors



Abu-Omar, Agrwal, Delgass, Kenttämaa, Mosier, Riberio (Purdue); Barnes, Bozell (Tennessee)

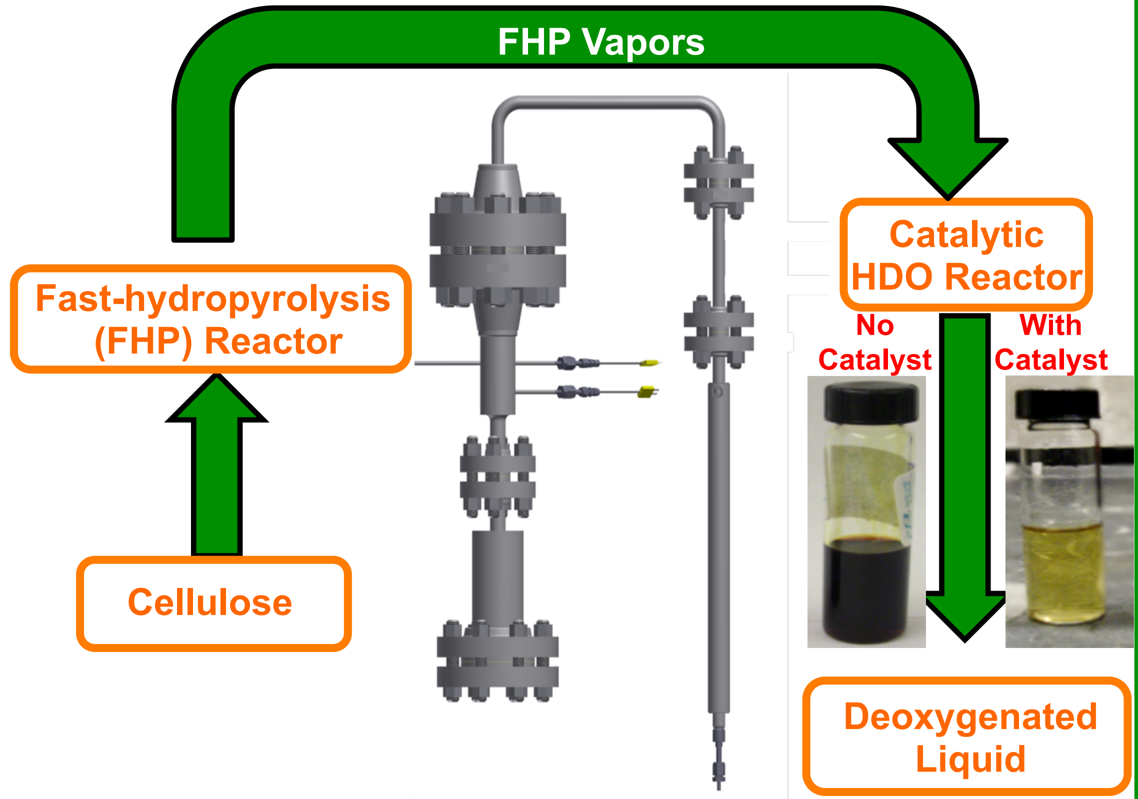
Catalytic Hydrodeoxygenation (HDO) upgrades hydropyrolysis vapors into fuel molecules



Abu-Omar, Agrwal, Delgass, Kenttämaa, Mosier, Riberio (Purdue); Barnes, Bozell (Tennessee)

Cellulose fast-hydropyrolysis and catalytic hydrodeoxygenation (HDO): Reactor and analytic system

- High-pressure, rapid-heating, continuous-flow, reactor and solids feeder.
- LC/MS method for complex product mixture analysis.
- High pressure (50 bar) H_2 did not significantly affect fast-hydropyrolysis without a catalyst, but is beneficial for catalytic HDO.

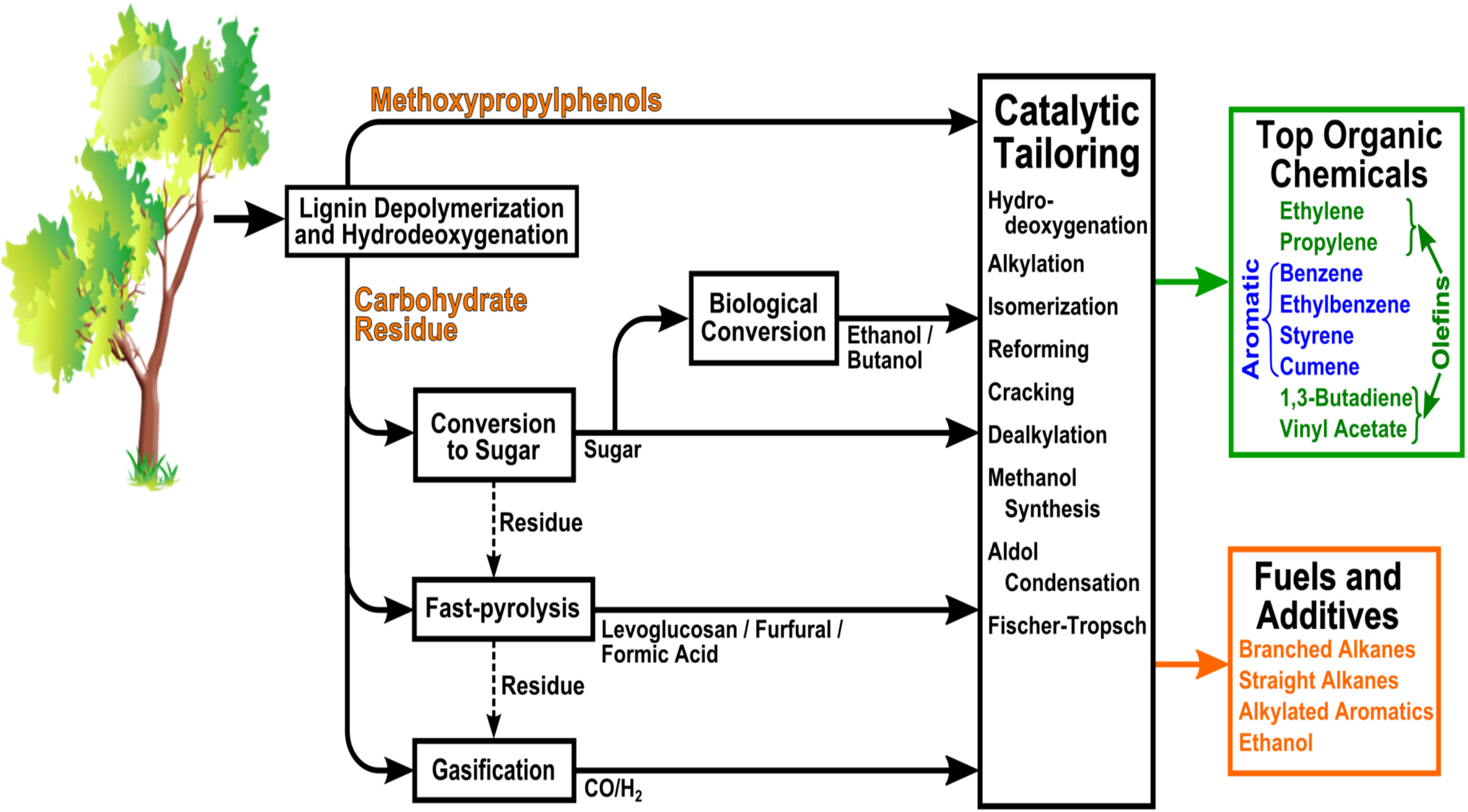


Schematic of reactor system and conversion pathway

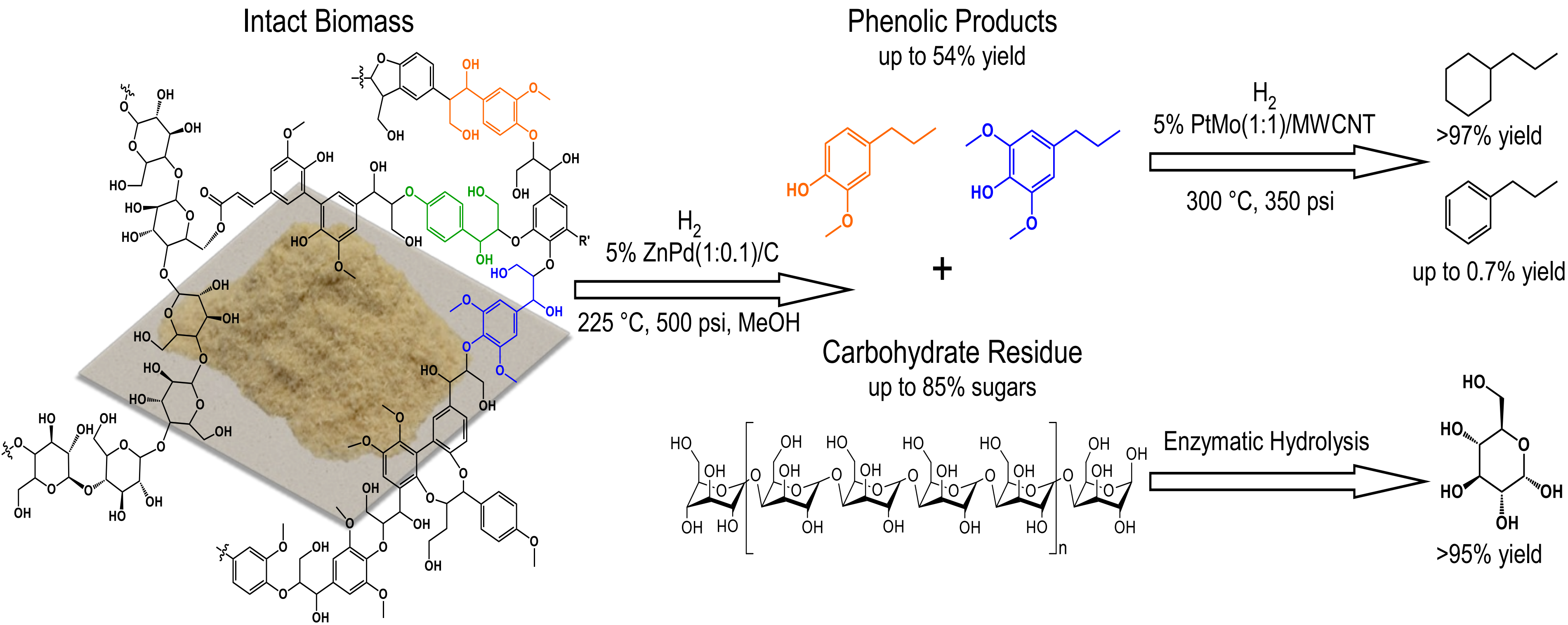
We have recently developed new catalysts which can directly produce complete hydrocarbons by 100% deoxygenation of cellulose.

Venkatakrishnan et al. (2014)

Turning the biorefinery on end: A synergistic biorefinery disassembling lignin first



Selective depolymerization and HDO of lignin directly from wood biomass.

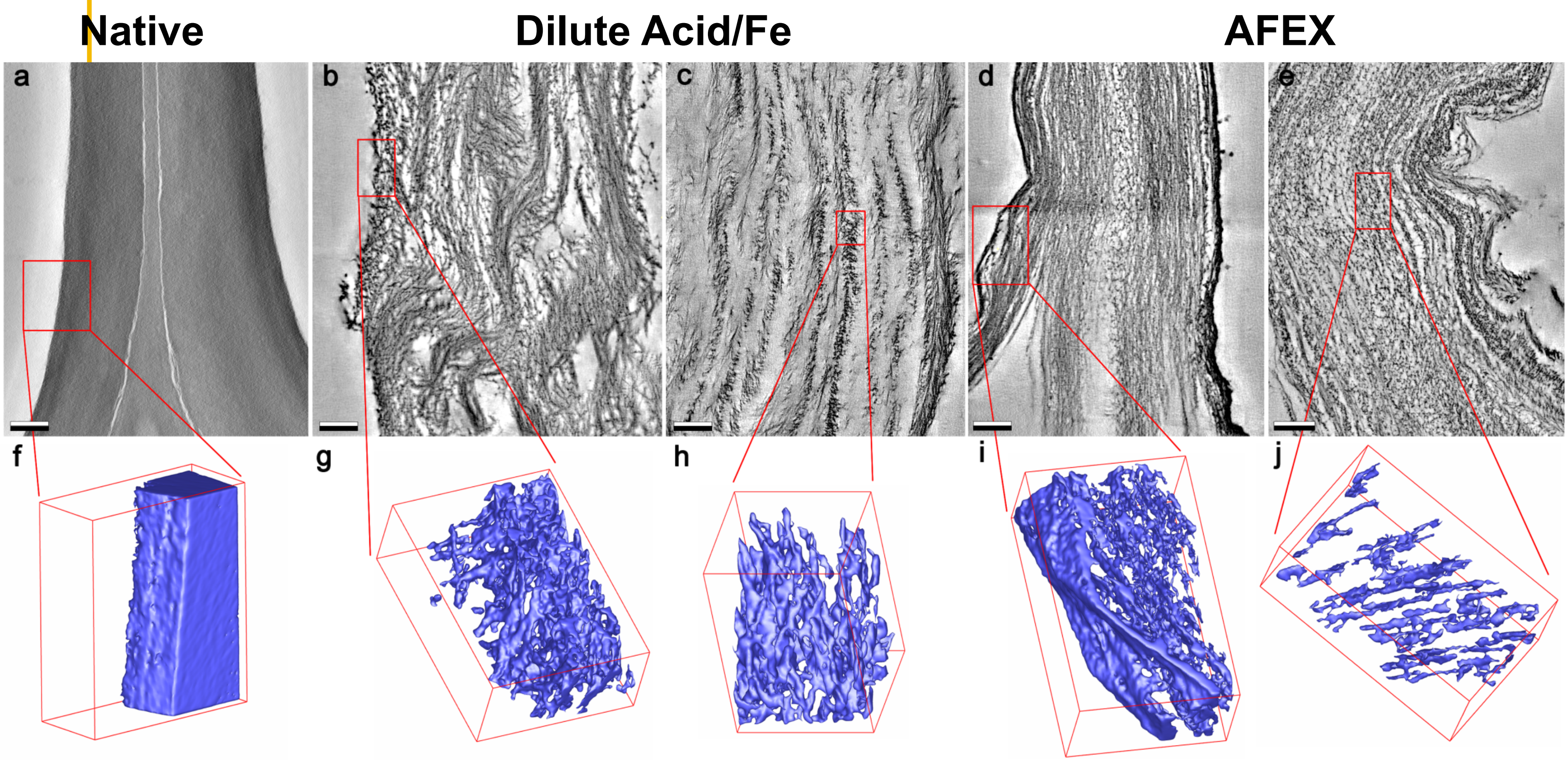


- Current methoxypropylphenols annual production volume of >30 M lbs and market value of $450 M.
- Methoxypropylphenols are manufactured from petroleum feedstock and toxic chemicals via a multi-step process

What were we thinking?

- **Plant cell walls may be overbuilt and can be engineered to be chemically and structurally less complex.**
- **Plants could be coerced into sowing the seeds of their own deconstruction by delivering catalysts to cell walls (the *Trojan horse* concept).**
- **Plants could meet engineers halfway on the road to conversion by producing more labile polymers leading to highly specific conversion with high yield.**

Analysis of 3D images designed to identify structural motifs and patterns that remain throughout the processing and provide clues as to the nature of the highly recalcitrant residue

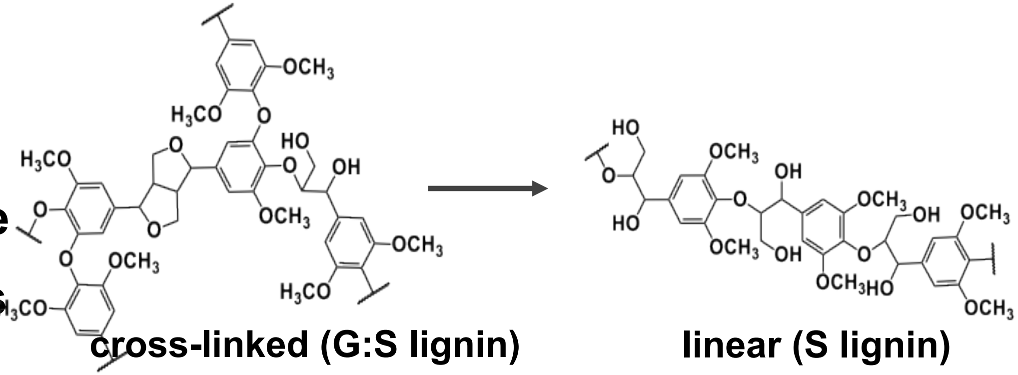


Scale Bars 200 nm

Donohoe, Ciesielski, Himmel (NREL)

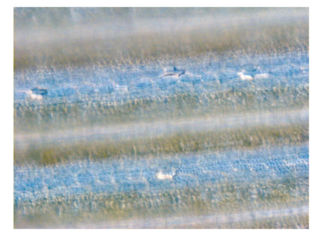
What has tailored biomass come to mean at C3Bio?

- **Lignin**
  - high-S, high-H, high-aldehyde
  - chemically induced synthesis



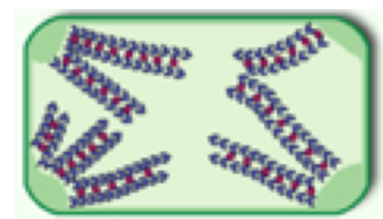
cross-linked (G:S lignin) linear (S lignin)

- **Catalysts**
  - ferritin expression in poplar
  - transition metal accumulation in cell walls



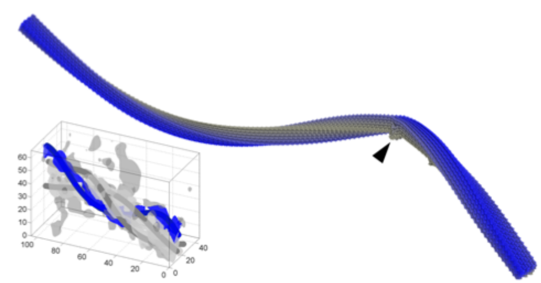
visualization of iron in cell walls of rice OPT3 knockdown plants

- **Cell Walls**
  - stabilized actin bundles
  - control trafficking infrastructure for cell wall modification and targeted delivery

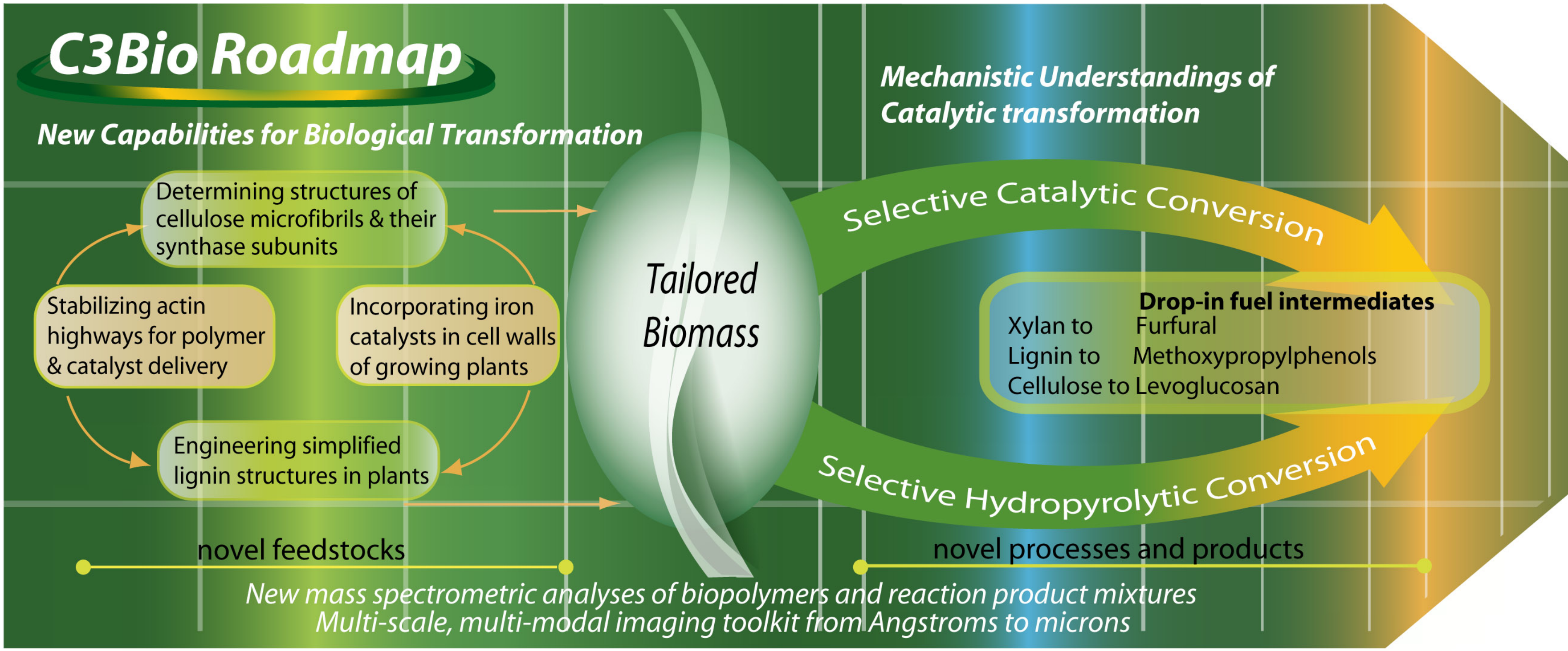


superhighways for directed cell wall deposition

- **Cellulose**
  - concepts for microfibril modifications
  - Chemical: rare sugars physical: defects



C3Bio research achievements



C3Bio

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PURDUE UNIVERSITY Discovery Park

M. McCann (Director), M. Abu-Omar (Associate Director), C. Huetteman (Project Manager), R. Agrawal, N. Carpita, C. Chapple, K. Clase, N. Delgass, H. Kenttämaa, N. Mosier, A. Murphy, W. Peer, F. Ribeiro, G. Simpson, C. Staiger, D. Szymanski.

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

M. Himmel, S-Y. Ding, M. Tucker, M. Crowley, B. Donohoe

THE UNIVERSITY of TENNESSEE UT
KNOXVILLE

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