



# Overview of Catalytic Biomass Conversion Activities At PNNL For IIC Open House

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15 & 16 March 07

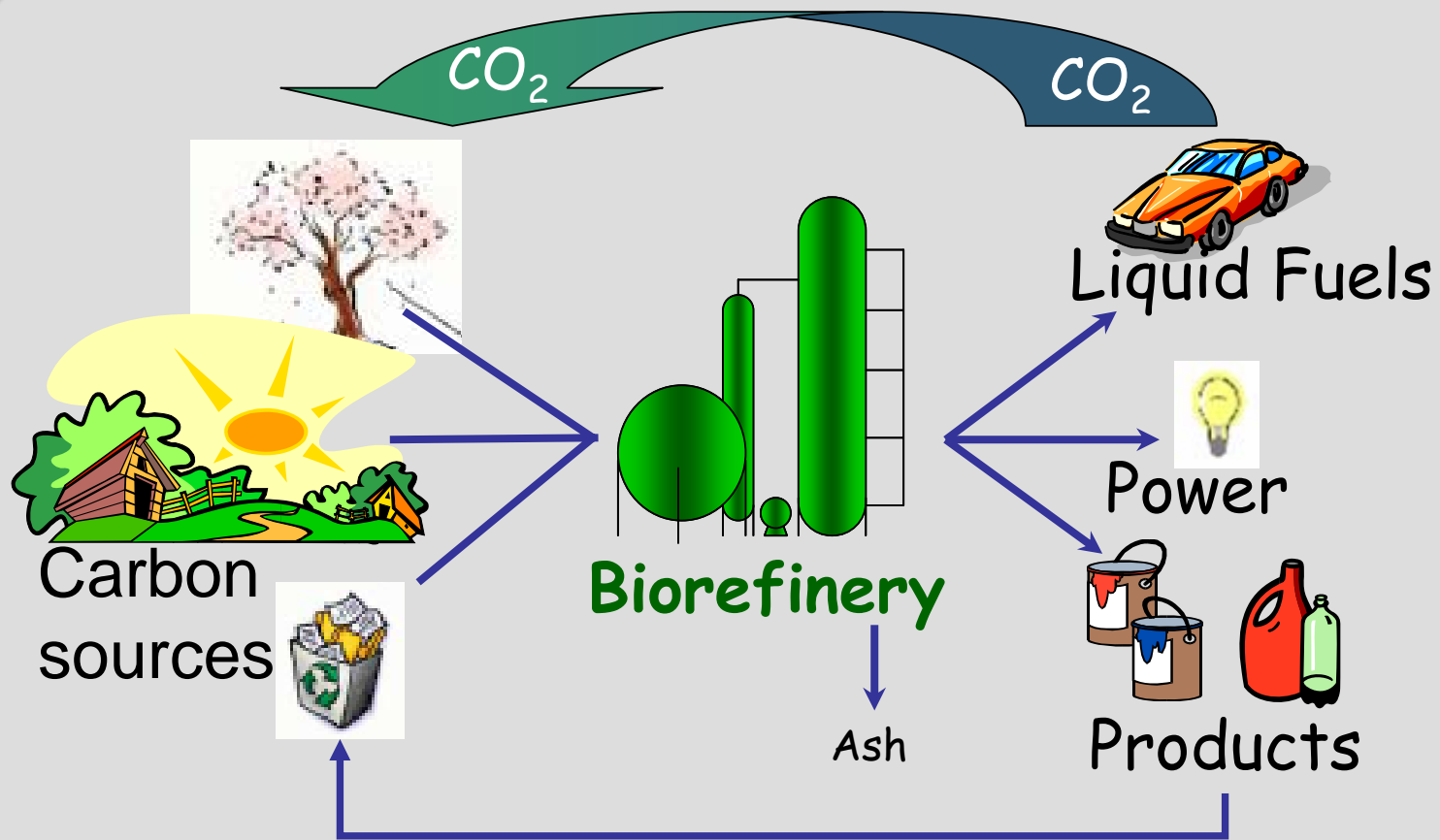


**Battelle**

Open House – March 15 & 16, 2007



**Pacific Northwest National Laboratory**  
U.S. Department of Energy 1

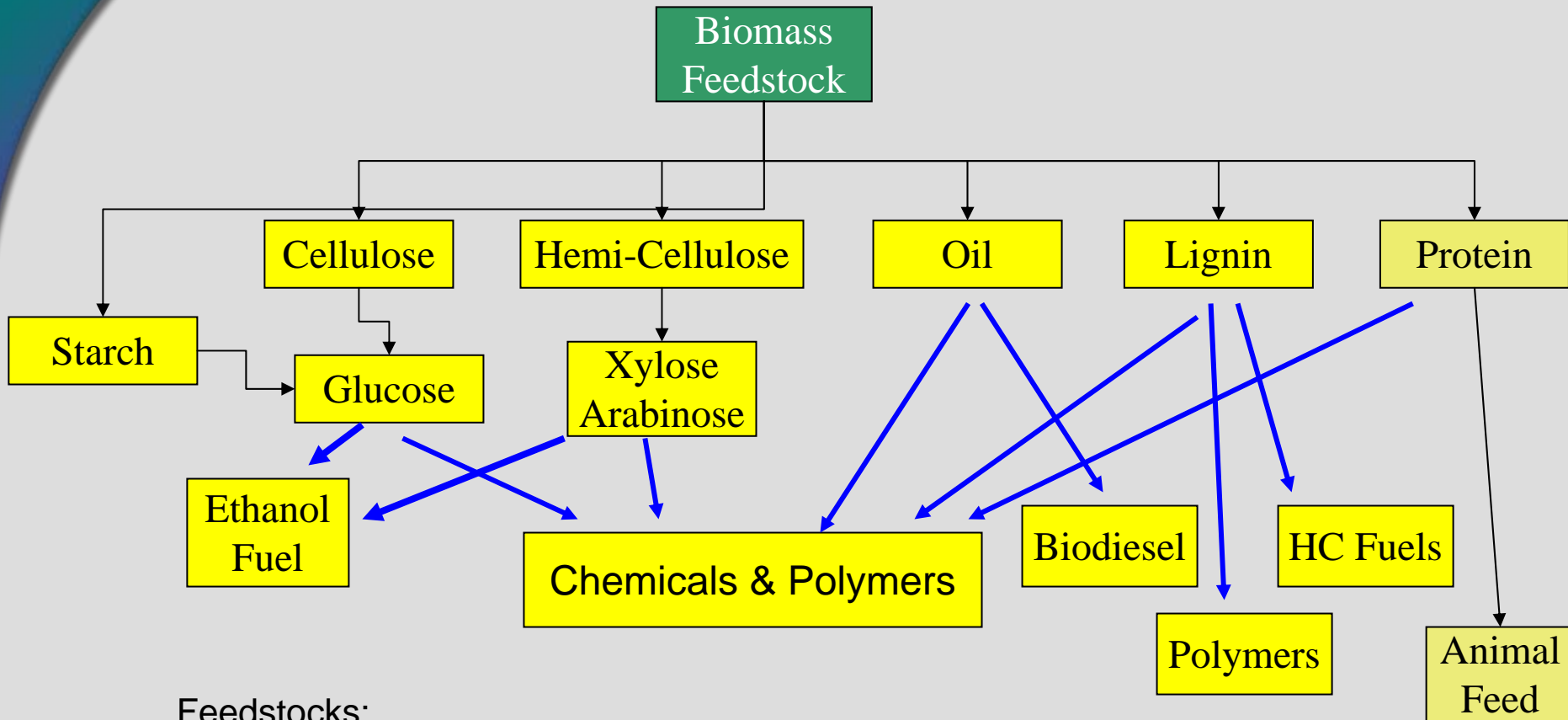


# CONCEPTUAL BIOREFINERY

# Program Strategy

- ▶ Analysis is used to **identify major cost barrier** areas in each element of the program
- ▶ Research is dedicated to **overcoming these barriers and reducing the cost** of each process as well as the final integrated biorefinery
- ▶ Program is driven by private - public partnerships to ensure integrity of the program
- ▶ Regular reviews are undertaken to ensure progress and fiduciary responsibility
- ▶ Program is based on both near term and long R&D objectives

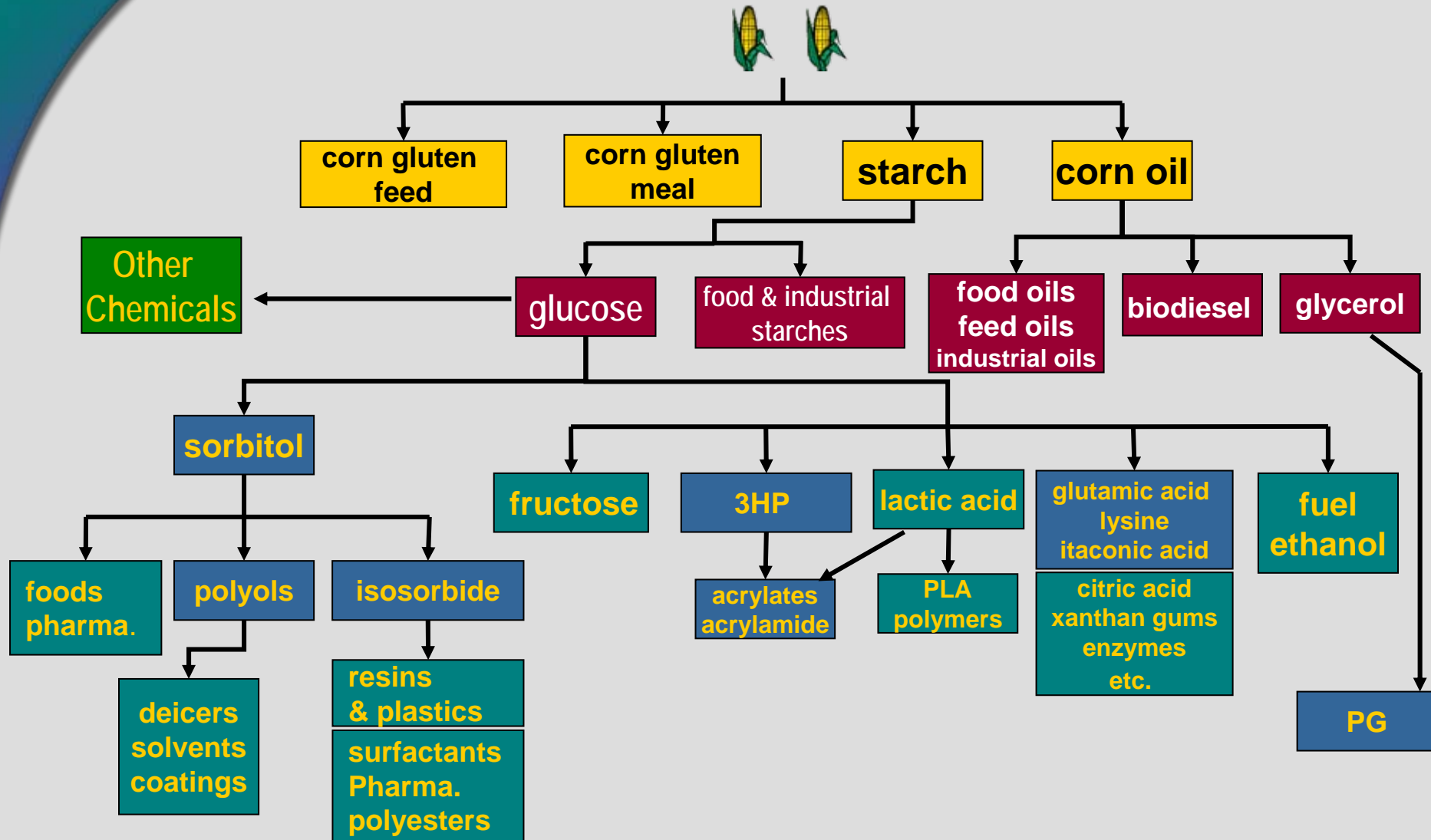
# Potential Feedstocks



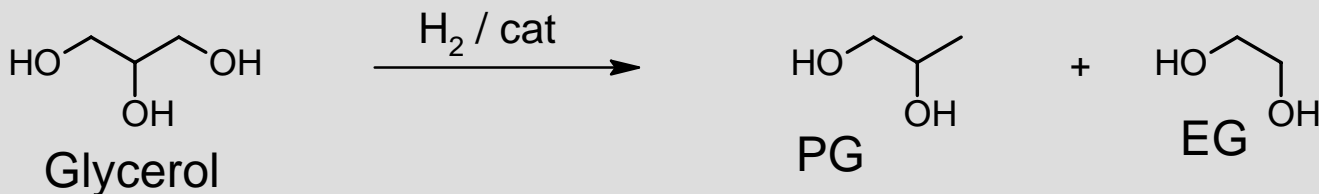
## Feedstocks:

- Rotational Crop Residues (stover, wheat straw, rice straw etc.)
- Forest Thinnings and Wastes
- Oil crops
- Traditional Rotational & New Crops
- Energy Crops (switch grass, poplar etc.)

# Example of a Bio-refinery: Corn Wet Mill



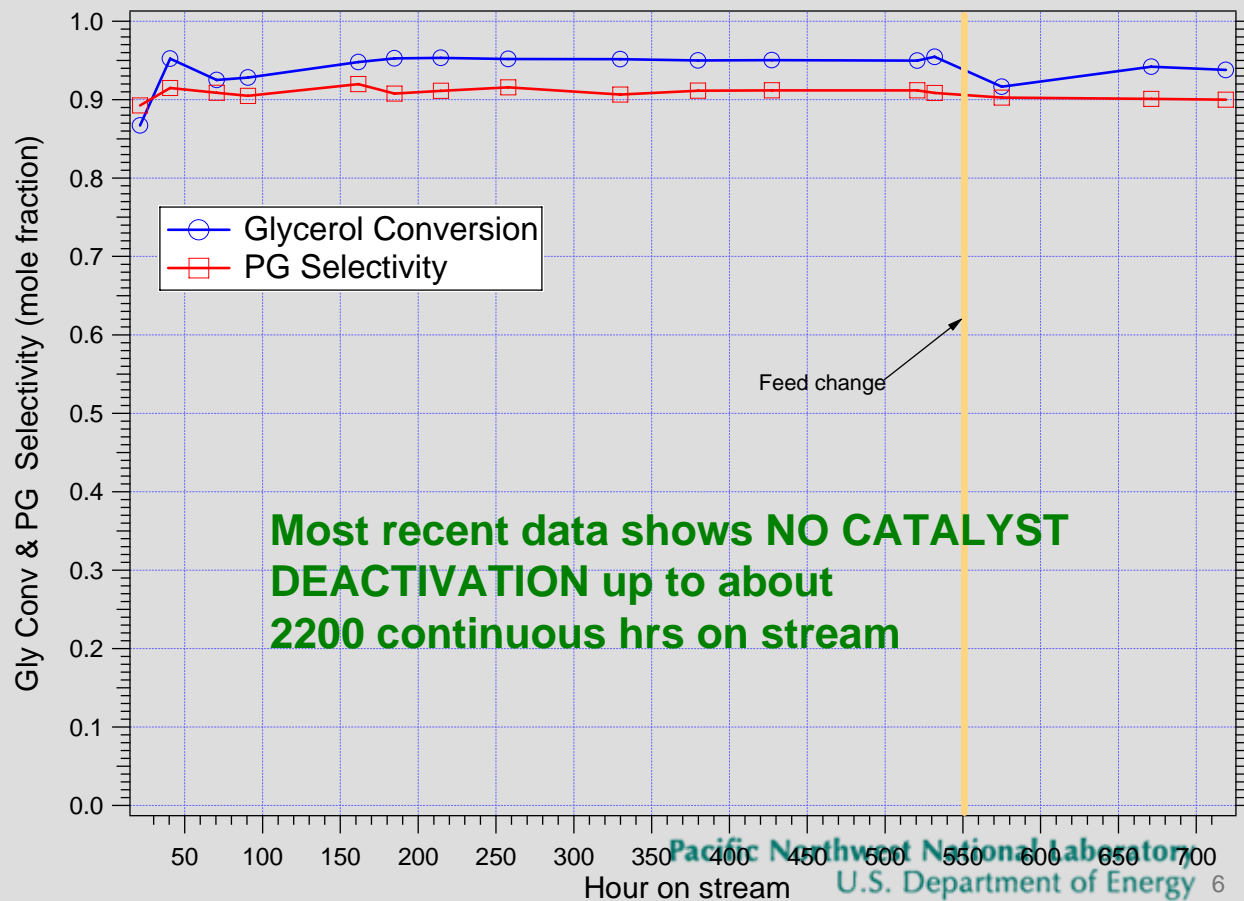
# Glycerol to PG chemistry—the bottom line



PG Market is 3.5 billion lbs globally

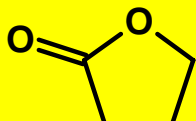
1 billion gallons of biodiesel affords about 700 million pounds of glycerol

PG Process requires catalysts with multiple functionality able to withstand rather severe hydrothermal conditions



# Succinic Acid - C4 Platform

Yield > 90%



**γ-Butyrolactone**

$C_4H_6O_2$  MW = 86.09

Yield > 90%



**1,4-Butanediol**

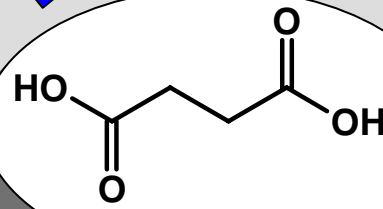
$C_4H_{10}O_2$  MW = 90.12

Yield > 90%



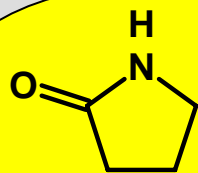
**Tetrahydrofuran**

$C_4H_8O$  MW = 72.11



**Succinic acid**

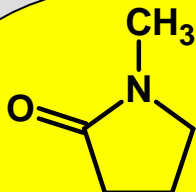
$C_4H_6O_4$  MW = 118.09



**2-Pyrrolidone**

$C_4H_7NO$  MW = 85.11

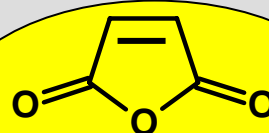
Yield >= 95%



**NMP**

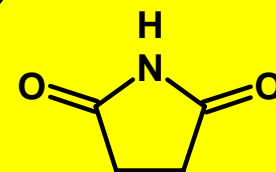
Yield > 95%

$C_5H_9NO$  MW = 99.13

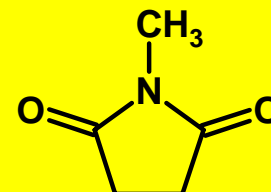


**Maleic Anhydride**

Yield ca. 80%



**Succinimide**

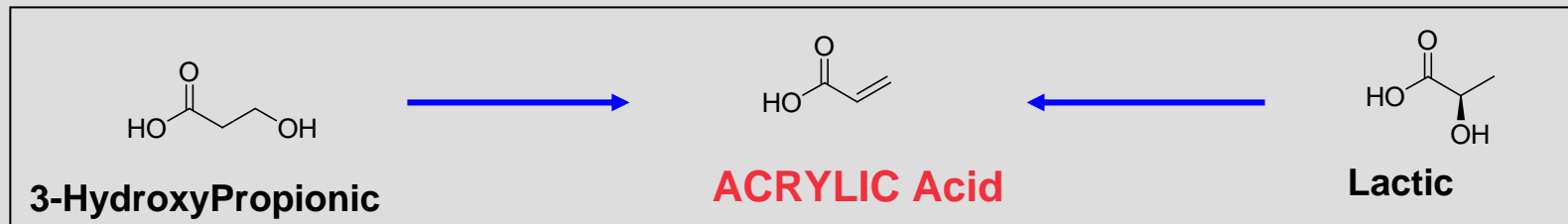


**N-methyl succinimide**

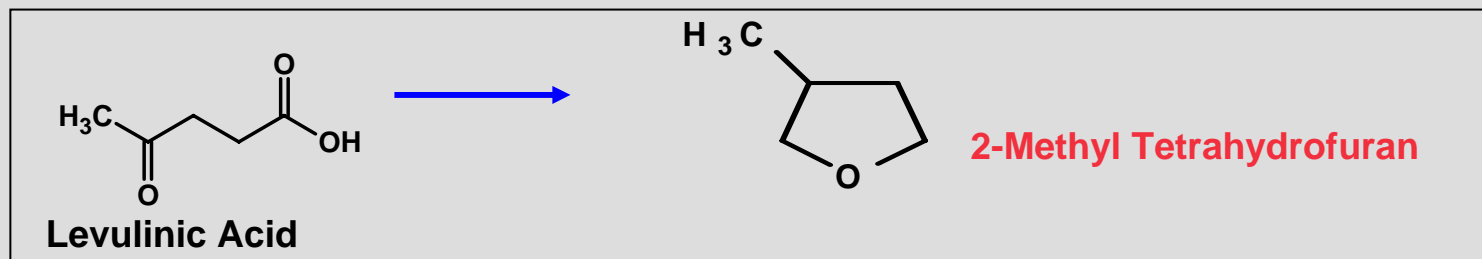
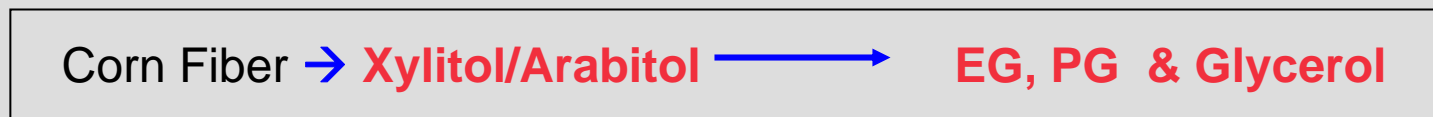
Yields ca 98%

# OTHER CATALYTIC PROJECTS by CARBON #

## C-3



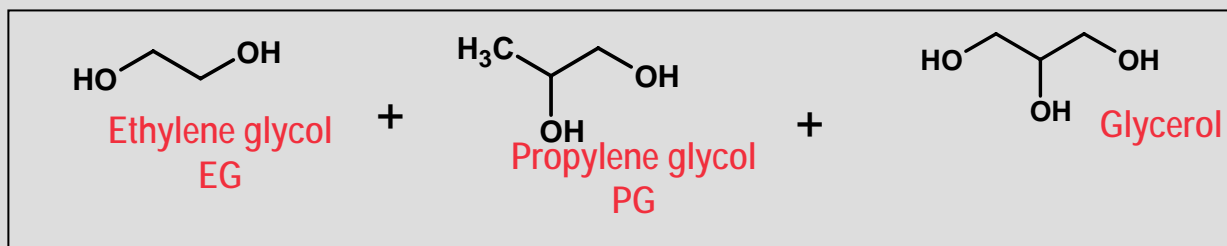
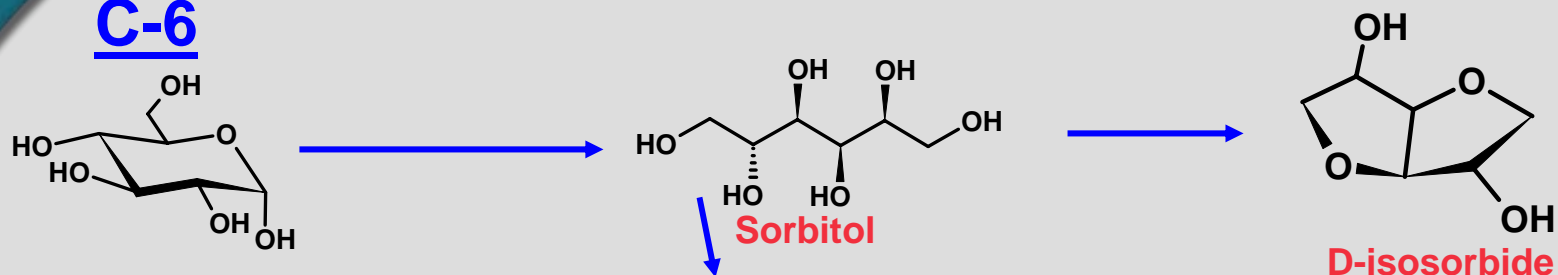
## C-5



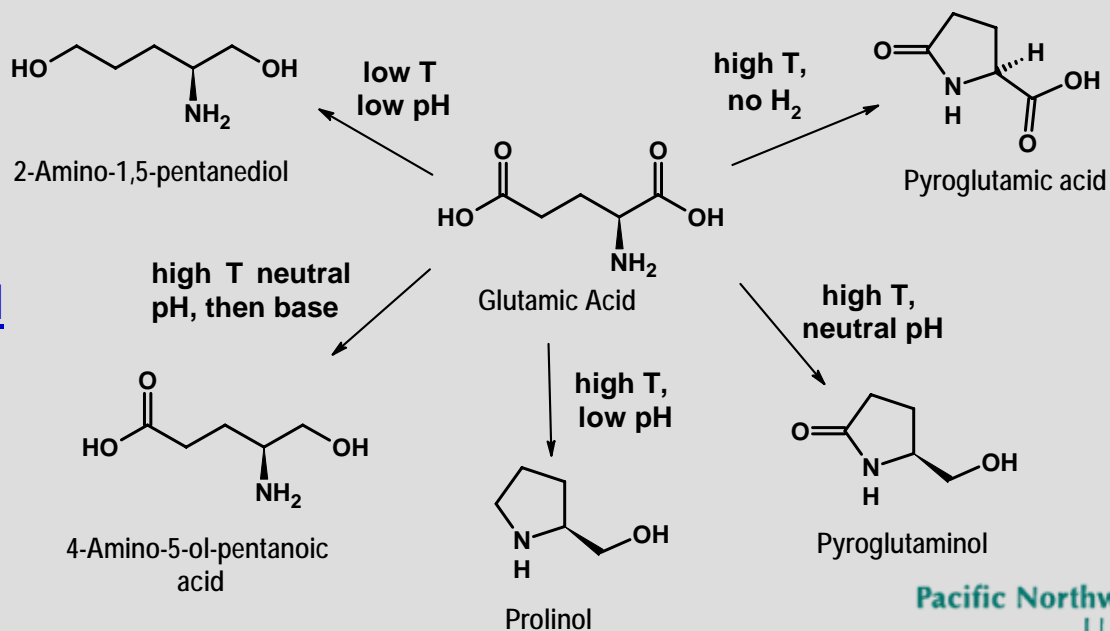


# OTHER CATALYTIC PROJECTS by CARBON #

## C-6



## C-5 AMINO ACID CONVERSION



# Integrated Ethanol, Pyrolysis and Mixed Alcohols

Stover, Forest  
Materials,  
Switchgrass

Ethanol via  
bioconversion

**PNNL has or had catalyst projects  
Inside the red circles**

Residues

Pyrolysis

Pyrolytic  
lignin

Stabilization  
&  
Hydrotreating/  
hydrocracking

“Green” Gasoline

“Green” Diesel

Water soluble  
pyrolysis oil

Reforming

Syngas

F-T  
Synthesis

Hydrocarbon  
Fuels

Alcohol  
Synthesis

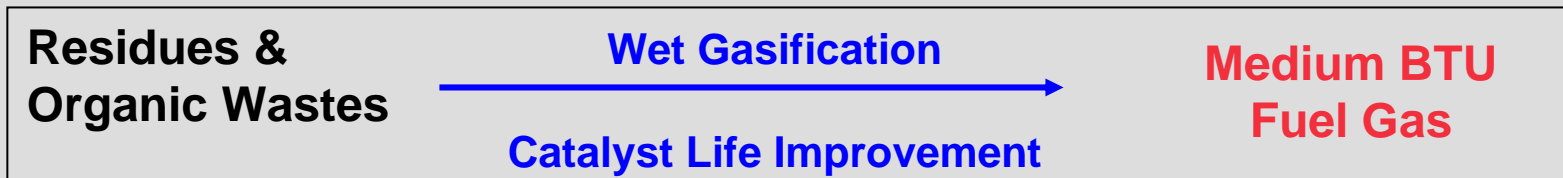
Ethanol

Methanol  
n-Propanol  
n-Butanol  
n-Pentanol

**Catalytic Conversions  
Of Bio-Oil to Fuels &  
Chemicals, F-T &  
Alcohols synthesis**

# OTHER CATALYTIC PROJECTS by CARBON #

## C-X



**Aqueous wastes clean-up yields fuel gas & clean water**



**Low Cost carbon fiber for better fuel mileage via cars lightweighting**

# Combinatorial Catalysis

Not a just better shotgun, but a very sophisticated discovery tool.

- ▶ High speed screening/optimization process
  - tens or hundreds of experiments in parallel
  - time is drastically reduced
- ▶ In catalysis research...
  - the number of possible combinations is virtually infinite
  - It is not possible to try all of them
- ▶ In performing numerous experiments, the need remains for
  - intelligent design of experiments
  - Informatic tools for analyzing experiments

# Integration of Combinatorial Discovery Experimental Rational

## Discovery\*

**Combinatorial  
Laboratory**



## Verification

**Batch  
Reactor**



## Scale Up

**Continuous  
Reactor**

\*System provided by Symyx®  
With PNNL Design Input

# PNNL Offers Unique Capabilities

## ► Condensed phase catalysis

- Reaction pathway selection – hydrogenation, hydrogenolysis, dehydration, oxidation
- Catalyst synthesis & characterization
- Process definition – continuous vs. batch, high conversion efficiency, high product selectivity

## ► Bio-Process development

- “Discovery” – screening, gene selection, etc.
- Molecular biology applied to fermentation process development
- Bio-process laboratory with protein/DNA analytical and purification systems
- Production of unique enzymes as biocatalysts

## ► Complete process and product characterization

# Novel Bio-Processes: Developing & Exploiting New Organisms

- ▶ Battelle's objective is to exploit fungi to create new biological processes that:
  - Support production of new products
  - Utilize single, highly-effective production host to selectively produce multiple end products
  - Offer reduced costs by
    - operating at very low pH
    - using lower-cost media
    - achieving very high yield and fermentation rates
- ▶ Battelle research focuses on two primary tasks
  - Reducing the time and cost to control and manipulate a new organism
  - Reduce the time and cost of defining a new process