

2019 AIChE Annual Meeting
Orlando, FL

**Superior performance biodiesel
from biomass hydrolysate fusel
alcohols and bio-oils: fatty acid
fusel esters (FAFE) and combustion
behaviour**



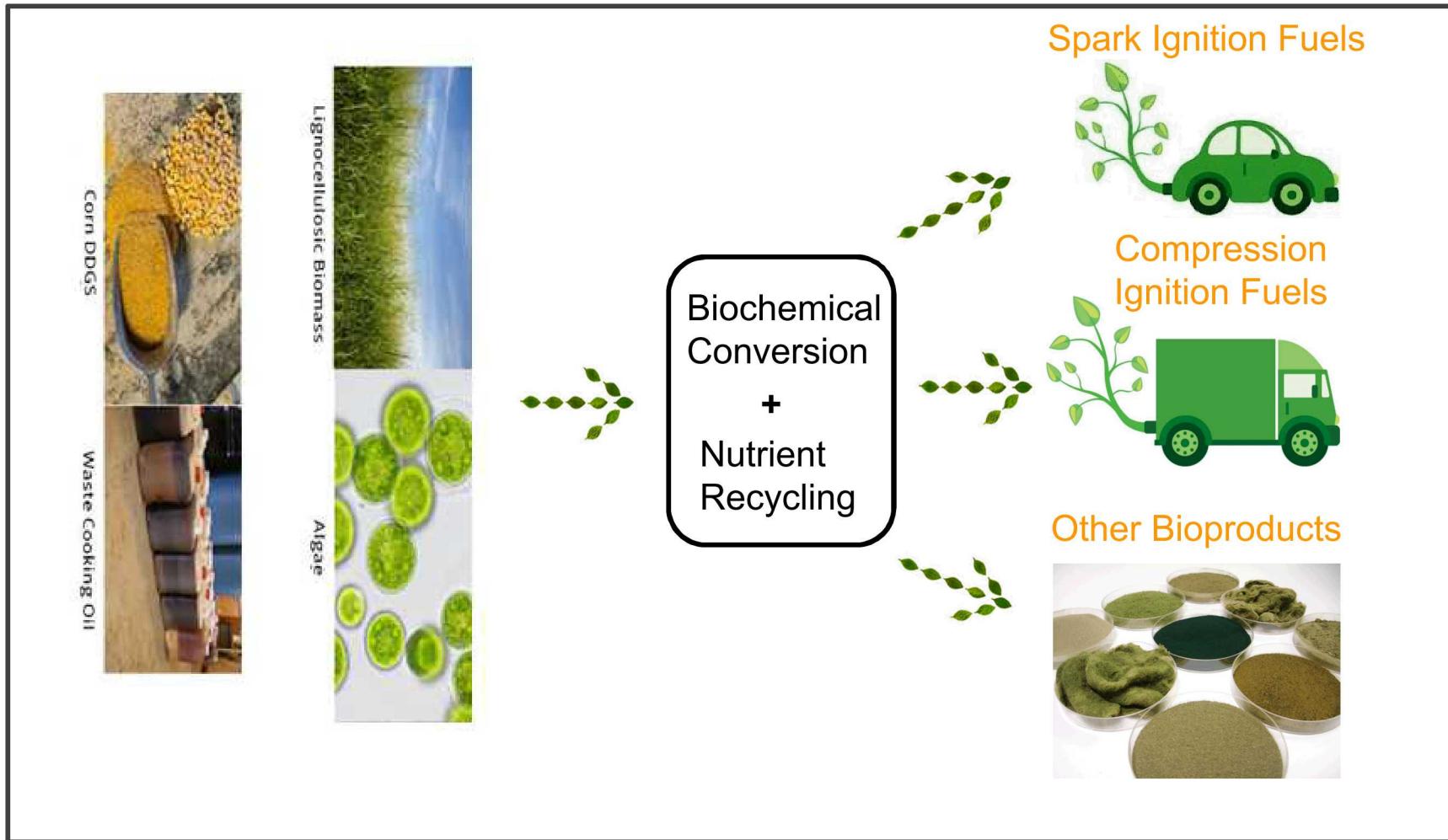
**Sandia National
Laboratories**

Somnath Shinde

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Sandia's perspective on biofuel production



Sandia's perspective on biofuel production

Biomass Production



What can we grow?

Conversion to Fuel Products



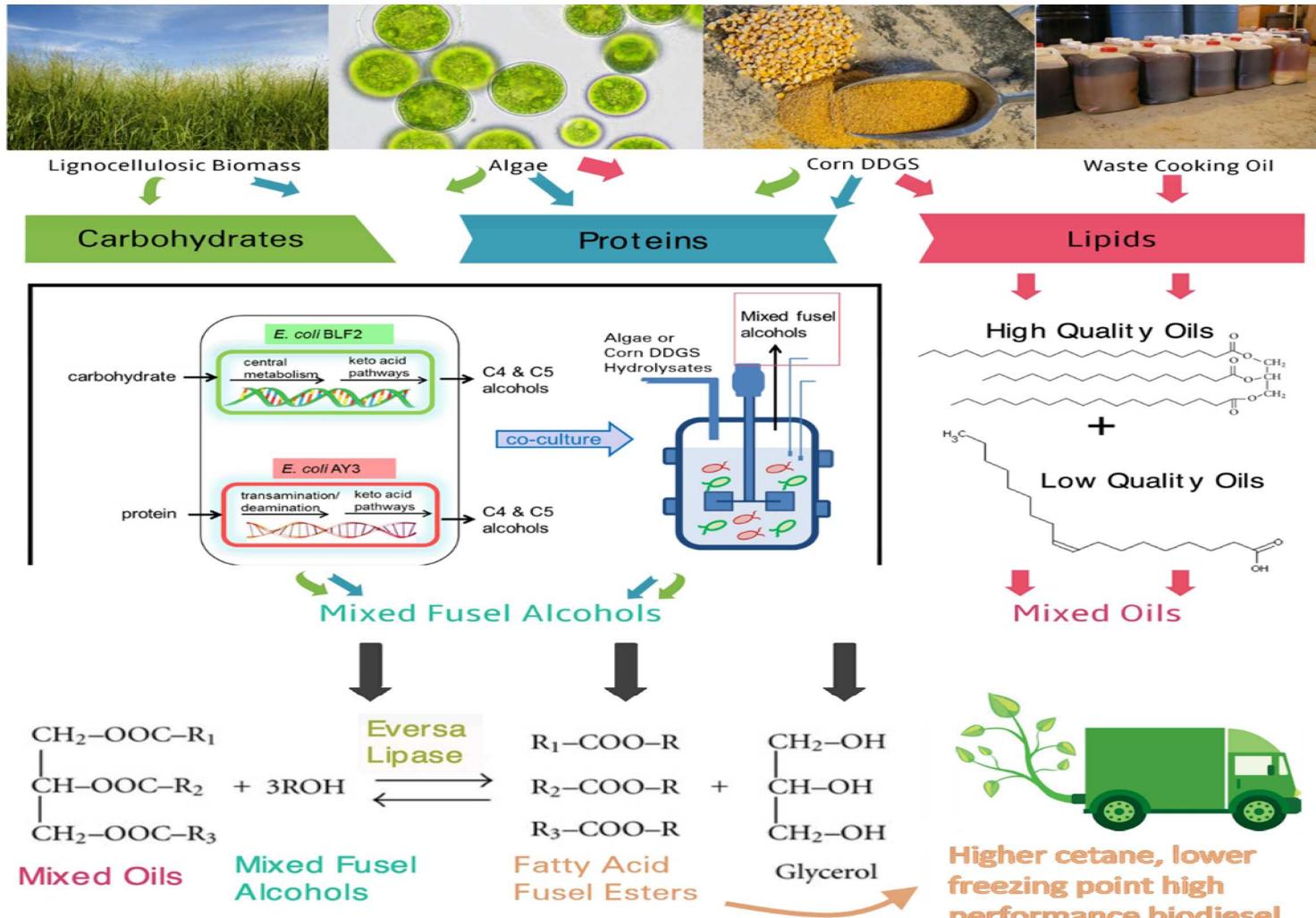
High performance fuel products can strengthen the value proposition of biofuels

Co-optimization of Fuels and Engines

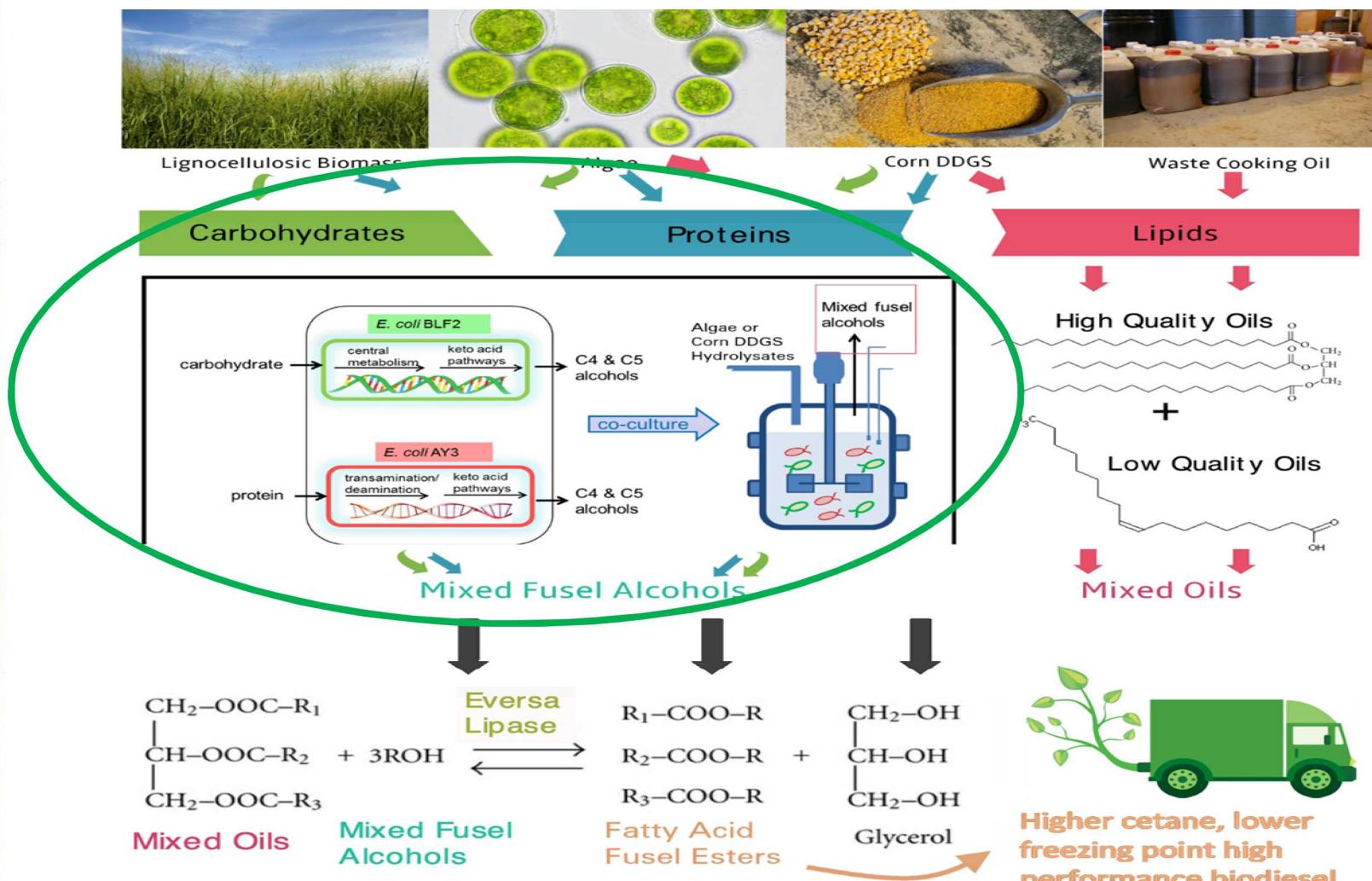


What is the best fuel?

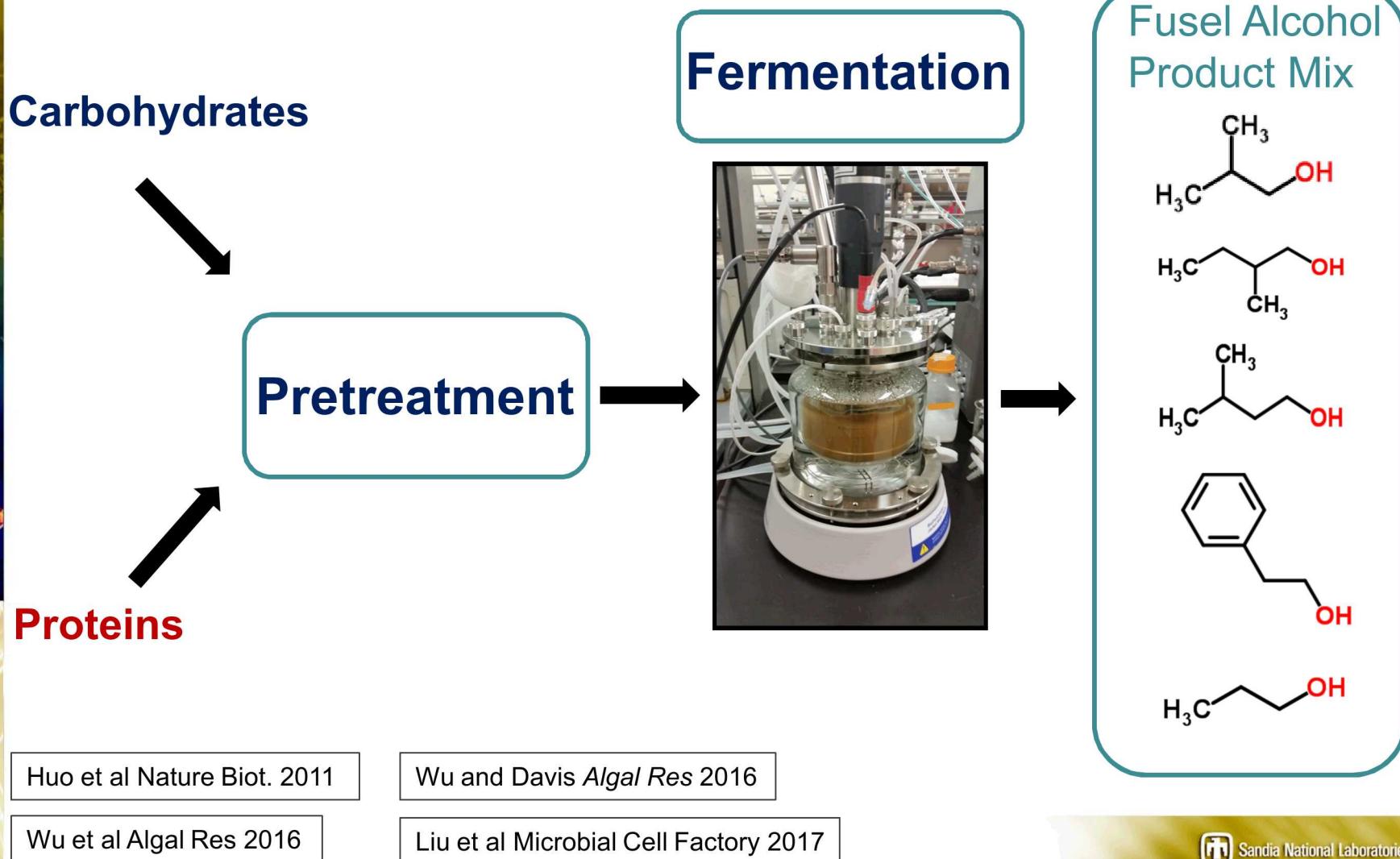
Our goal: a robust, feedstock agnostic bioconversion process to utilize this biomass



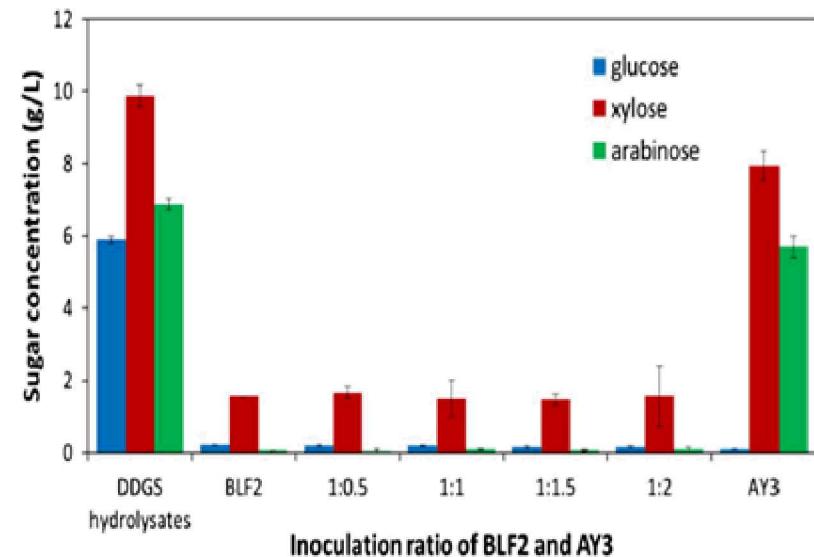
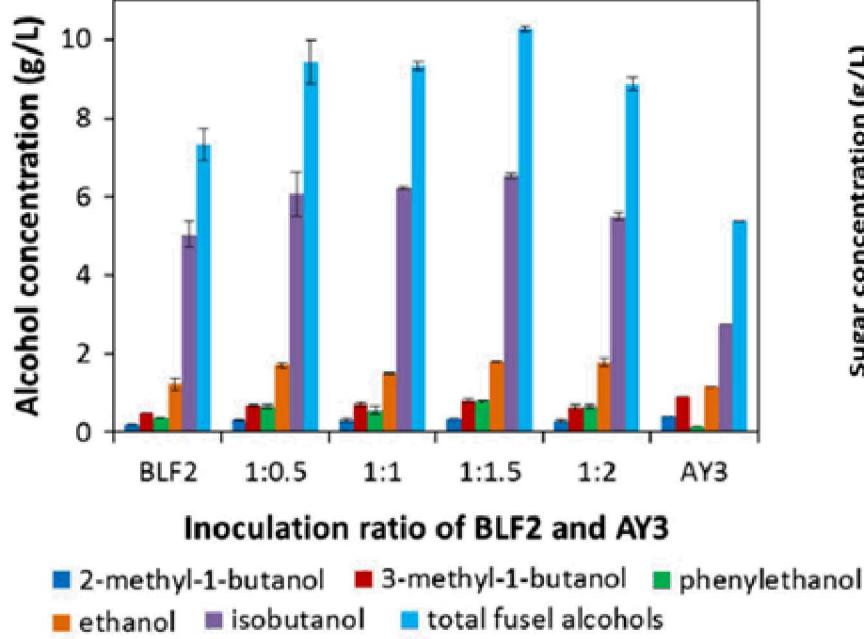
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Development of *E. coli* strains for protein conversion and carbohydrate conversion to fusel alcohols in co-culture system

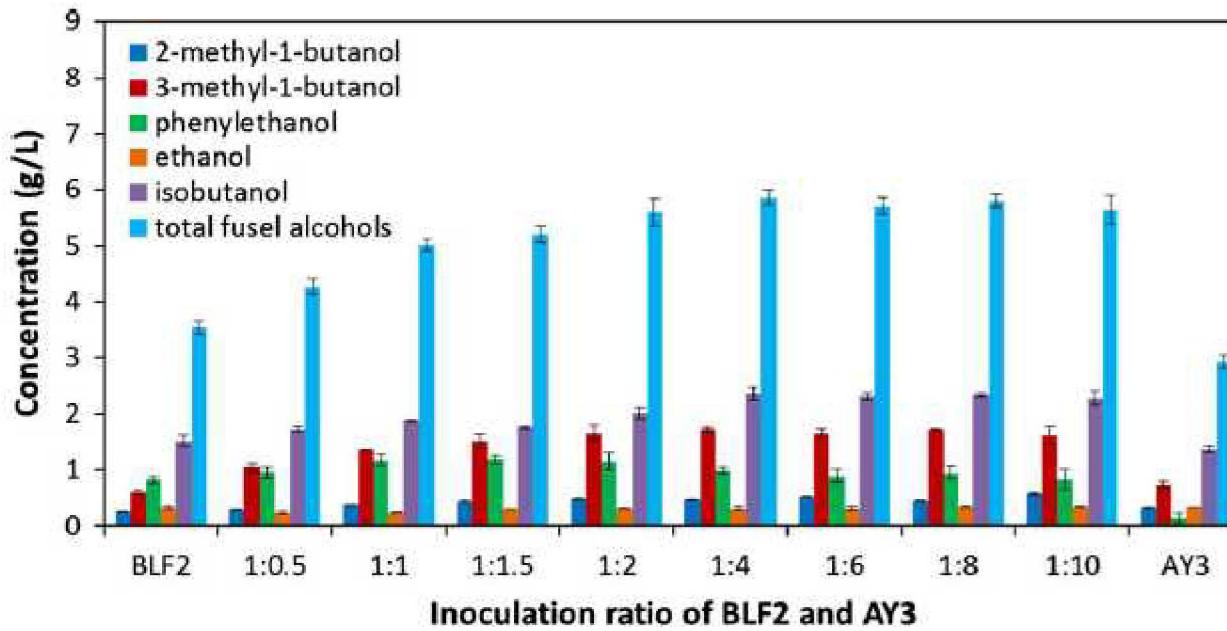


Fusel alcohols production from DDGS



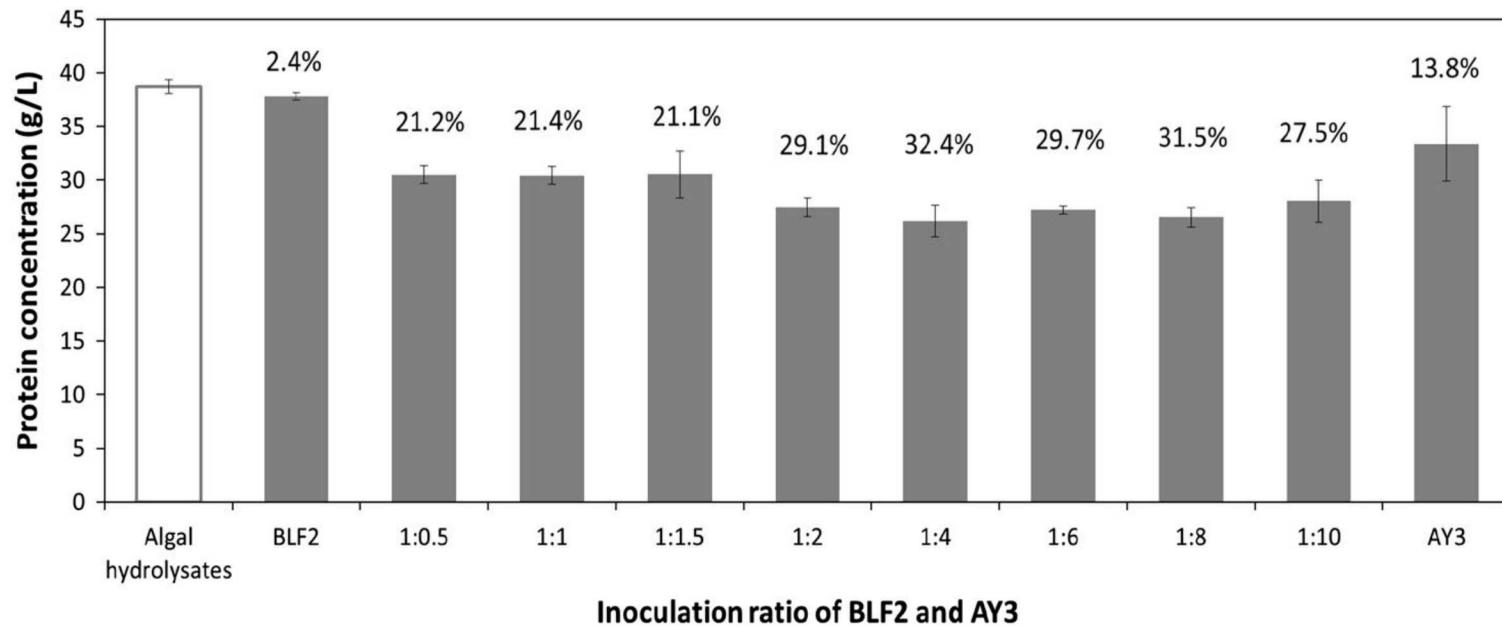
- The co-culture with an inoculation ratio of 1:1.5 of *E. coli* BLF2 and AY3 achieved the highest total fuel titer of up to 10.3 g/L from DGS hydrolysates.

Fusel alcohols production from *Nannochloropsis sp.* algae hydrolysates



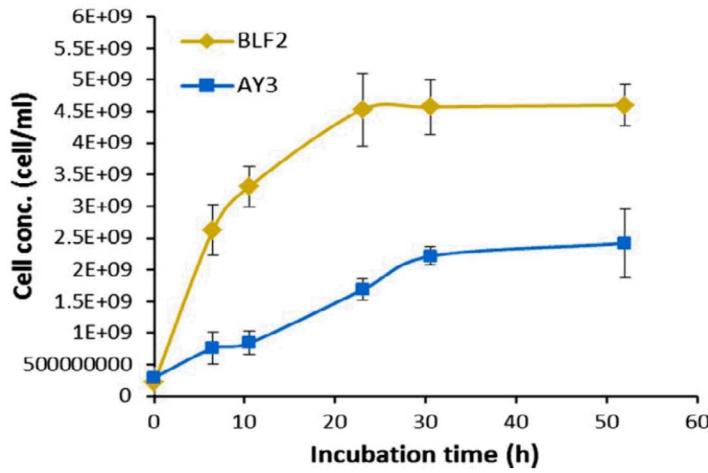
- The composition of the fusel alcohols products from algae hydrolysates included isobutanol (40.3% (w/w)) and mixed isopentanols (2-methyl-1-butanol and 3-methyl-1-butanol (37.3% (w/w)), indicating significant enrichment of the C5 alcohols compared to the product spectrum produced from DGS, where isobutanol was the major product (63.1% (w/w))

Fusel alcohols production from *Nannochloropsis sp.* algae hydrolysates

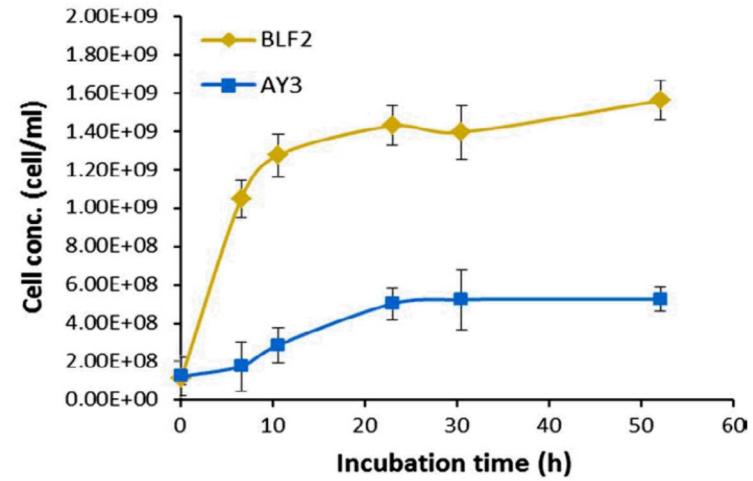


- Up to 32.4% of the initial 38.7 g/L proteins in the algae hydrolysates were converted by the co-culture with an inoculation ratio of 1:4

Growth dynamics of individual populations in the co-culture



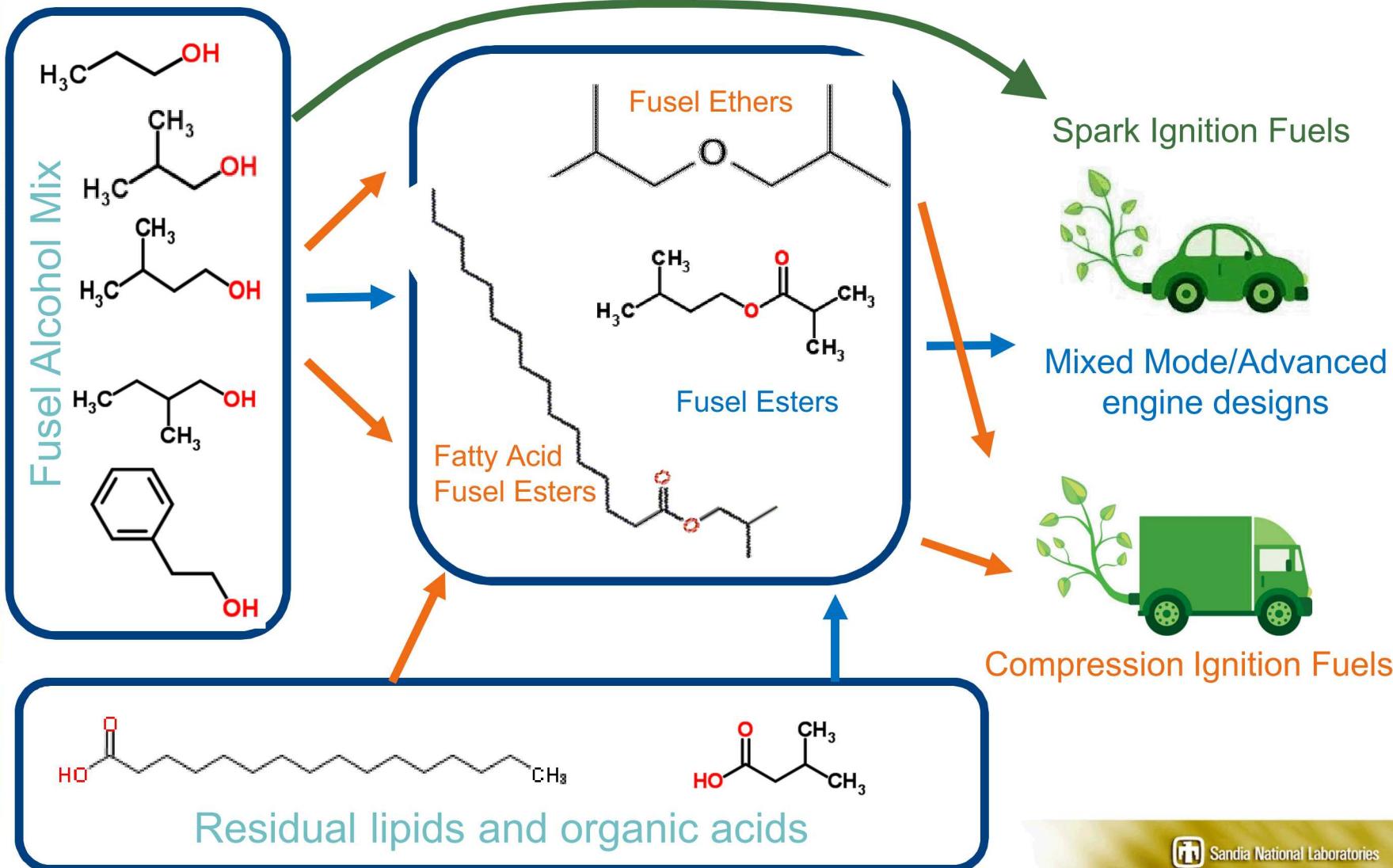
DGS hydrolysate with a BLF2/AY3 inoculation ratio of 1:1.5



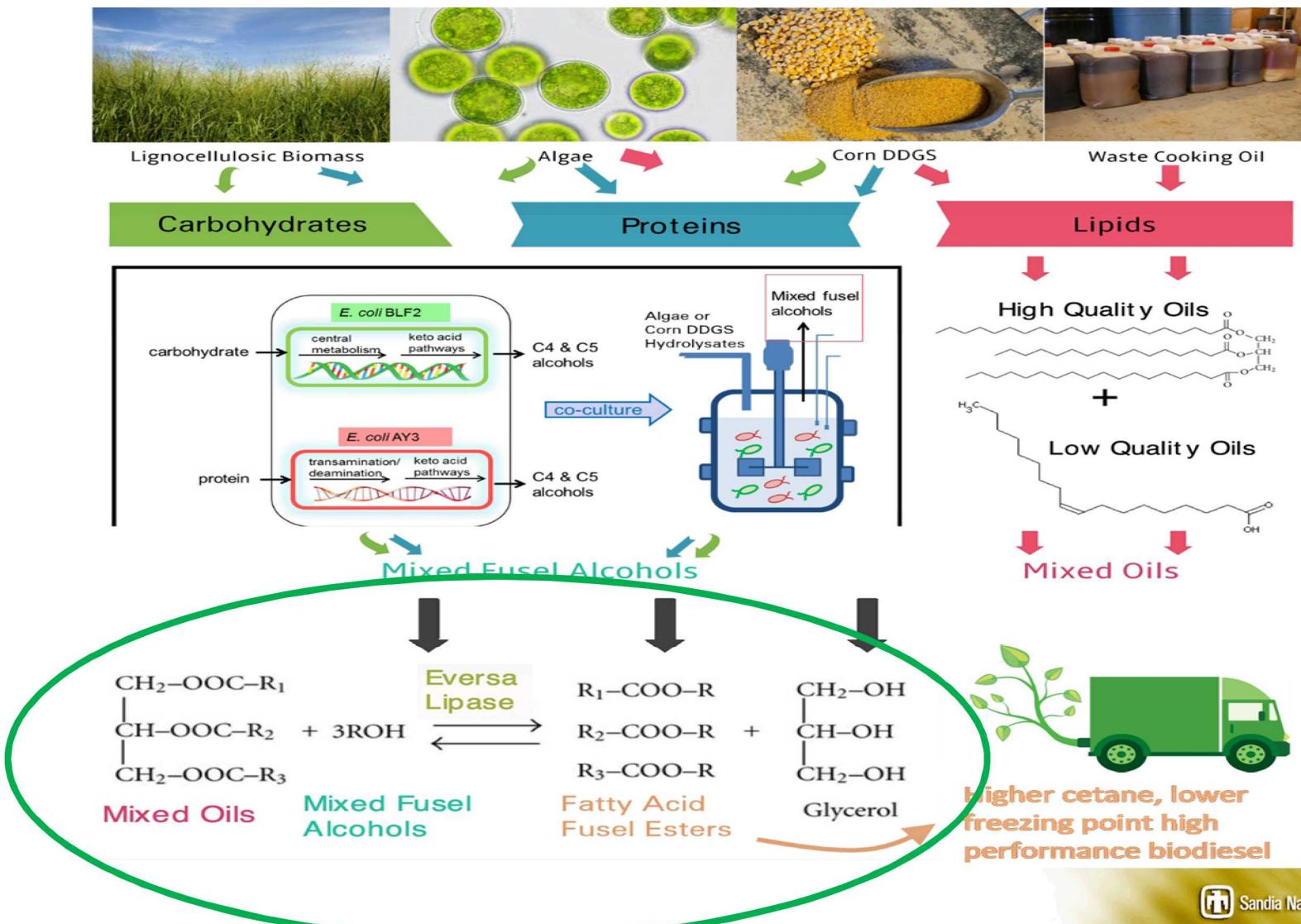
Algae hydrolysate with a BLF2/AY3 inoculation ratio of 1:4

- In both of the hydrolysates, the cell number of the two strains continuously increased until reaching plateau, which indicated that despite the growth rate difference between the two strains, the co-culturing didn't adversely affect the growth of each strain.
- The final cell numbers of AY3 in the co-cultures at proper inoculation ratios of BLF2/AY3 were no less than the cell number of AY3 monoculture in the hydrolysates.

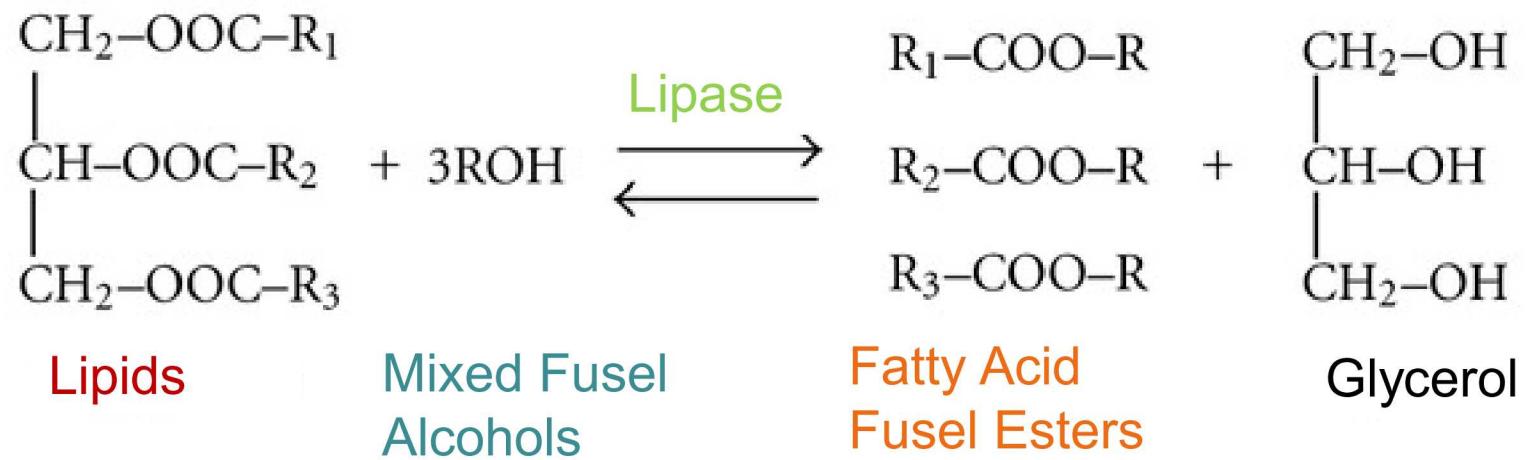
Fusel Alcohols as a platform for a diverse suite of high performance fuels



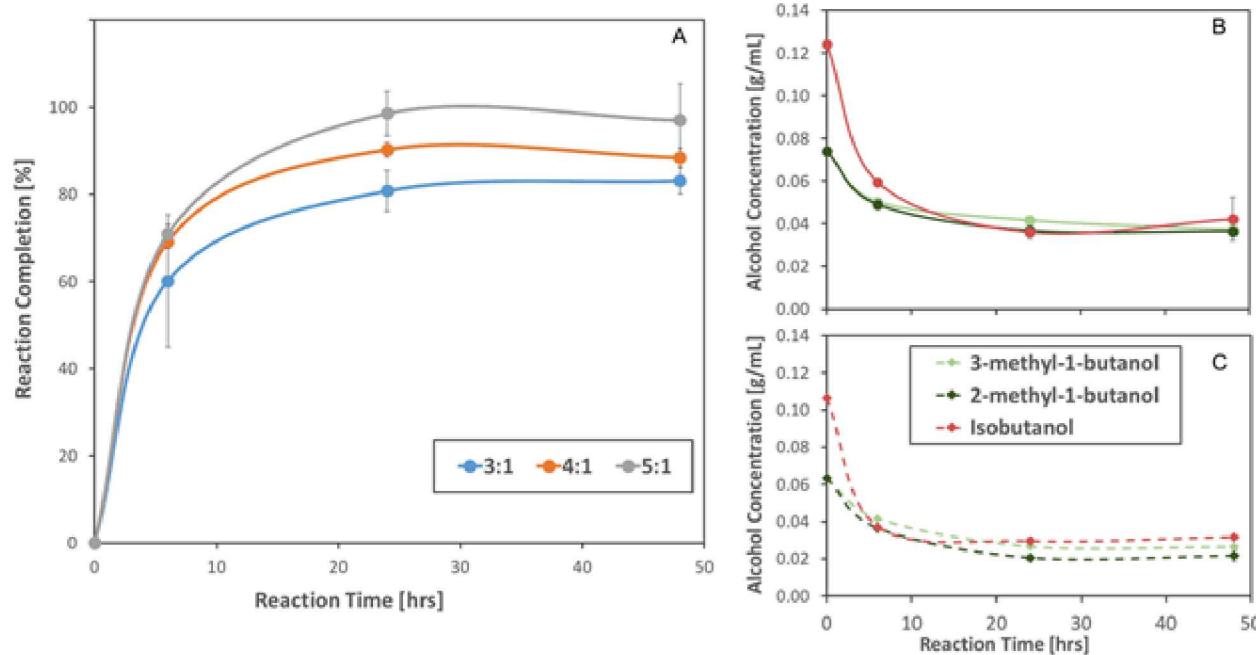
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Fusel alcohols upgrading to Fatty Acid Fusel Esters



Fatty Acid Fusel Esters



- >97% Yield after 24 hrs using 5:1 molar ratio of alcohol:oil and fusel alcohol mixture.

Understanding what makes a biofuel good

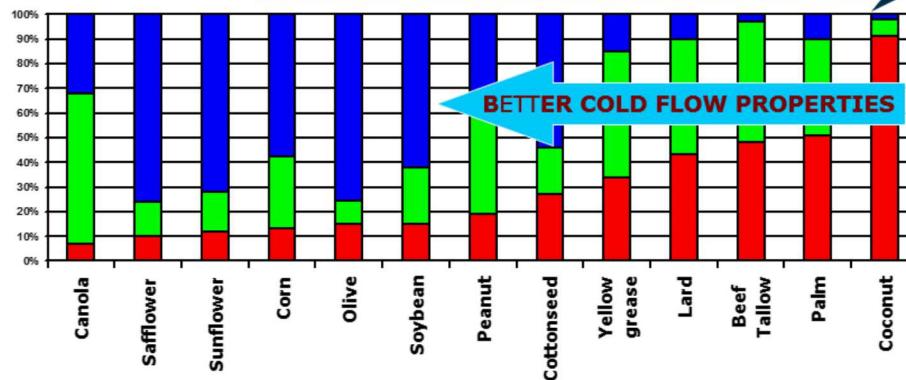
Evaluating a fuel is about more than just combustion

Compression
Ignition Fuels



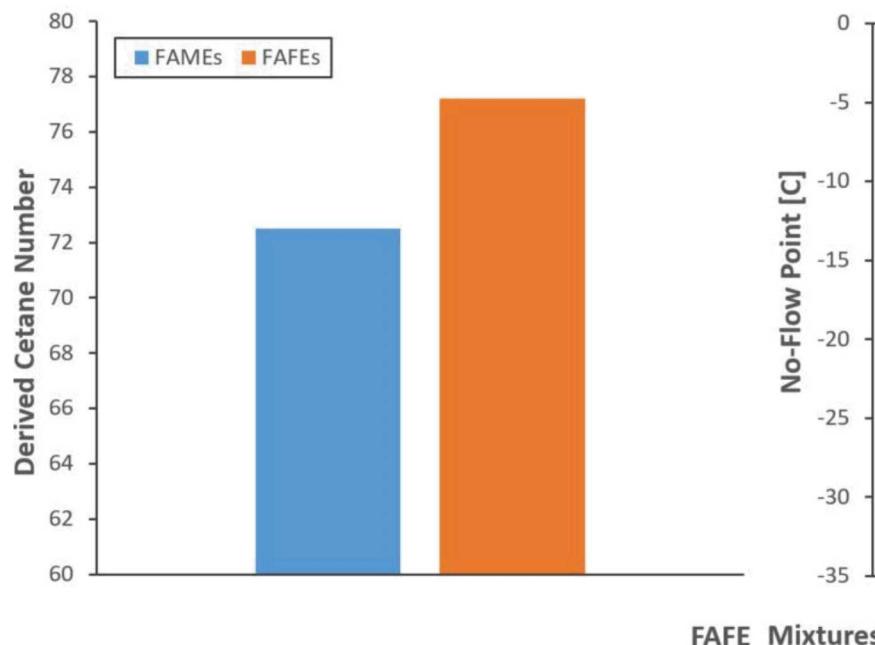
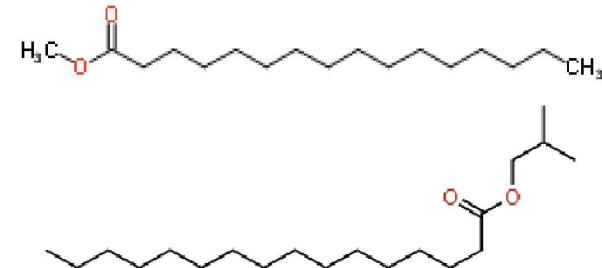
Criteria	Greatly Exceeds	Exceeds Criteria	Meets Criteria	Barriers Exist
Cetane	>50	46 to 50	40 to 45	<40
LHV (MJ/Kg)	>40	31 to 40	25 to 30	<25
Flash Point (°C)	>70	61 to 70	52 to 50	<52
Melting Point (°C)	<-50	-50 to -26	-25 to 0	>0
Water Solubility (mg/L)	<5	5 to 501	500 to 1000	>1000
YSI	<50	50 to 151	150 to 200	>200

INCREASING CETANE NUMBER (CN) AND STABILITY

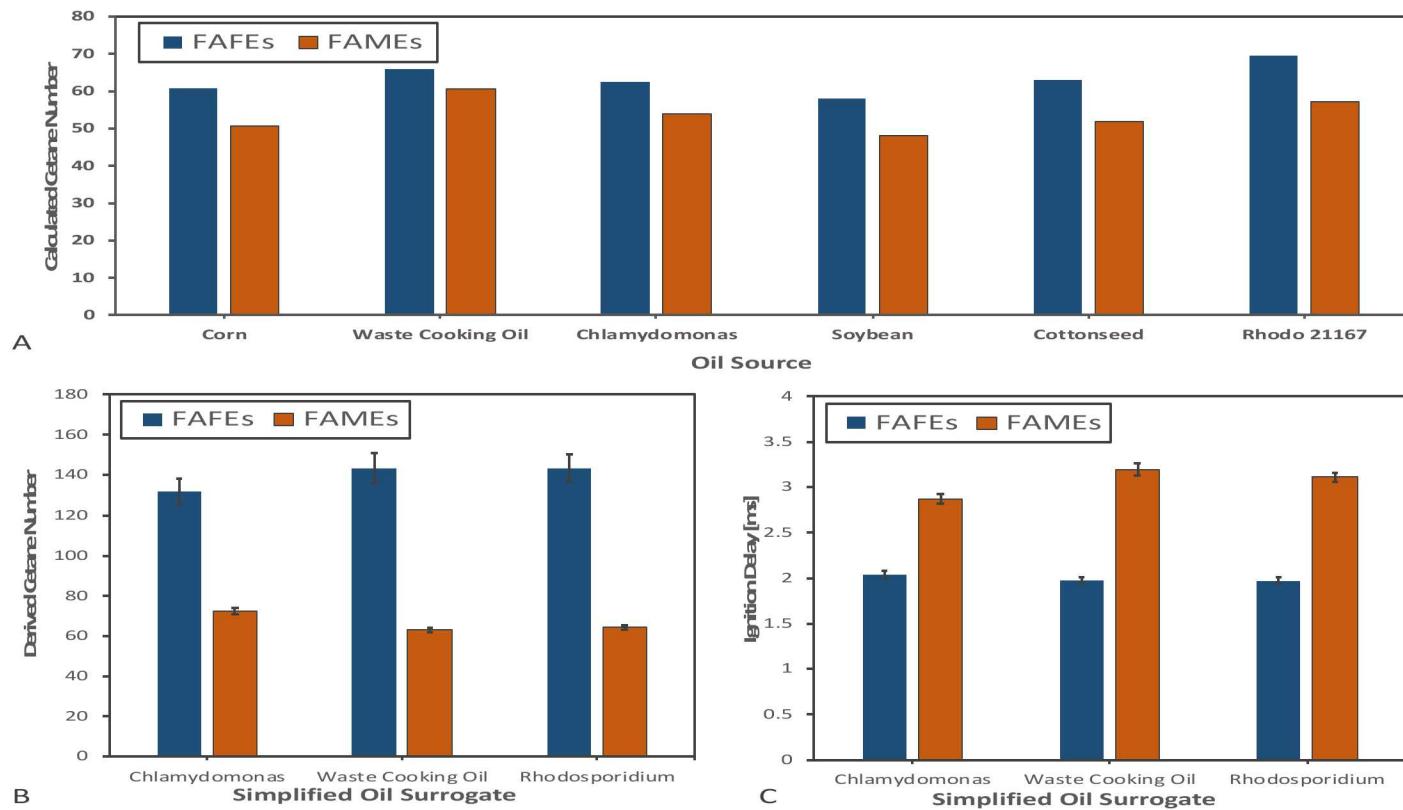


FAFEs as high performance compression ignition fuels

- Results shown are based on fusel surrogates reacted with corn oil.
- 5 point increase in Derived Cetane Number
- No-Flow point improved by >12 C which addresses biodiesel's significant cold-flow performance issues.

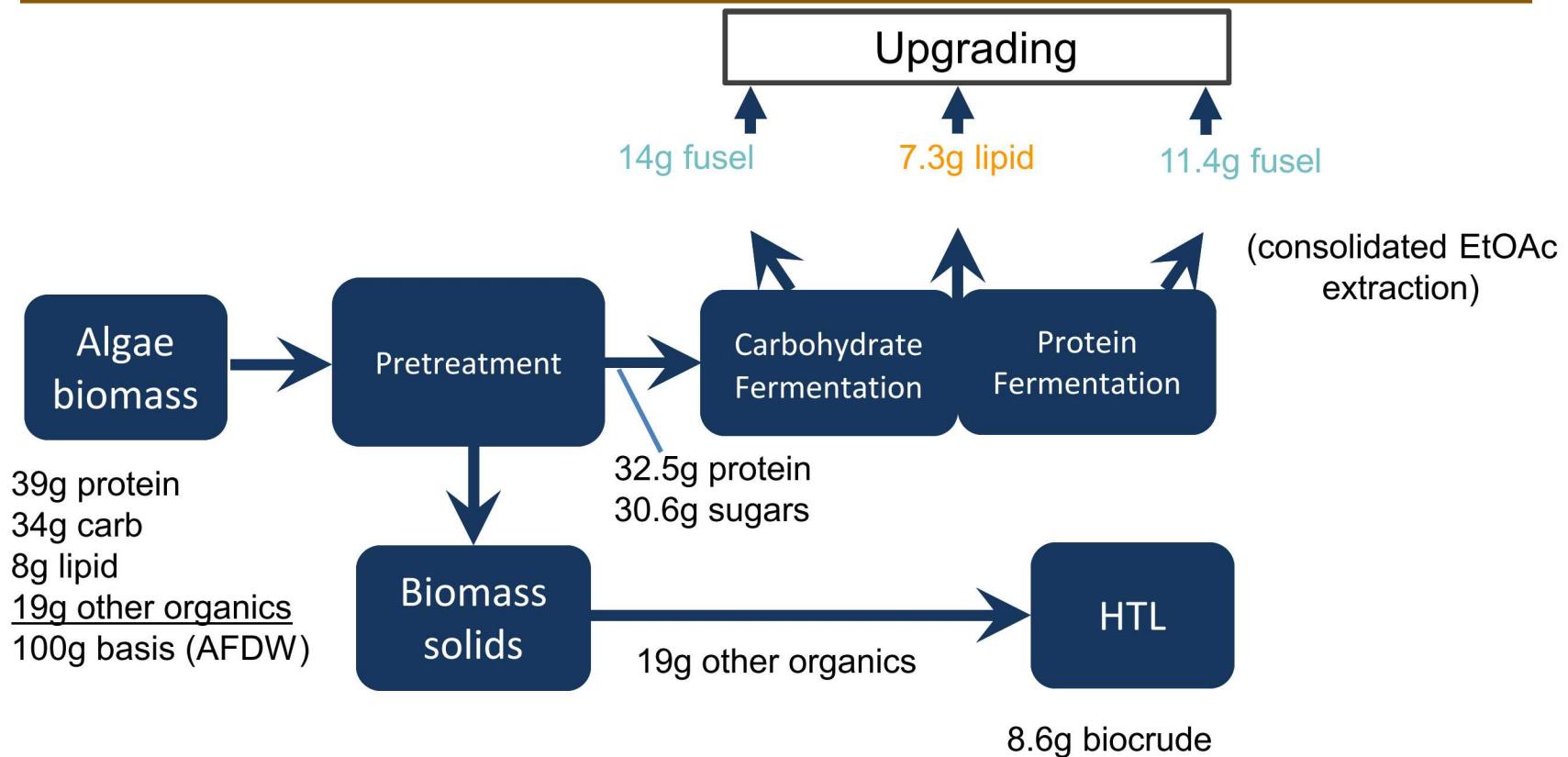


FAFEs as high performance compression ignition fuels



FAFE showed superior combustion and cold-flow properties, a 34.6% shorter ignition delay time (leading to higher cetane values)

Is the loop closed and what biomass is going where?



- High yields from consortium fermentations
- Titers > 12 g/L
- TEA Modeling underway

Conclusions

- A key bottleneck for large-scale biofuel feasibility is sustainable growth of high productivity biomass, which often means high protein and carbohydrate fractions.
- We have developed a proof of concept “one-pot bioconversion” with engineered *E. coli* for efficient production of mixed fusel alcohols from a wide variety of biomass sources.
- These fusel alcohols show promise as drop in fuels or as blending agents with gasoline for SI engines with properties comparable or better than ethanol.
- Fusel alcohols can further be upgraded to other high performance fuel compounds or reacted with residual lipids to utilize all major biochemical components of the biomass and “close the loop” allow for tunability to different engine architectures.
- **Fusel alcohols represent one example of this, but the co-optima effort has identified a variety of biofuel molecules that each have slightly unique value propositions as industrial fuels.**

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Co-Optimization
of
Fuels & Engines

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Thank you

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