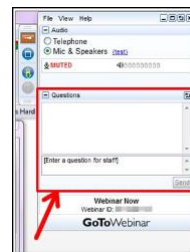
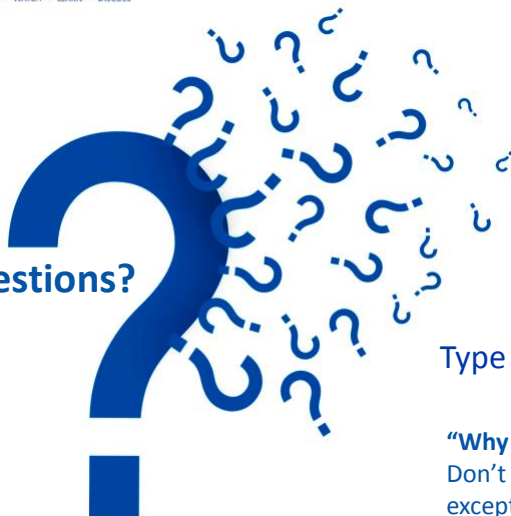




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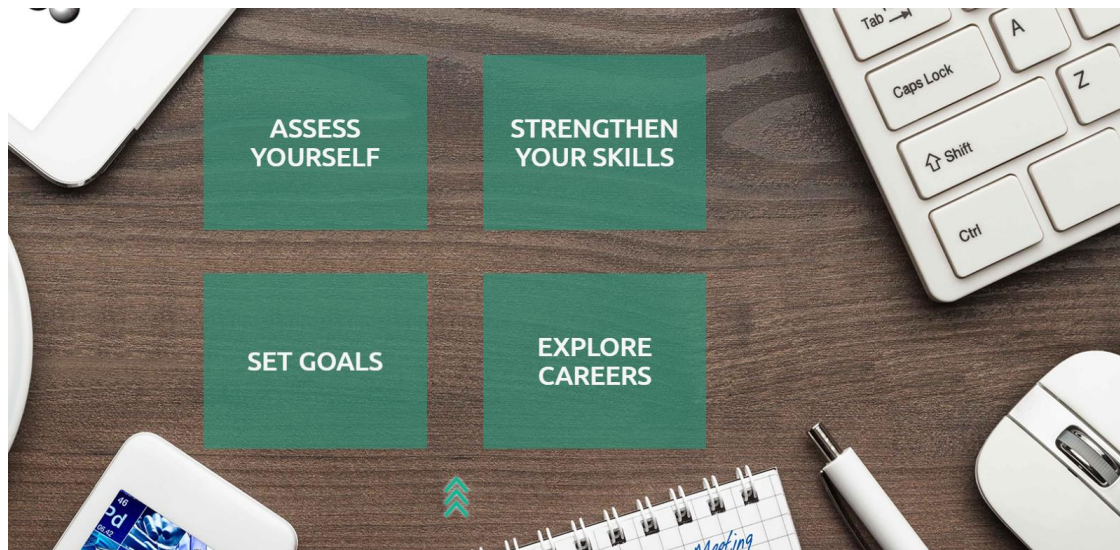
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## *Bioprivileged Molecules: A New Paradigm for Biobased Chemical Development*



**Peter Keeling**  
Industrial Collaboration and Innovation Director,  
NSF Engineering Research Center for Biorenewable  
Chemicals (CBIRC), Iowa State University



**Brent Shanks**  
Distinguished Professor, Engineering and  
Chair, Chemical and Biological Engineering,  
Iowa State University  
Director, NSF Engineering Research Center for  
Biorenewable Chemicals, Iowa State University



**Joe Fortunak**  
Professor of Chemistry, Howard University

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## **Bioprivileged Molecules**

## **A New Paradigm for Biobased Chemical Development**



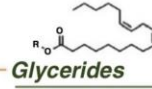
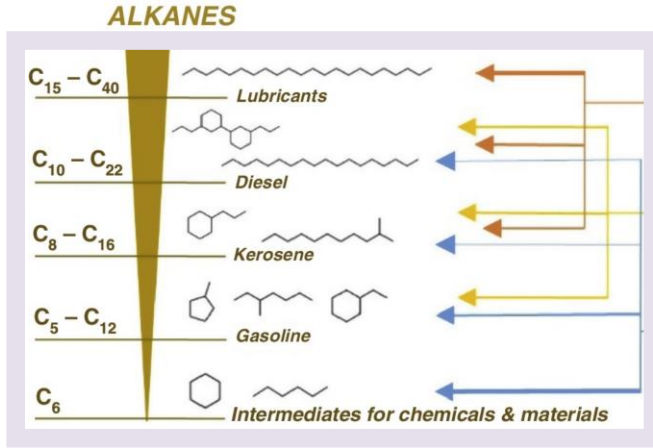
**Peter Keeling & Brent Shanks**  
*Iowa State University*



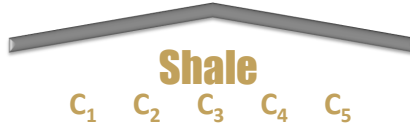
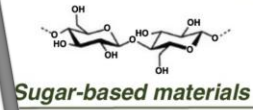
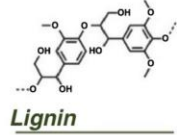
# Carbon Sourcing



Petroleum



Biomass



Adapted from: Deneyer et al., (2015) Current Opinion in Chemical Biology 29, 40-48



# Biobased Chemicals



circa 2013

Source: ICIS

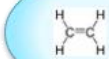




# Petrochemicals

## ETHYLENE

maleic anhydride  
ethanol  
ethylene  
ethylene dichloride  
vinyl chloride  
ethylene oxide  
ethylene glycol  
α-olefins  
vinyl acetate  
ethanolamines  
diethylene glycol  
butene-1  
1,4-butanedio



## PROPYLENE

propylene  
acrylonitrile  
propylene oxide  
acrylic acid  
n-butanol  
isopropanol  
propylene glycol  
2-ethylhexanol  
methyl ethyl ketone



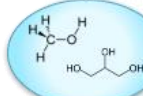
## BENZENE

benzene  
nitrobenzene  
cyclohexane  
adipic acid  
caprolactam  
linear alkylbenzene  
cumene  
phenol  
acetone  
bisphenol-A  
methyl diphenyl diisocyanate  
aniline  
ethylbenzene  
styrene



## METHANOL/GLYCEROL

glycerol  
methanol  
methyl tert-butyl ether  
formaldehyde  
acetic acid  
methyl chloride  
chloroform  
methyl methacrylate



## XYLENE

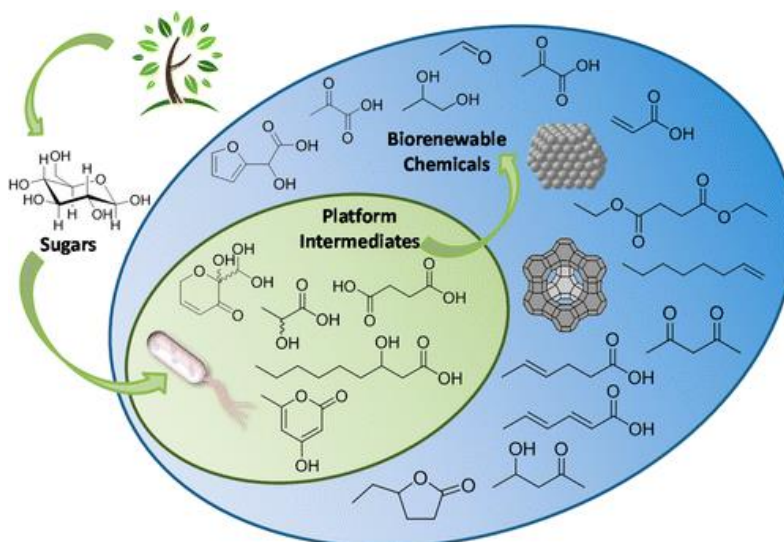
toluene diisocyanate  
phthalic anhydride  
o-xylene  
terephthalic acid  
p-xylene  
butadiene



Alkanes/Cycloalkanes/Aromatics



# Integrating Biology/Chemistry



Schwartz et al. *ACS Catal.* 4:2060-2069 (2014)







## Biobased Chemicals



How can this address so many chemical targets?

One Branch at a Time

One Leaf at a Time



Biology Branches

Chemistry Leaves



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## Risks, Costs and Return



**Risks:** Transition from lab to pilot to semi-works and full scale is frequently difficult.

- *Need to focus on fewer biological systems & combine with chemical catalysis for diversification.*

**Costs:** Capital costs are very significant and not fully derisked.

- *Need to find ways to move step-wise through scale levels for commercialization.*

**Return:** Competing with commodity chemicals is challenging

- *Need to identify higher value opportunities*



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## Bioprivileged Molecules



*Bioprivileged molecules are defined as biology-derived chemical species that can be efficiently converted to a diversity of chemical products including both novel molecules and drop-in replacements.*

Shanks, Keeling *Green Chem.* **19**:3177-3185 (2017)



PERSPECTIVE  
From G. Stano and Peter L. Leadley  
Bioprivileged molecules, creating value from biomass

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### Audience Challenge Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

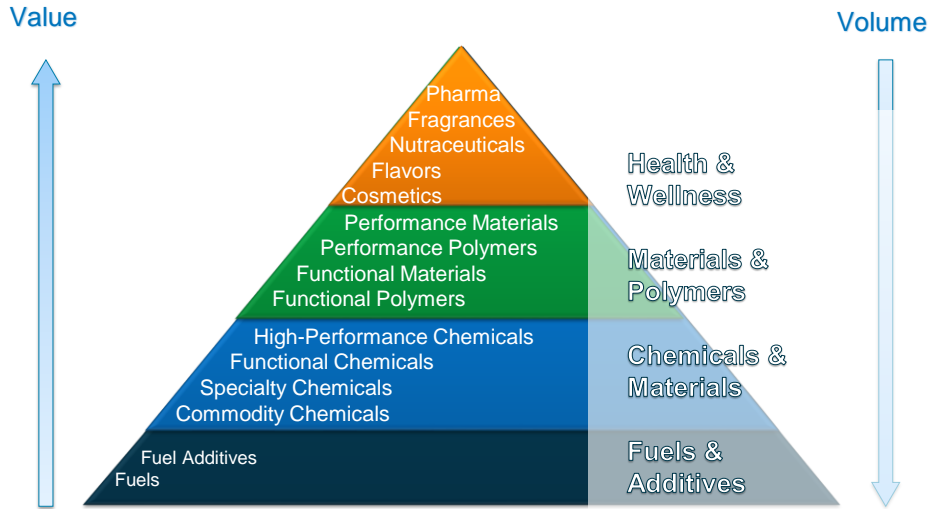


**When was the last new petrochemical compound commercialized?**

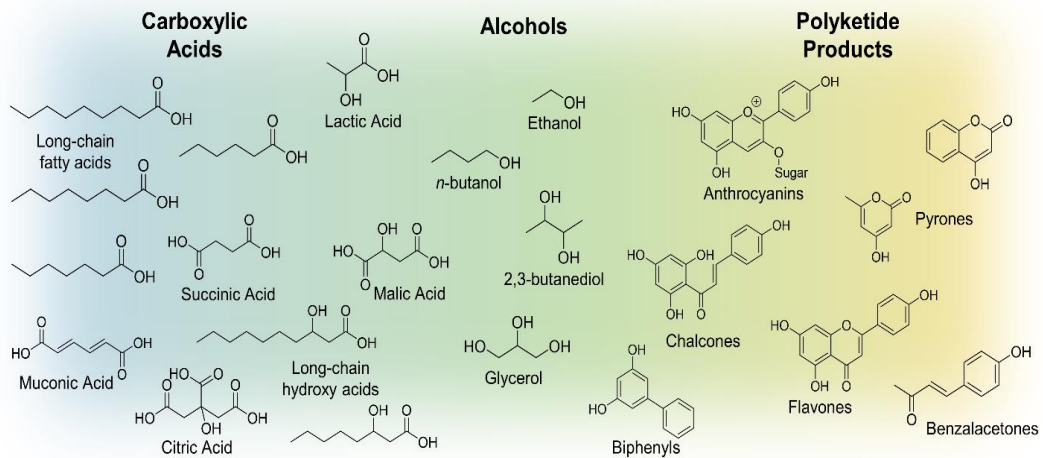
- 1-5 years
- 6-10 years
- 11-15 years
- 16-20 years
- Greater than 20 years



## Start with Higher Value MVP



## Biology-Derived Molecules



## Audience Challenge Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT



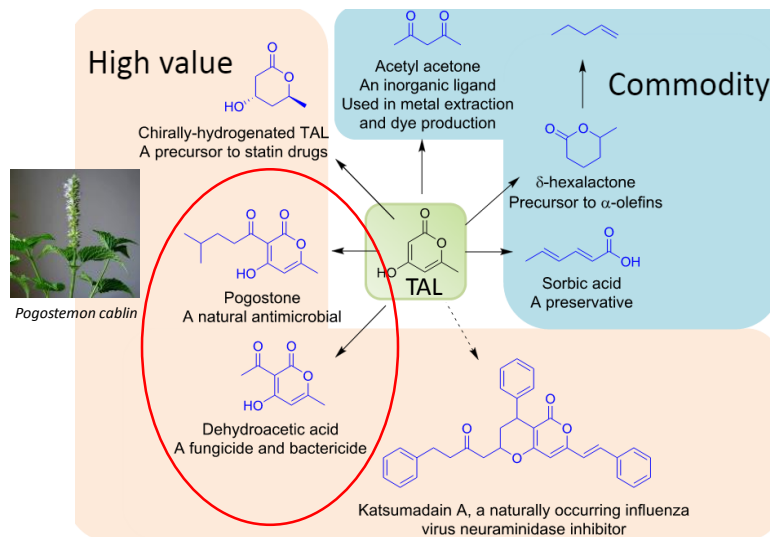
What are the number of possible  $C_6H_xO_y$  chemical compounds?

- About 30,000
- About 20,000
- About 15,000
- About 10,000
- About 5,000

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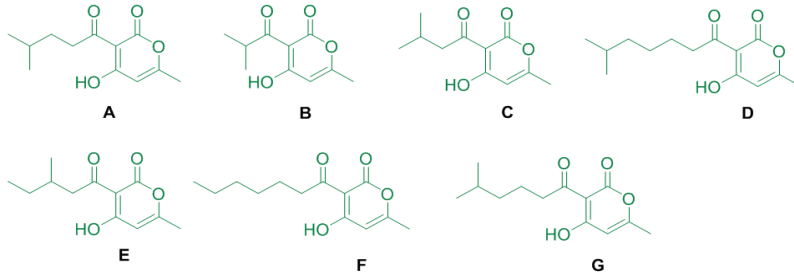
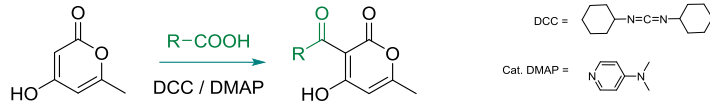


## Triacetic Acid Lactone





# Synthesis of Pogostone and Analogues



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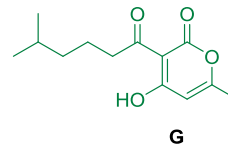
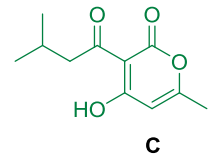
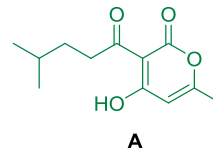
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# Antimicrobial Activity



Organisms	A	B	C	D	E	F	G
<i>Cryptococcus neoformans</i>	+						+
<i>Geotrichum capitatum</i>	+		+				+
<i>Candida kefyr</i>	+					+	
<i>Candida geochares</i>	+						+
<i>Candida krusei</i>	+		+				+
<i>Yarrowia lipolytica</i>	+		+				+
<i>Trichosporon mucoides</i>			+	+			+
<i>Prototheca wickehamii</i>	+	+	+	+	+	+	+
<i>Ogataea polymorpha</i>	+		+				+
<i>Candida intermedia</i>	+		+				
<i>Candida dubliniensis</i>	+		+				
<i>Cyberlindnera fabianii</i>	+		+				+
<i>Candida tropicalis</i>	+		+				+
<i>Rhodotorula mucilaginosa</i>							+
<i>Candida glabrata</i>	+		+				
<i>Candida parapsilosis</i>							
<i>Saccharomyces bayanus</i>	+		+				+
<i>Hanseniaspora guilliermondii</i>	+		+				+
<i>Cornebacterium glutamicum</i>							+
<i>Staphylococcus saprophyticus</i>							+
<i>Staphylococcus haemolyticus</i>							+
<i>Enterobacter cloacae</i>							+
<i>Chryseobacterium indologenes</i>							+



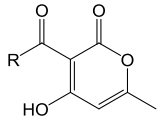
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# Insecticidal & Repellency



Pogostone Analogs

Compound	Insecticidal				
	0.025%	0.05%	0.1%	0.15%	0.25%
Pogostone Analog 1	0		10	55 ± 5	77.1 ± 10.4
Pogostone Analog 2	0		30	55 ± 25	80
Pogostone Analog 3			0	5	0
Pogostone Analog 4				10	
<b>Natural Pyrethrins</b>	0	0	0	20	10



Repellent	Spatial Repellency		
	15 mins	90 mins	150 mins
Control (acetone treated & evaporated)	-7.5	5	-5
<b>DEET</b>	20	50	56.7
Pogostone A	7.5	45	25
Pogostone B	<b>KD</b>	<b>KD</b>	<b>KD</b>
Pogostone C	35	67.5	62.5
Pogostone F	30	15	22.5
Pogostone G	7.5	15	5



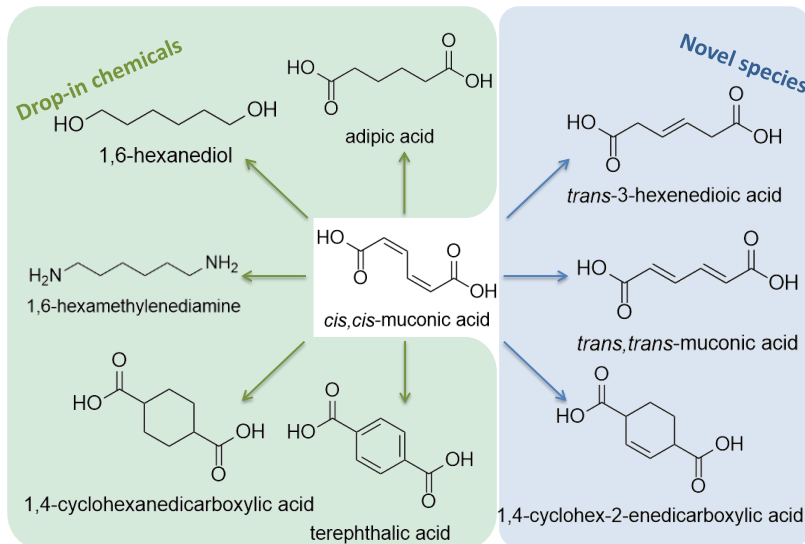
Norris and Coats, Pesticide Toxicology Lab

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# Muonic Acid Platform



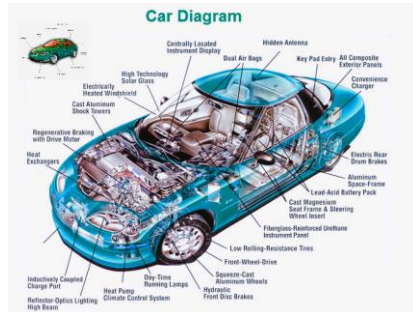
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## Bioadvantaged Nylon



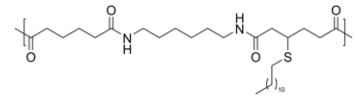
**Polymer:** Nylon 6,6

**Structure:** \*CC(=O)CCCCC(=O)NCCCCCCCCNC(=O)N\*

**Water Absorption:** 4.12 wt% increase



**Bioadvantaged Nylon 6,6 (5 wt% HDA)**



0.69 wt% increase

The mechanical properties of conventional Nylon 6,6 drop by 40% with the absorption of 2% moisture.

Application – Automotive Parts



## Physical Properties

Sample	$T_m$ (°C)	$\Delta H_m$ (J/g)	Crystallinity (%)	$T_{cr}$ Maxima	$\Delta H_c$ (J/g)	$T_{d50}$
BAN 0	254.92±1.98	76.285±1.68	51.9	226.16±1.79	75.19±2.34	431
BAN 5	249.47±0.75	62.06±0.80	53.6	224.06±0.02	64.06±4.56	430
BAN 20	229.27±0.94	43.55±1.50	44.0	196.86±0.93	47.98±0.53	437
BAN 40	194.80±1.60	26.94±3.03	31.6	156.85±0.45	34.55±4.13	444
BAN 50	170.02±0.04	23.26±0.30	23.4	114.29±1.69	21.78±2.27	447
BAN 60	-	-	21.0	-	-	448
BAN 80	-	-	0	-	-	451
BAN 100	-	-	-	-	-	452



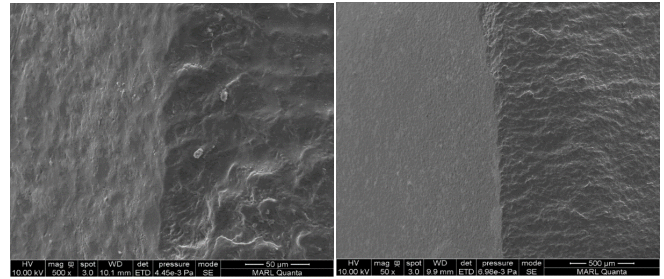
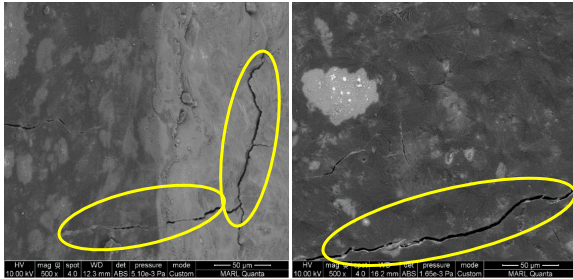


# Halide Resistance Test

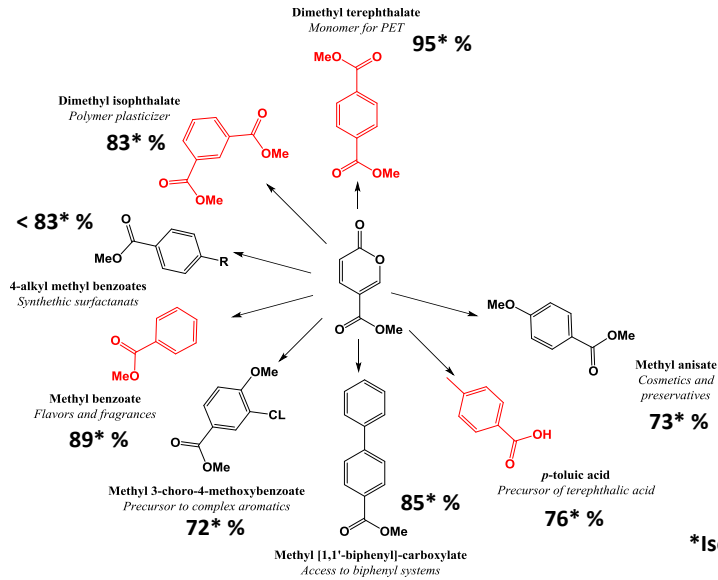


Conventional Nylon

Bioadvantaged Nylon



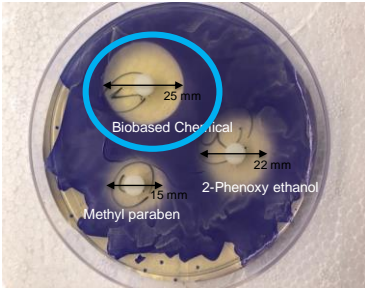
# Coumalate Platform







# MIC Testing



Compounds were tested against a wild type strain of *Escherichia coli* K-12 expressing a purple chromogenic protein to improve visualization.

Contaminating bacteria	Industry Standard Phenoxyethanol (PHE)	Pyrone Derivatives * < 0.5 wt% MIC (minimum inhibitory concentration)							
		A	B	C	D	E	F	G	H
<i>Escherichia coli</i>	*	*			*		*		*
<i>Aspergillus brasiliensis</i>	*				*		*		
<i>Pseudomonas aeruginosa</i>	*	*		*	*		*		
<i>Staphylococcus aureus</i>	*	*			*		*		
<i>Salmonella typhimurium</i>	*	*			*		*		
<i>Salmonella abony</i>	*	*			*		*		
<i>Clostridium sporogenes</i>	*	*			*		*		
<i>Candida albicans</i>	*	*			*		*		

\* *Salmonella Typhimurium* ATCC 14028, *Salmonella Abony* NCTC 6017, *Escherichia coli* ATCC 8739, *Pseudomonas aeruginosa* ATCC 9027, *Staphylococcus aureus* ATCC 6538, *Clostridium sporogenes* ATCC 11437, *Candida albicans* ATCC 10231 and *Candida albicans* ATCC 90028



# Novel Molecules



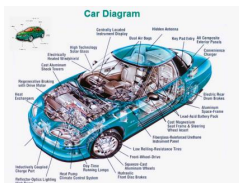
Consumer Goods, Materials, Chemicals

Petrochemicals

- Shifting consumer demand
- Lack of alternatives

Biobased Chemicals

- Consumer opportunity
- Novel alternatives





# Thank You



## *Bioprivileged Molecules: A New Paradigm for Biobased Chemical Development*



**Peter Keeling**  
Industrial Collaboration and Innovation Director,  
NSF Engineering Research Center for Biorenewable  
Chemicals (CBiRC), Iowa State University



**Brent Shanks**  
Distinguished Professor, Engineering and  
Chair, Chemical and Biological Engineering,  
Iowa State University  
Director, NSF Engineering Research Center for  
Biorenewable Chemicals, Iowa State University



**Joe Fortunak**  
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UCLA

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## Bioprivileged Molecules: A New Paradigm for Biobased Chemical Development



**Peter Keeling**  
 Industrial Collaboration and Innovation Director,  
 NSF Engineering Research Center for Biorenewable  
 Chemicals (CBIRC), Iowa State University



**Brent Shanks**  
 Distinguished Professor, Engineering and  
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 ACS member 1 year strong!

  
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