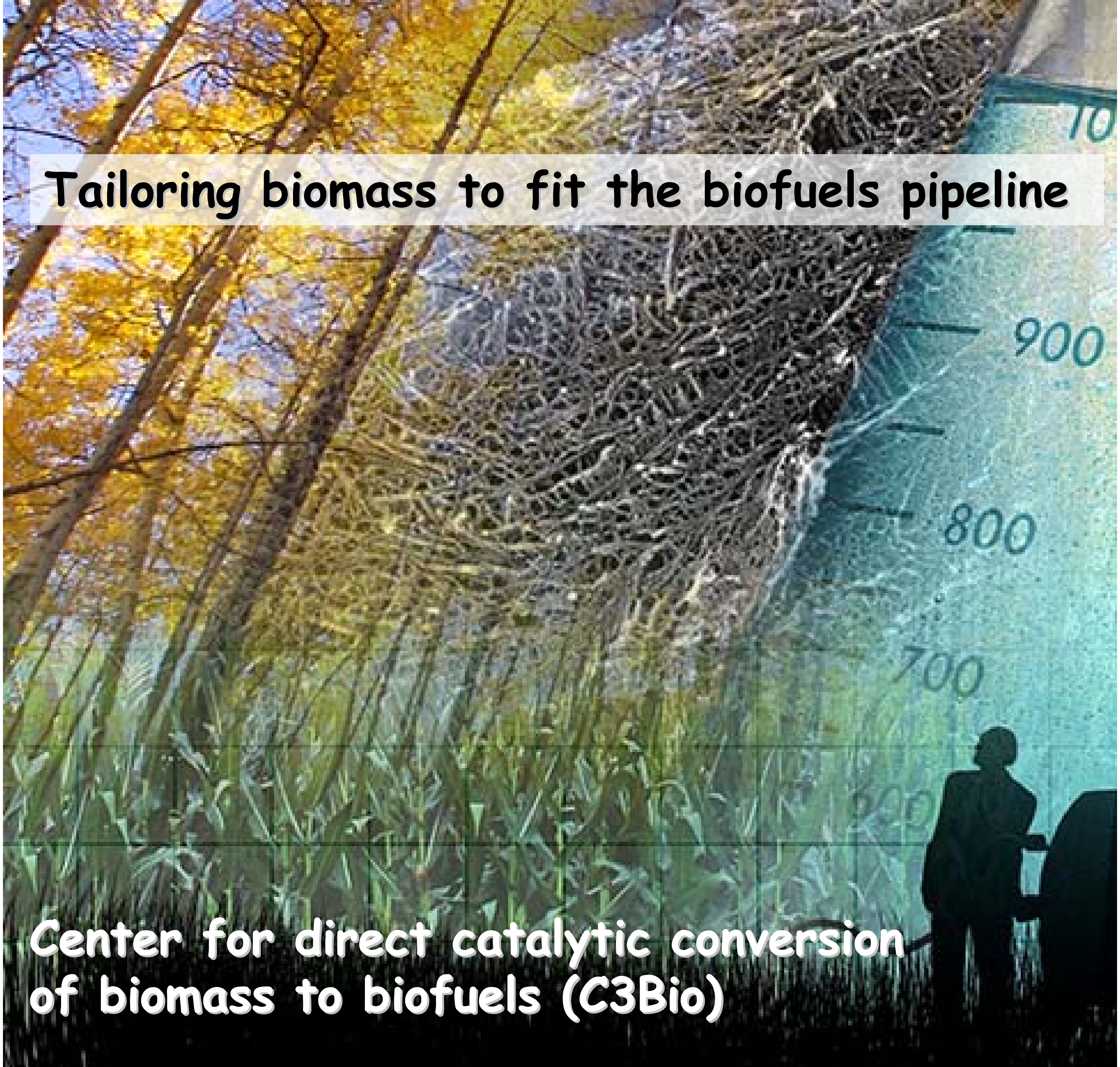
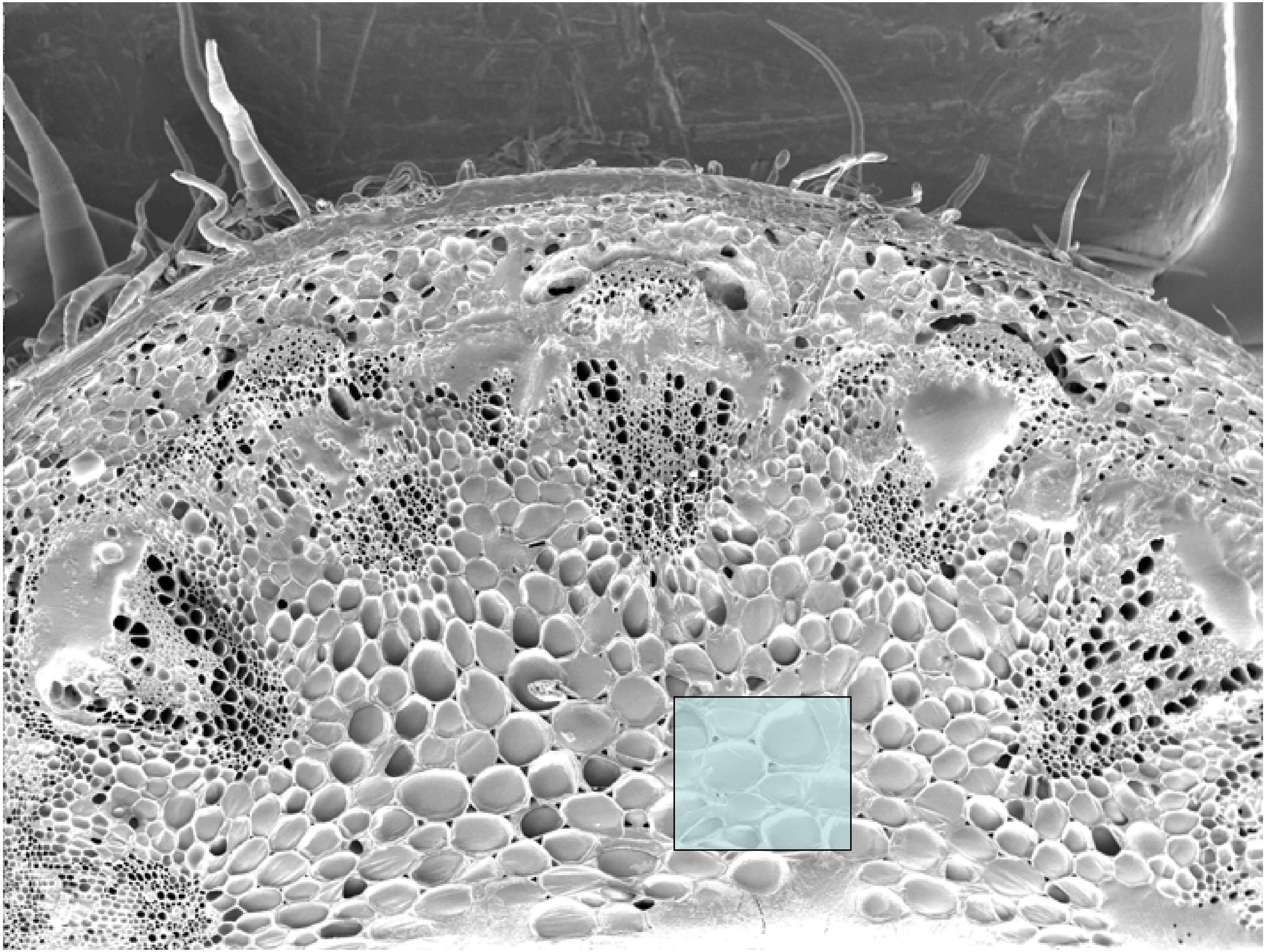
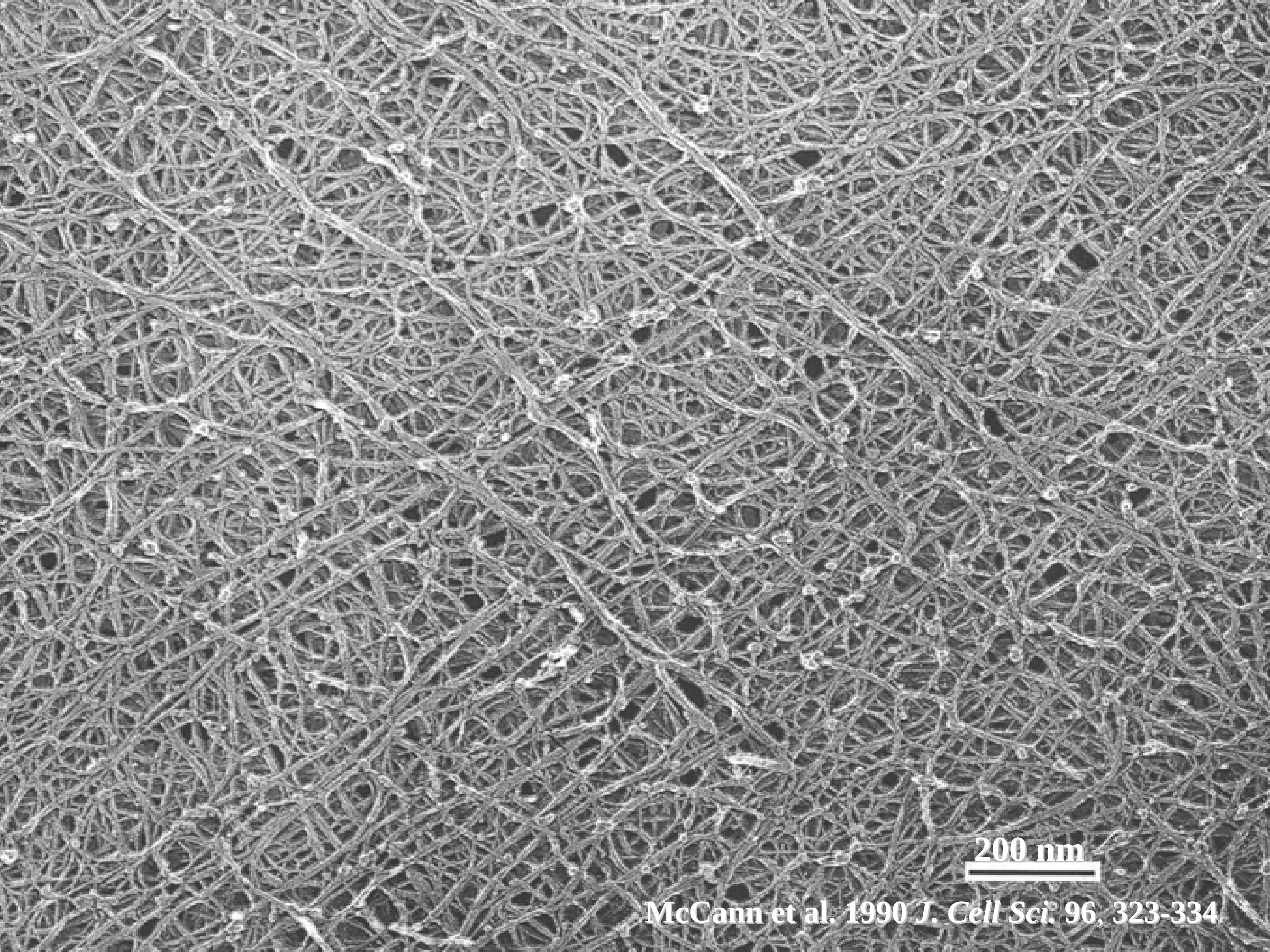

Tailoring biomass to fit the biofuels pipeline
Center for direct catalytic conversion of biomass to biofuels (C3Bio)

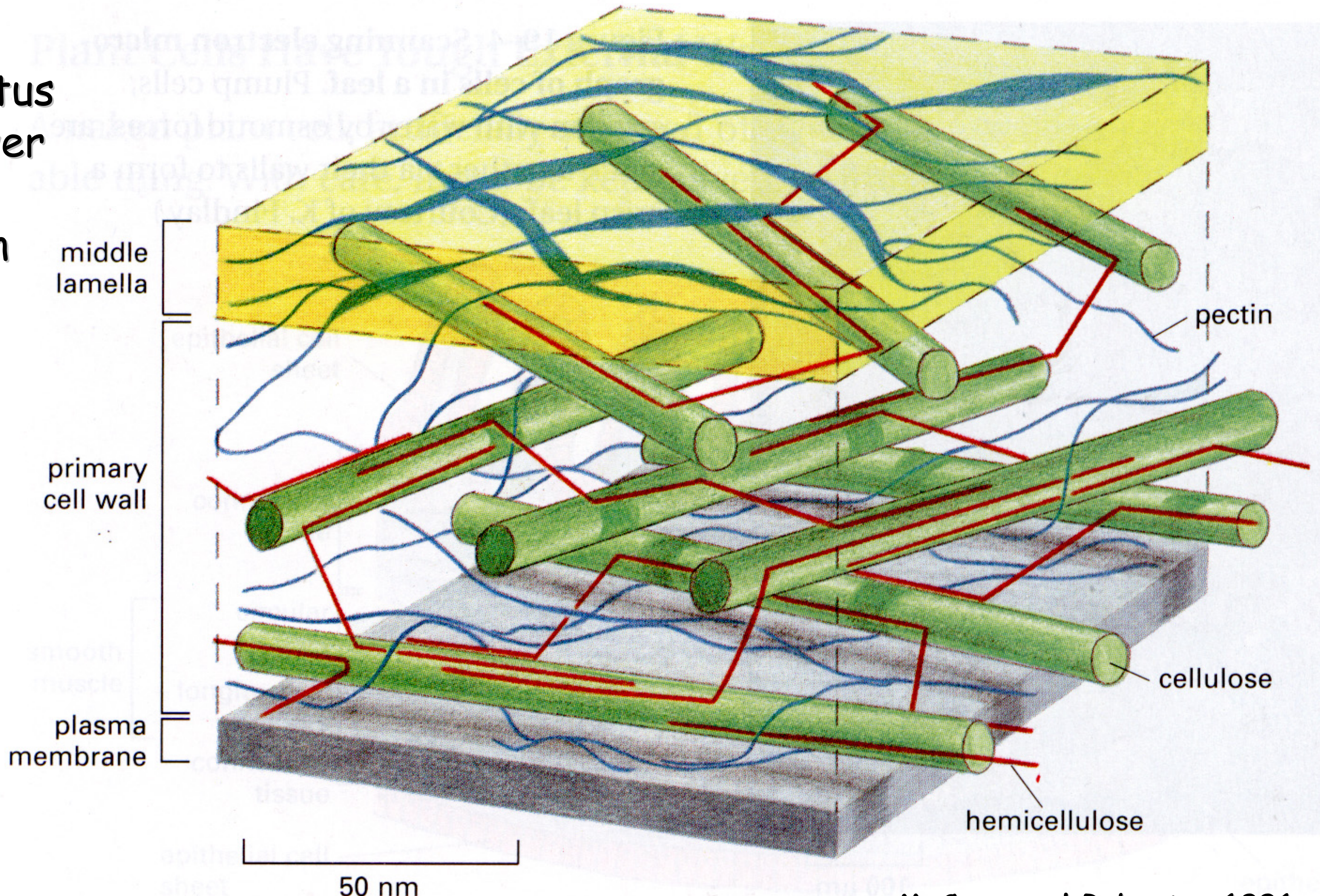




McCann et al. 1990 *J. Cell Sci.* 96, 323-334

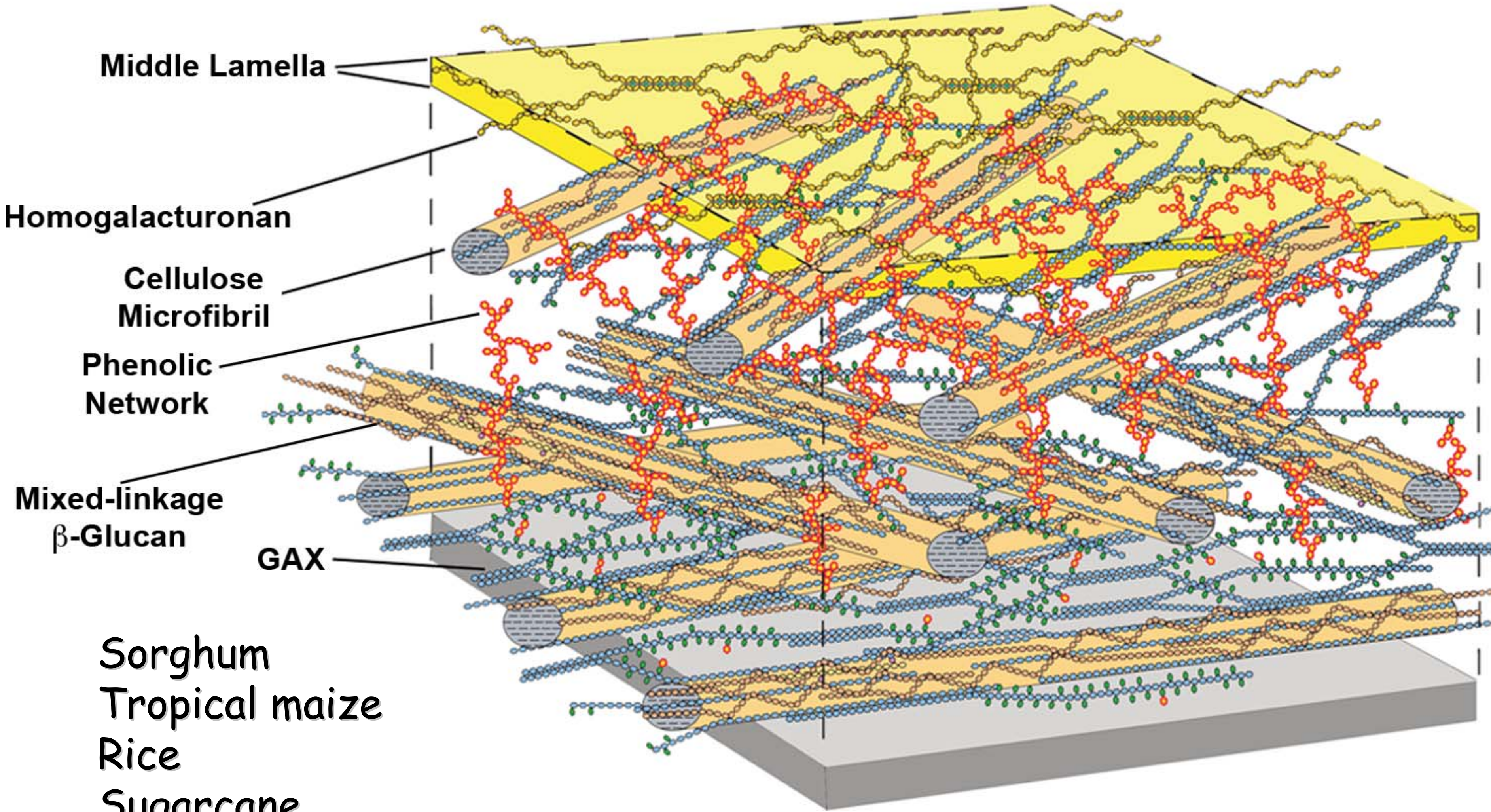
Model of a primary (growing) cell wall

Poplar
Willow
Eucalyptus
Sunflower
Canola
Soybean

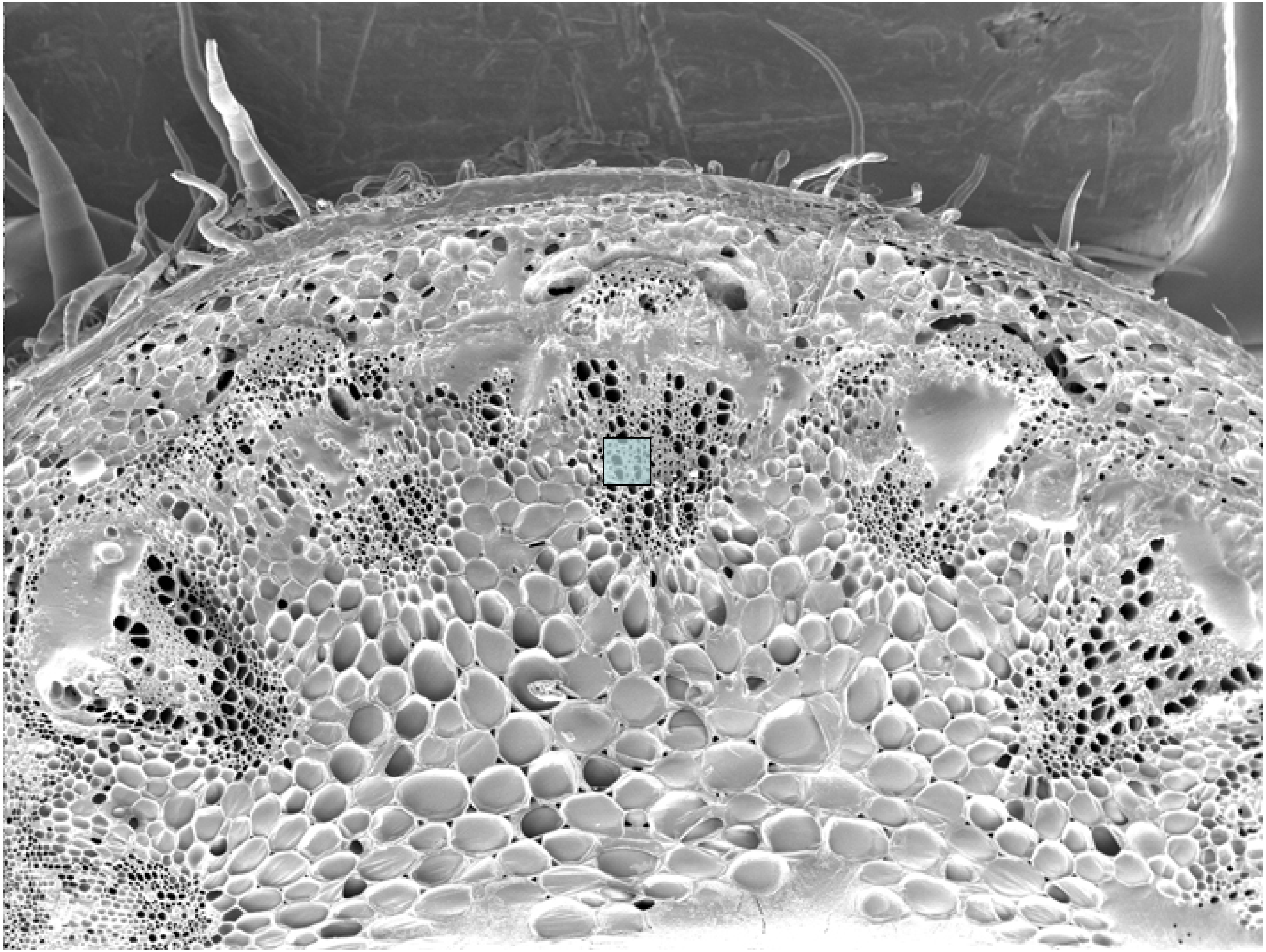


McCann and Roberts, 1991

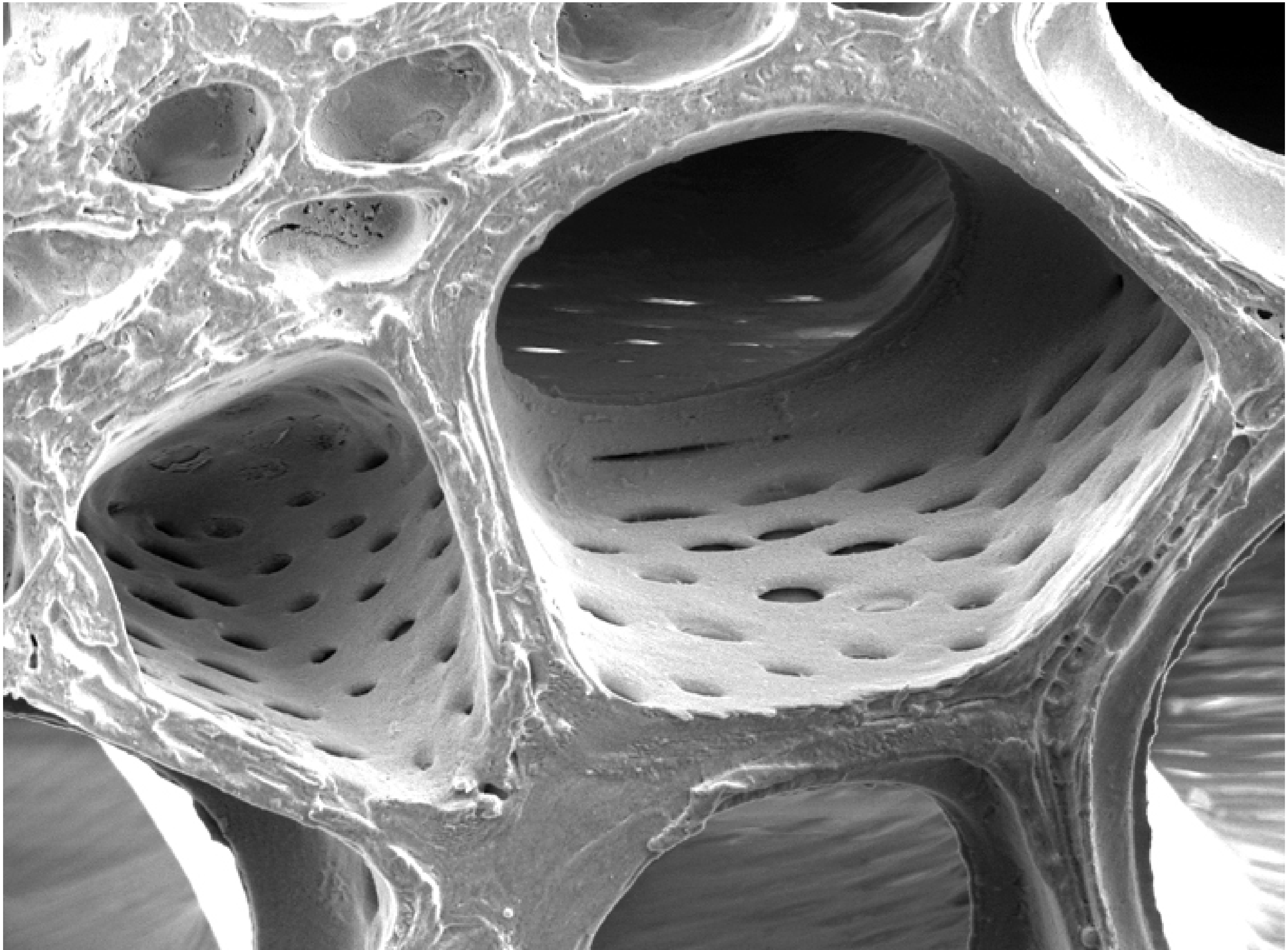
The cell walls of grasses are unique among the angiosperms



Sorghum
Tropical maize
Rice
Sugarcane
Miscanthus
Switchgrass
Big Bluestem

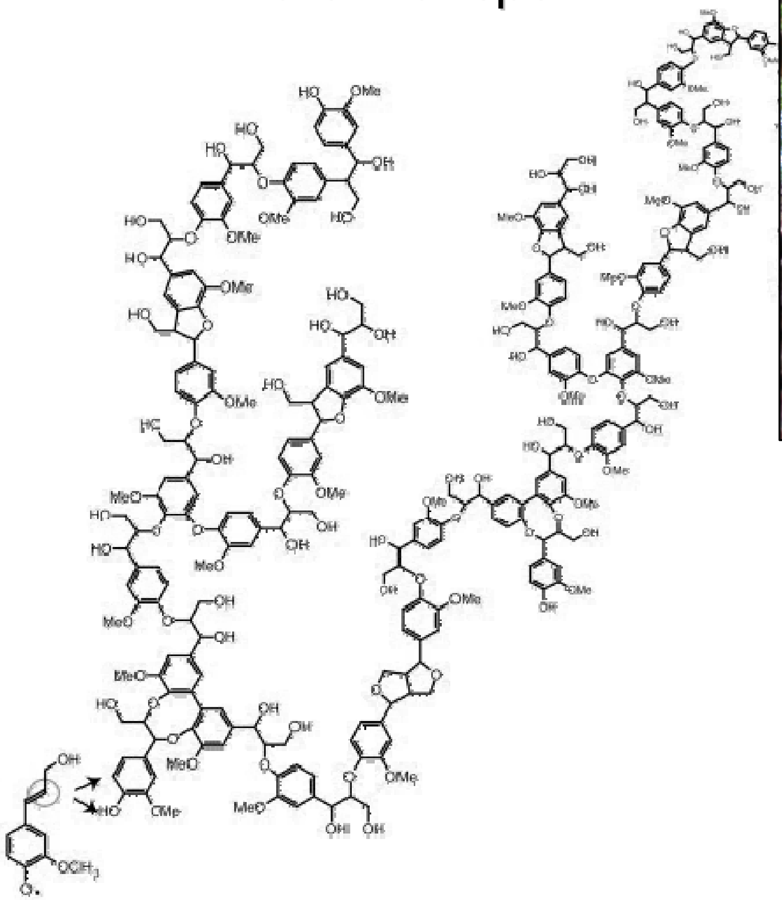


Lignified walls surround some specialized cell types but contribute greatly to the biomass

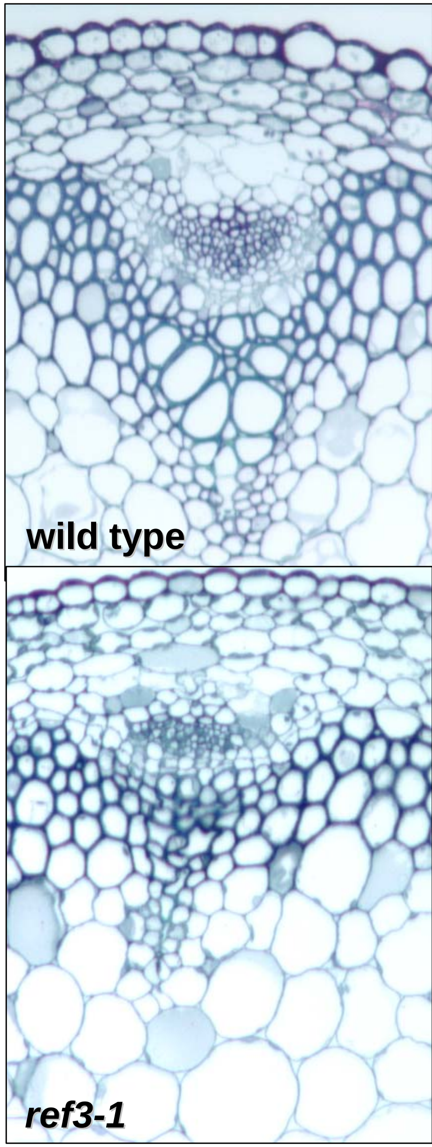


Phenylpropanoid metabolism is critical for plant survival

- UV resistance
- structural support
- water transport

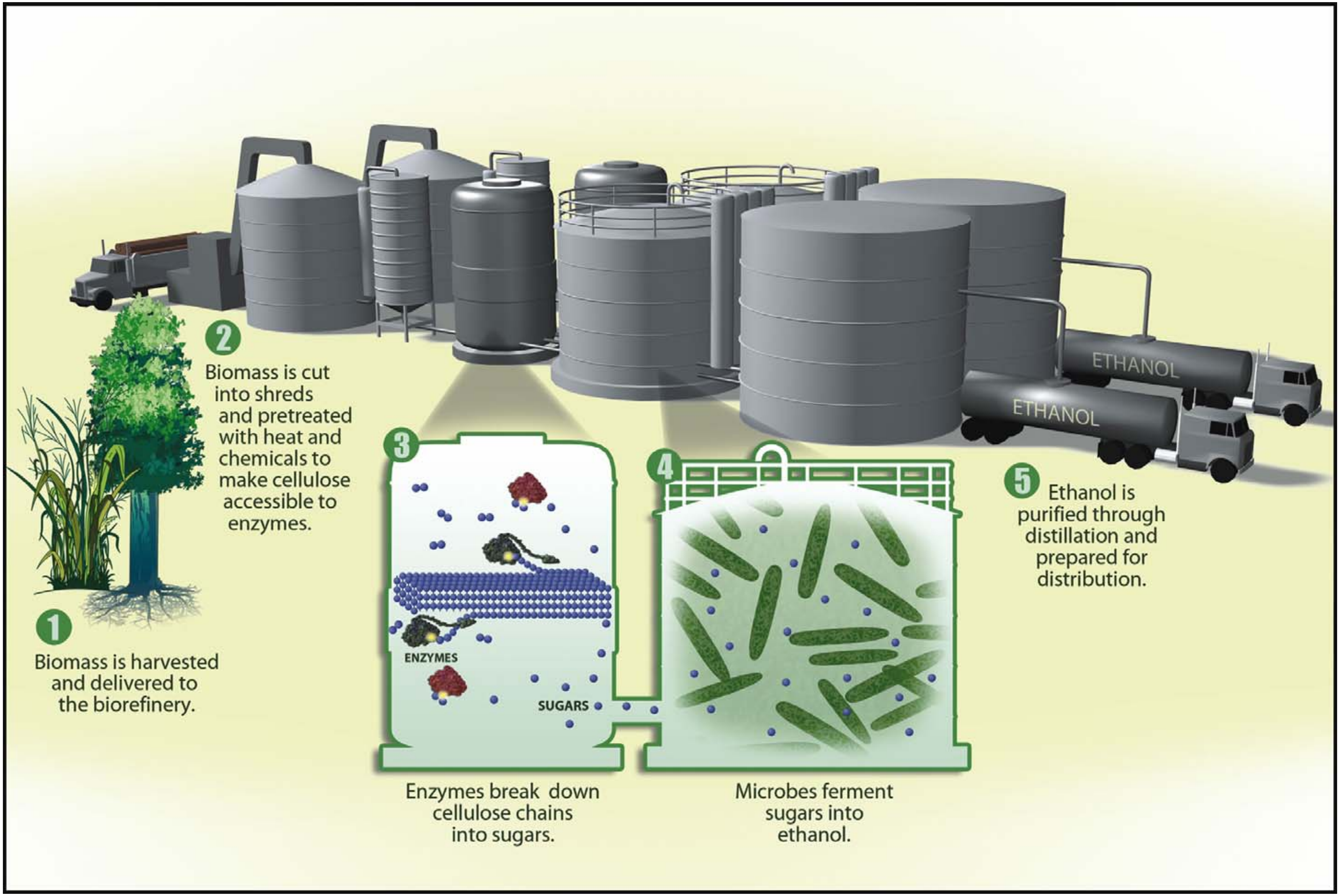


http://givingspace.org/benlomond/up%20redwoods.jpg

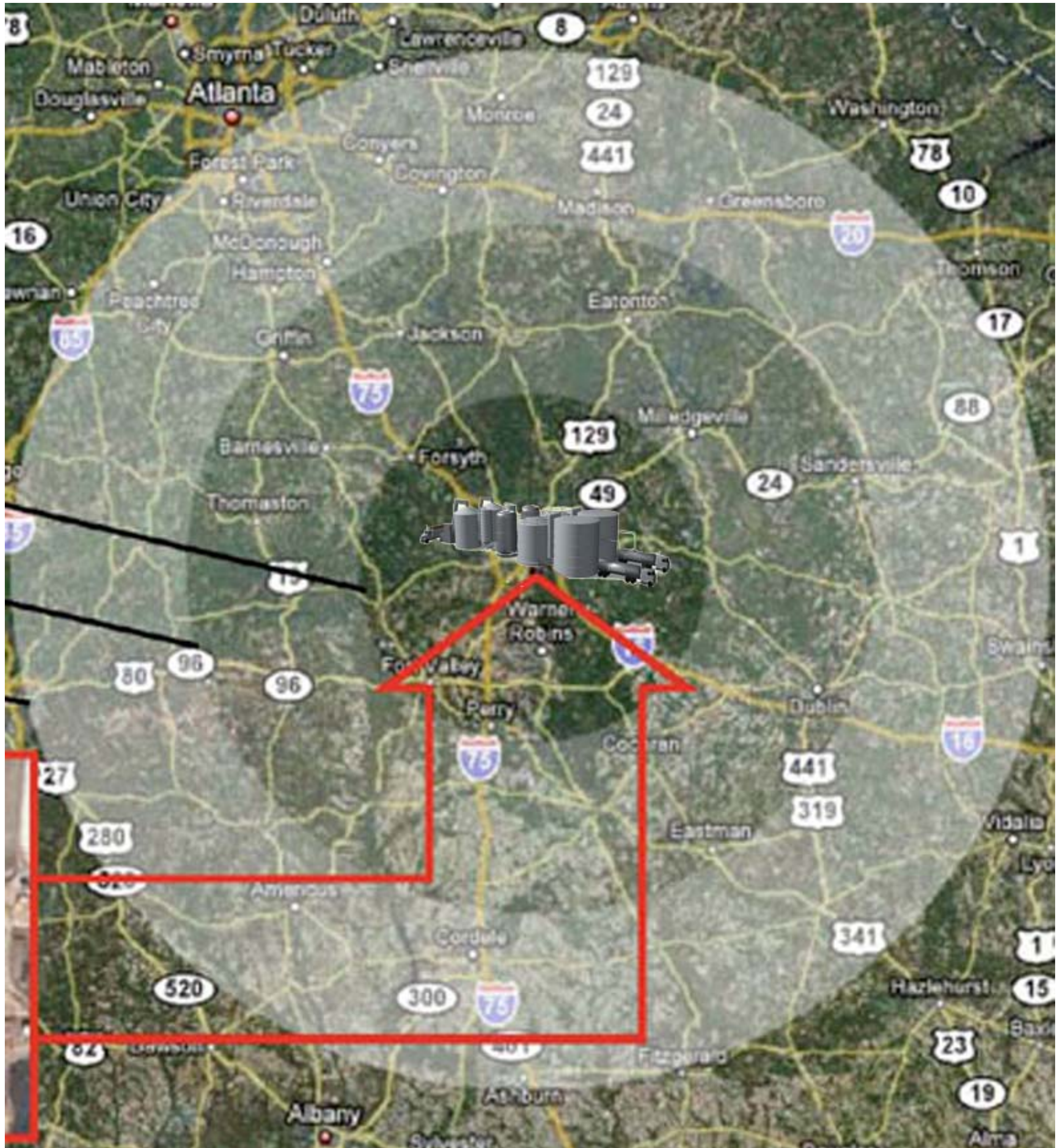


Hatfield R, Vermerris W. (2001). Plant Physiol. 126: 1351-1357

Biological conversion route for biomass to biofuel



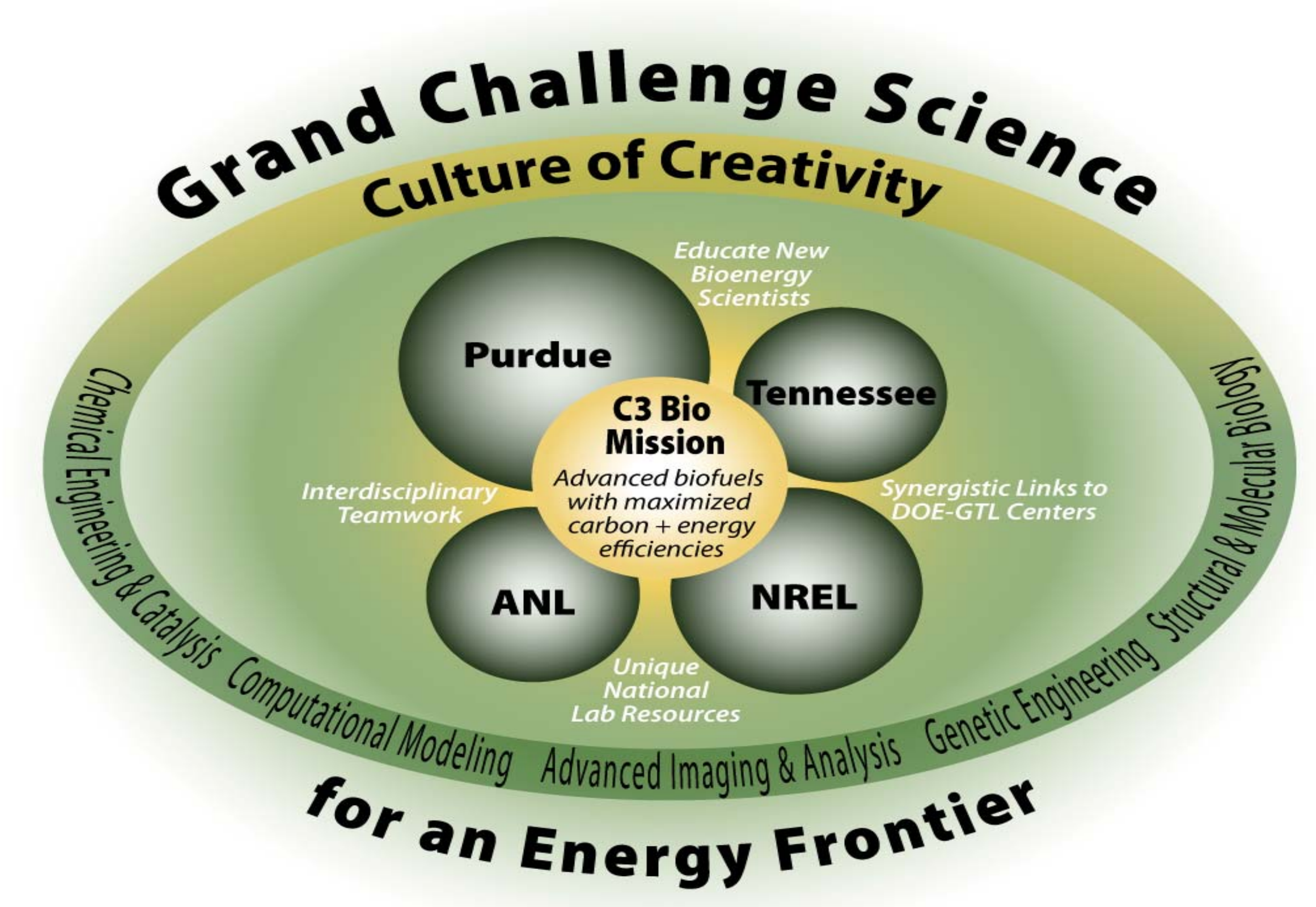
Transport costs will limit where biomass feedstocks are grown



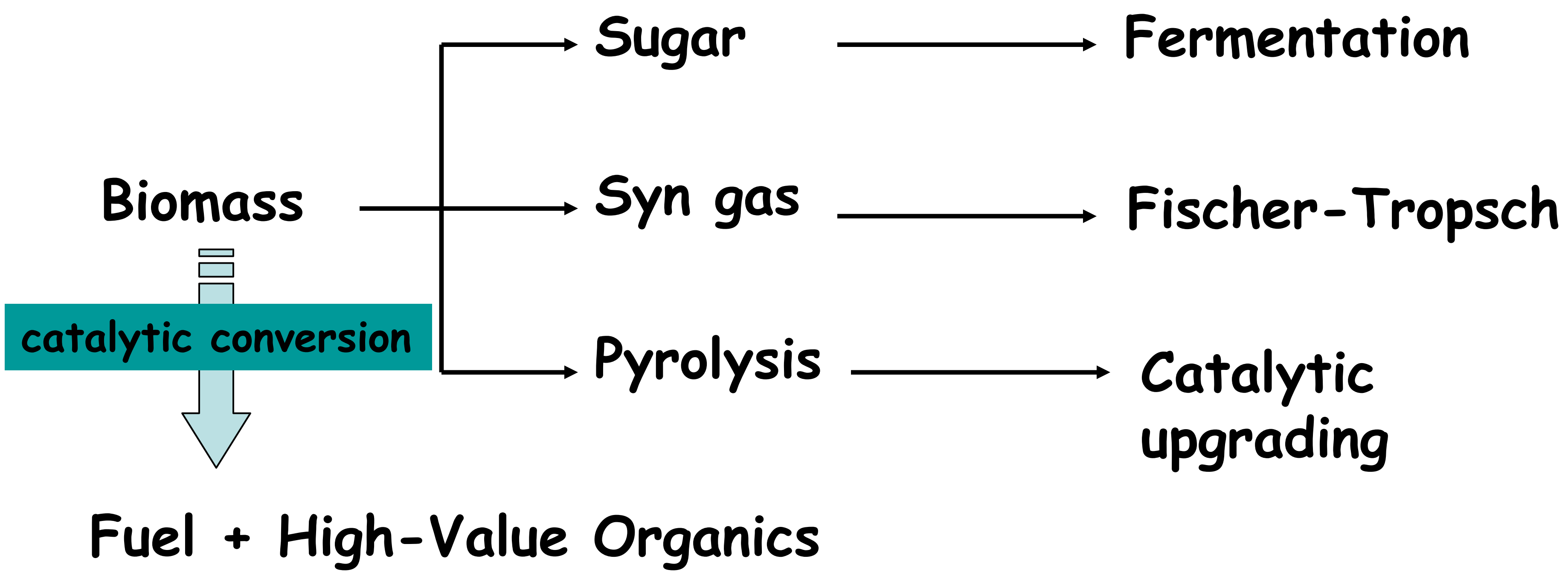
Understanding biomass biology is critical for biofuels production because……

- Cell wall architectures impact plant stature and form (biomass quantity)
- The architecture of cell walls limits their deconstruction to substrates for biofuel production (biomass quality)
- Plant cell walls may be optimized for their end-use in biofuel conversion processes (tailored biomass)

We need to increase dramatically the carbon and energy efficiencies of biofuels production

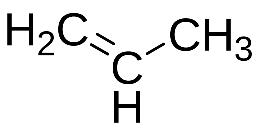


Conversion technologies for next-generation biofuels

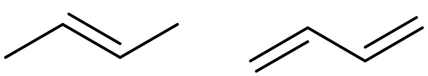


Magnificent six – the six chemicals used as starting materials in the petrochemical industry

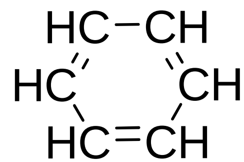
$H_2C=CH_2$ ethylene



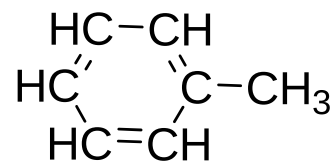
propylene



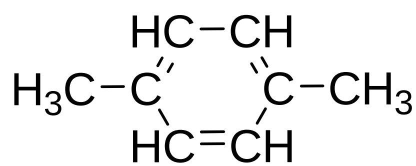
C4-olefins



benzene

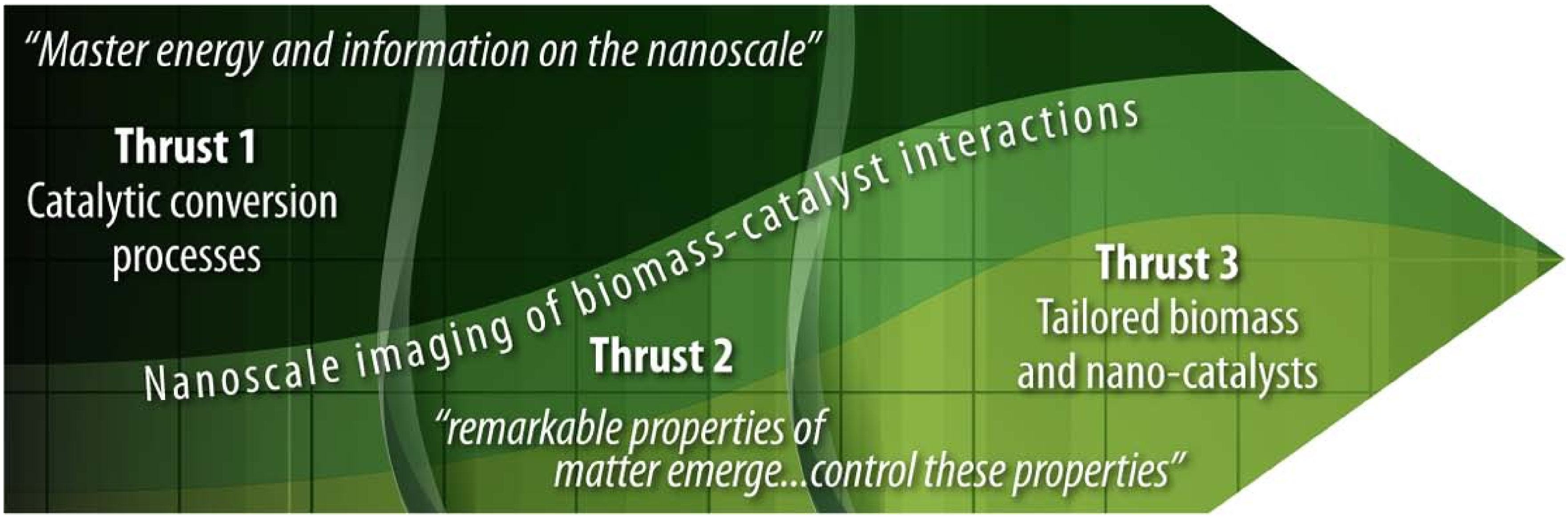


toluene



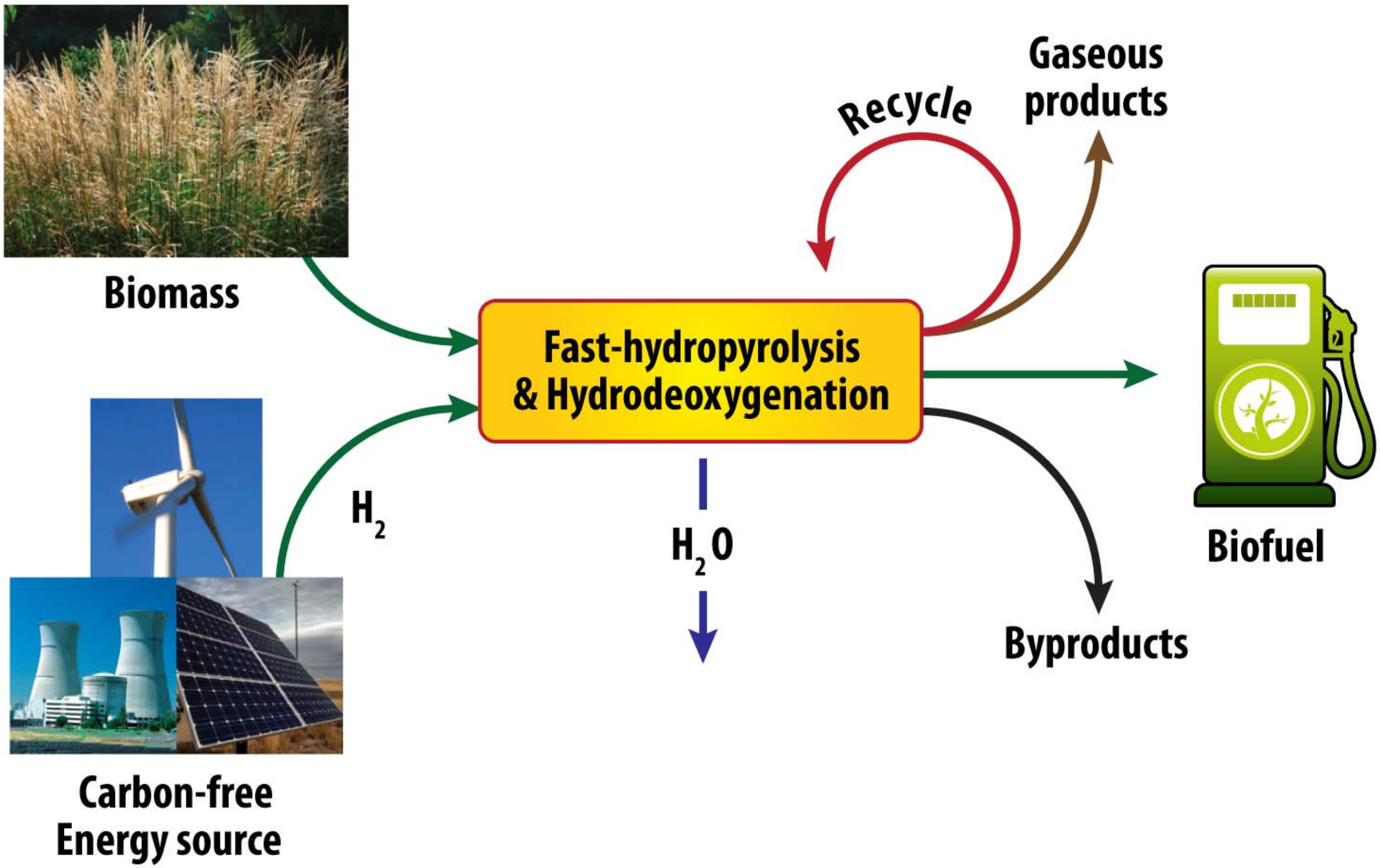
xylene (BTX)

C3Bio will build the knowledge base of biomass-catalyst interactions for optimized catalytic pathways and biomass tailored for its end-use



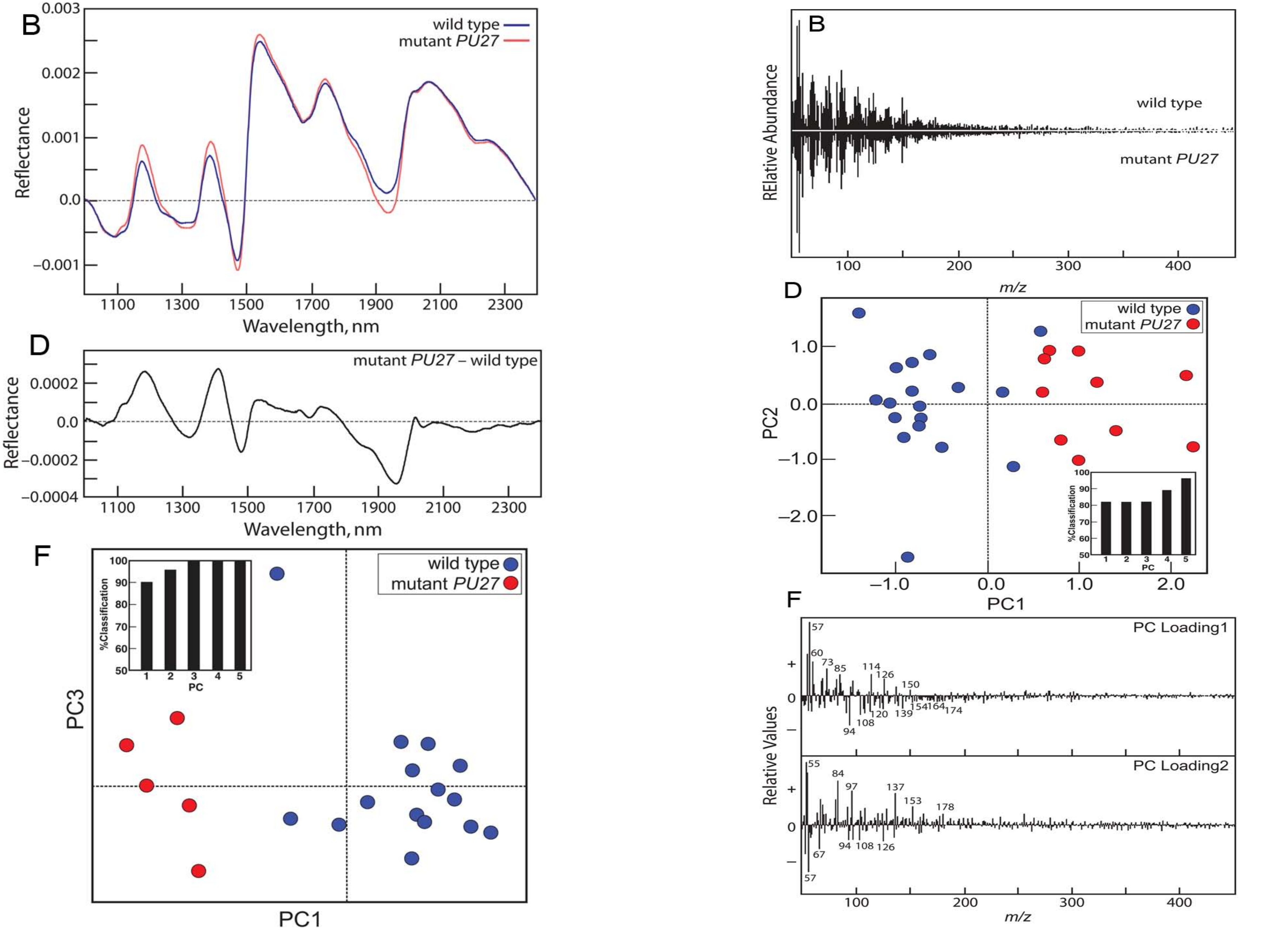
This knowledge will allow development of transformational technologies for the direct conversion of plant lignocellulosic biomass to biofuels and other biobased products, currently derived from oil, by the use of new chemical catalysts and thermal treatments.

Thermal treatments may produce a bio-crude oil for biorefinery fractionation

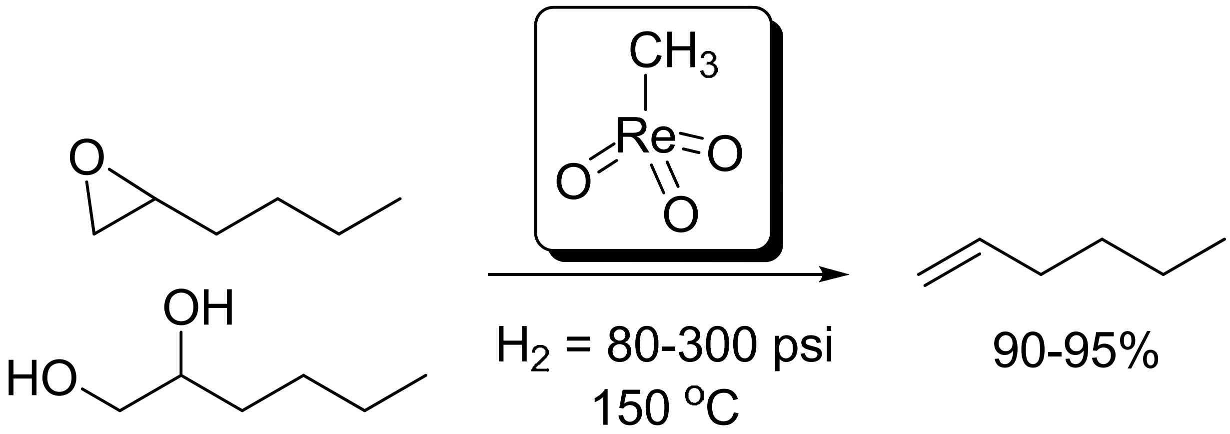


R. Agrawal and N. Singh, AIChE Journal, **55**, 1898 (2009)

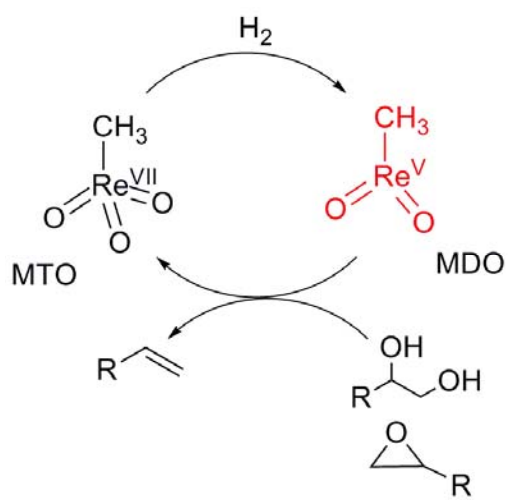
NIR and PyMBMS identify maize mutants with altered CHO-lignin interactions

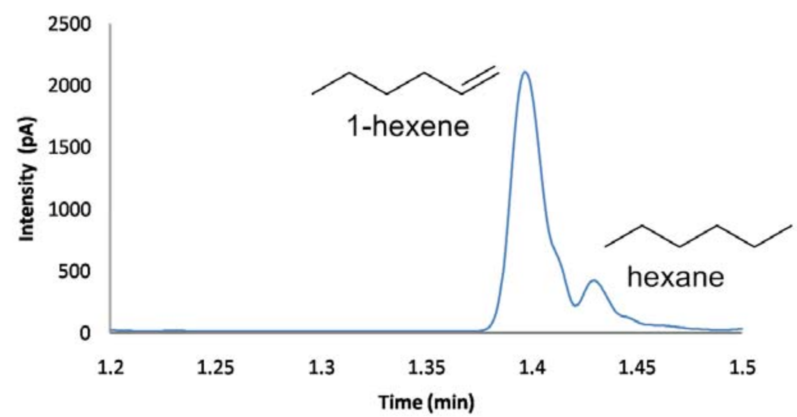


Converting sugars to alkenes: diol-to-alkene reaction



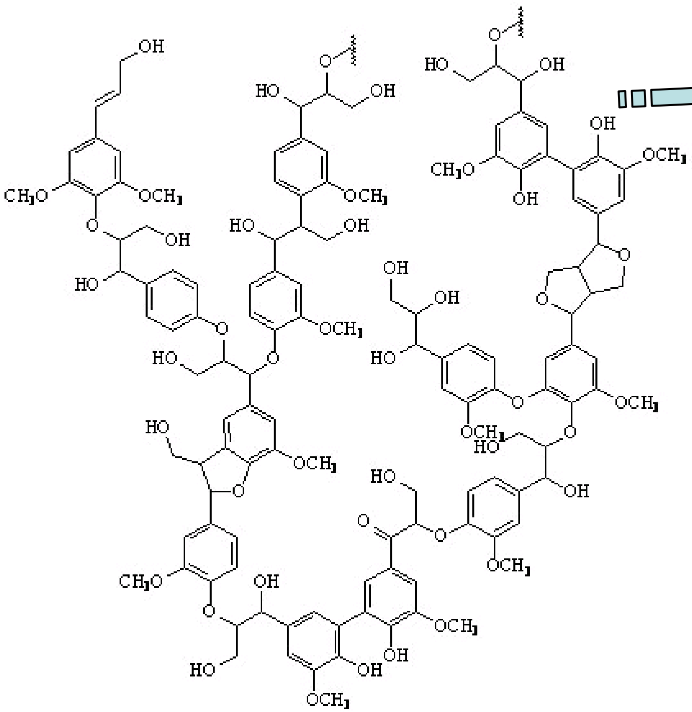
Mechanism



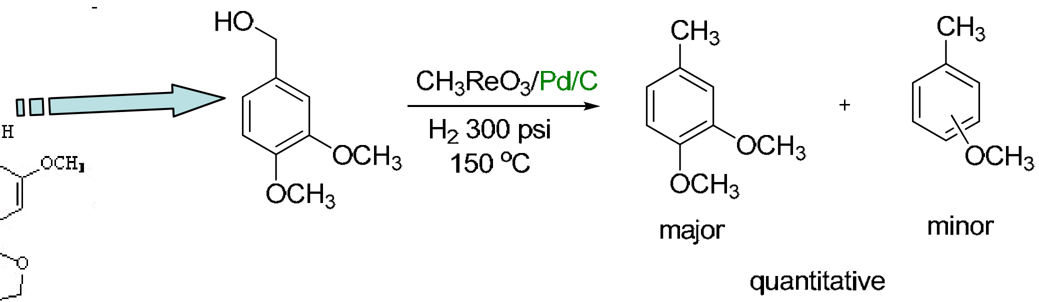


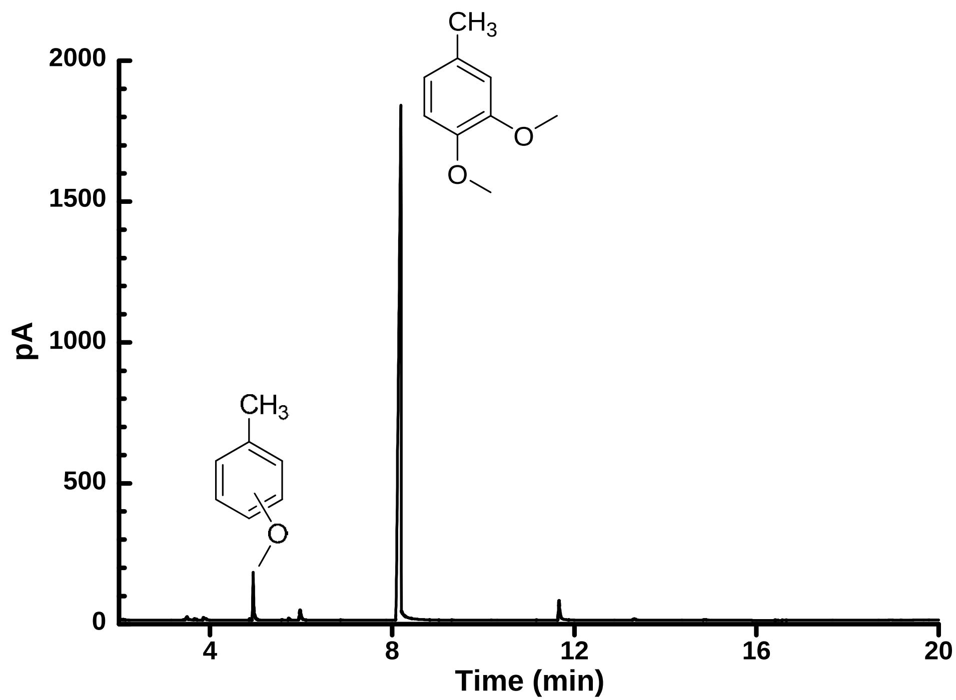
J. E. Ziegler, M. J. Zdilla, A. J. Evans, and M. M. Abu-Omar, "H_2-Driven Deoxygenation of Epoxides and Diols to Alkenes Catalyzed by Methyltrioxorhenium" *Inorg. Chem.* **2009**, *48*, Published on the Web October 6, 2009.

Partial deoxygenation of model compounds of lignin

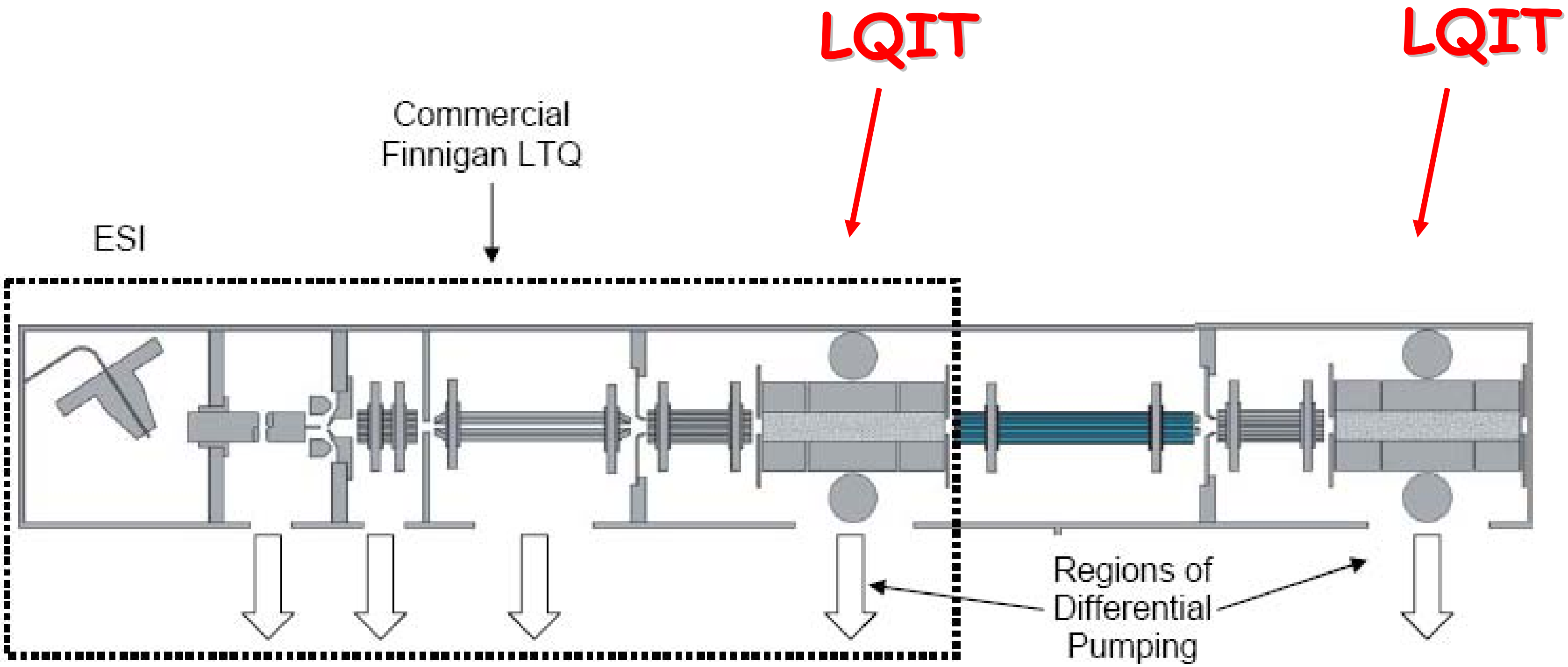


Lignin

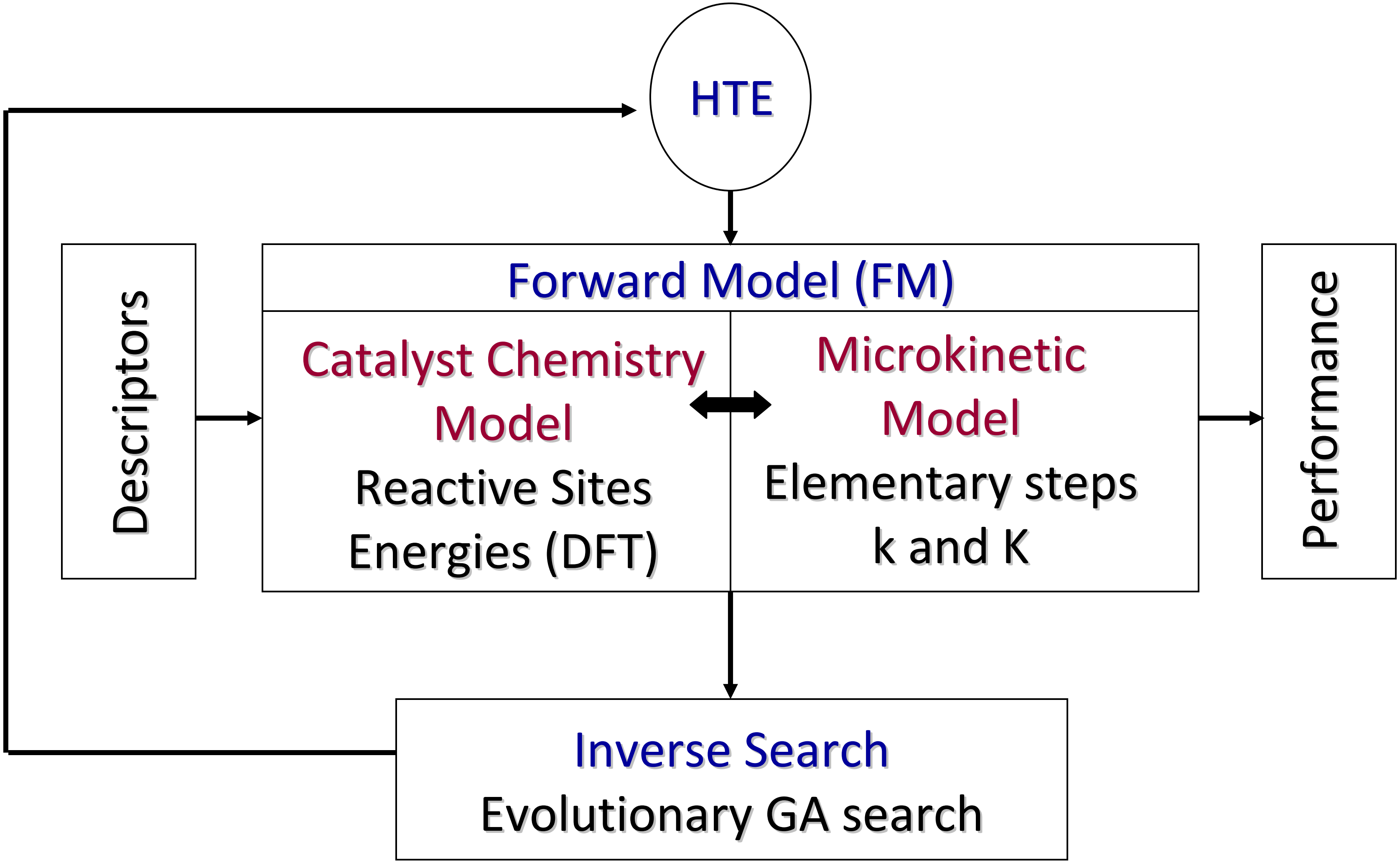




A new tandem-linear quadrupole ion trap (TWIN) to analyze highly complex mixtures of reaction products in MS^n experiments

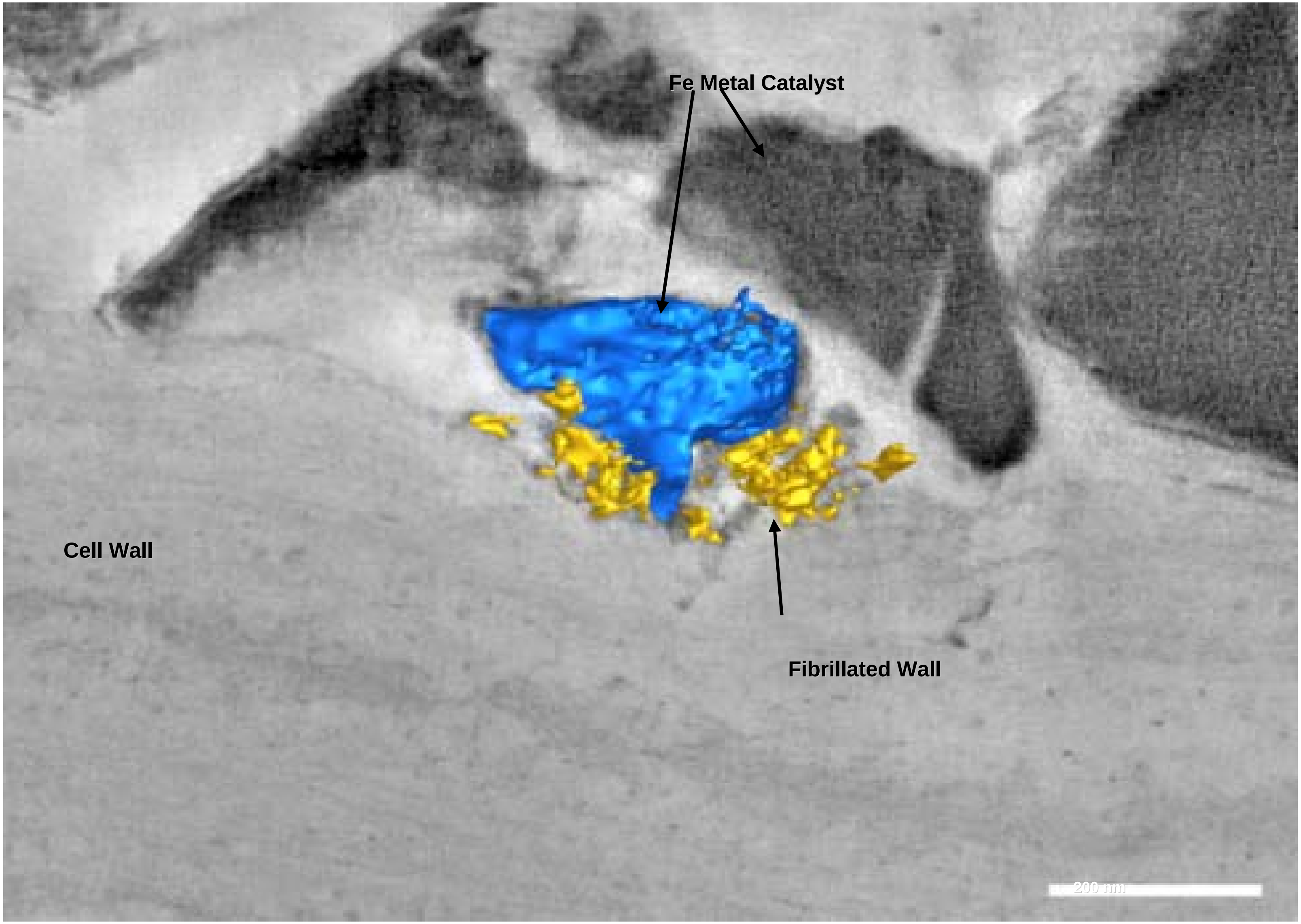


Computational modeling allows design of improved catalysts

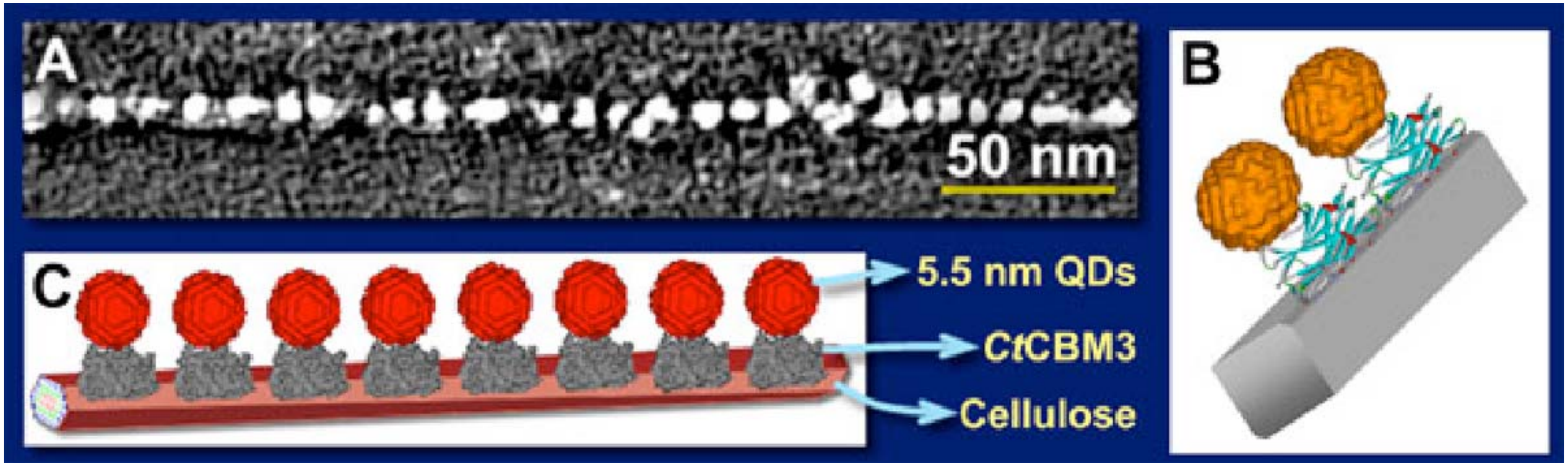


Iterative cycles lead to Convergence on an accurate FM

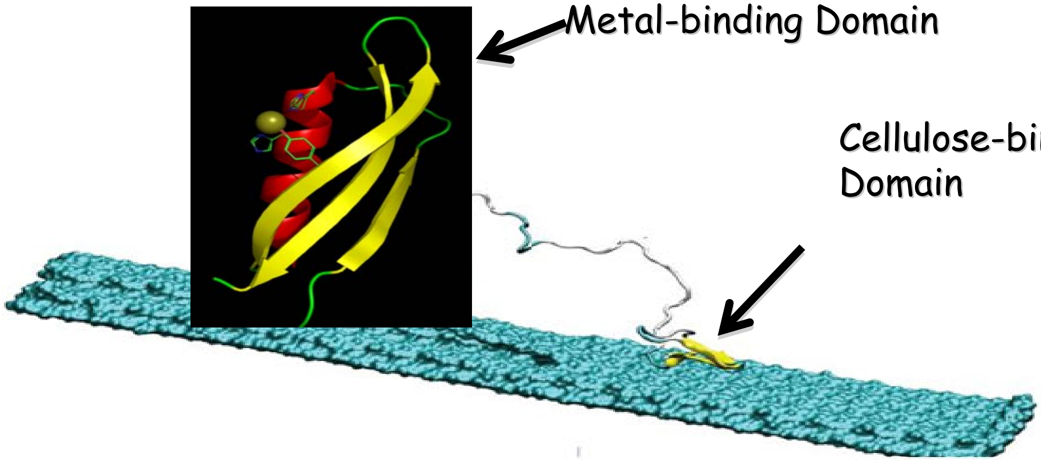
A metal catalyst contacts a very limited surface of cell wall. Can we deliver metal catalysts throughout the volume of the cell wall and target them to specific molecules?



Tailored biomass – introducing catalysts and catalytic sites as plants grow

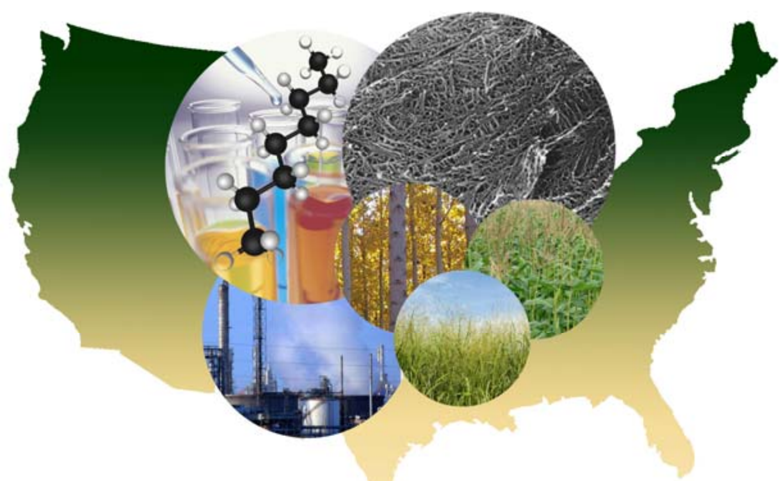


Quantum dots are specifically labeled on the planar face of crystaline cellulose directed by carbohydrate-binding module (CBM).



Long-term impacts of success

- *more than double* the carbon captured into fuel molecules compared to biological catalytic routes;
- *expand* the product range to alkanes and new energy-rich aromatic liquid fuels and other value-added molecules currently made through oxygenation of petrochemicals;
- *retain* the current liquid fuel infrastructure;
- *enable* the utilization of engineered energy crops;
- *minimize* the agricultural footprint through scalable and distributive hydrocarbon refineries that substitute for the present-day oil refinery.



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Argonne National Laboratory

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University of Tennessee

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