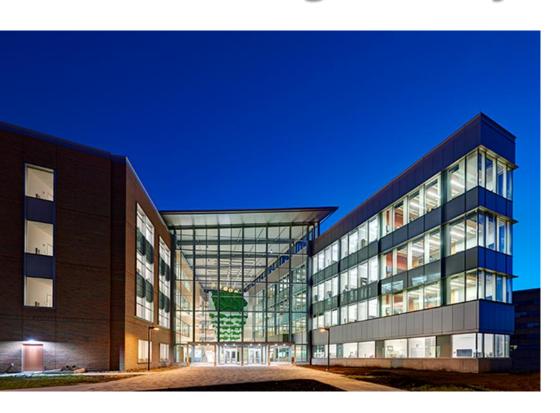




Bioprivileged Molecules: Creating Value from Biomass



Brent Shanks
Iowa State University

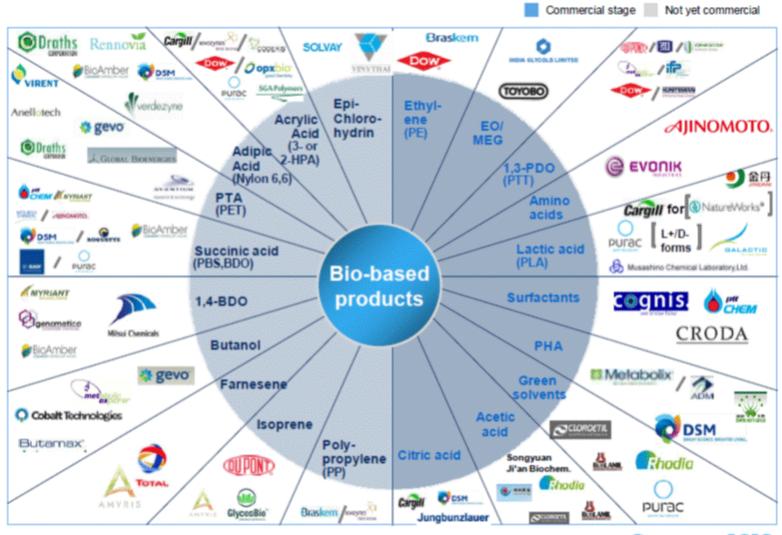
Bioeconomy 2017
July 11, 2017





Biobased Chemicals





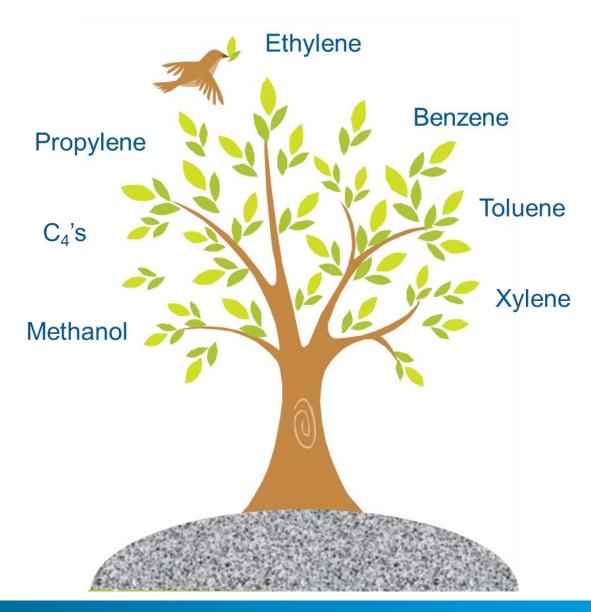
Source: ICIS





Petrochemicals



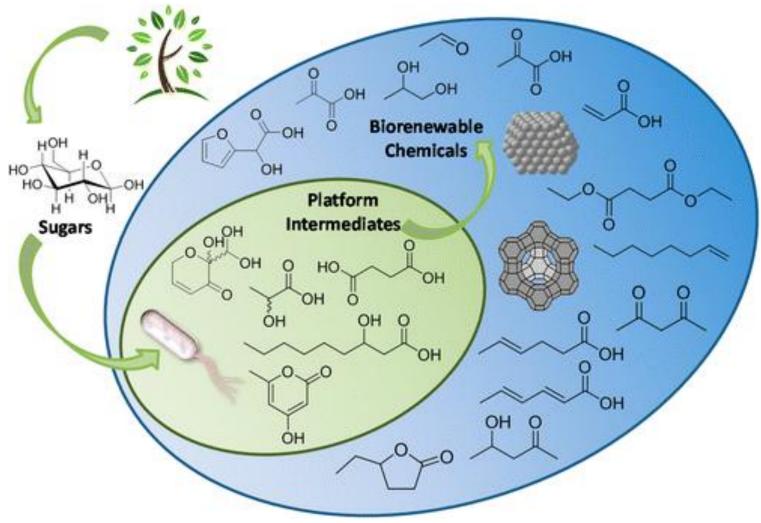






Integrating Biology/Chemistry





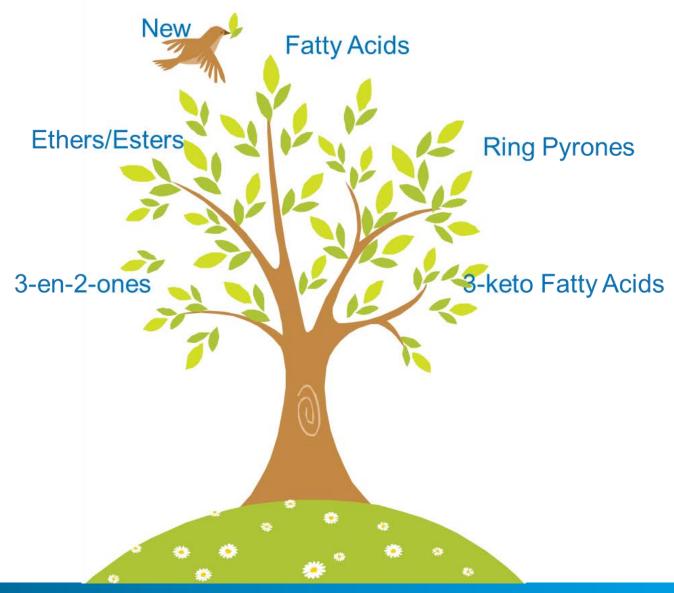
Schwartz et al. ACS Catal. 4:2060-2069 (2014)





CBiRC Strategy







Bioprivileged Molecules



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



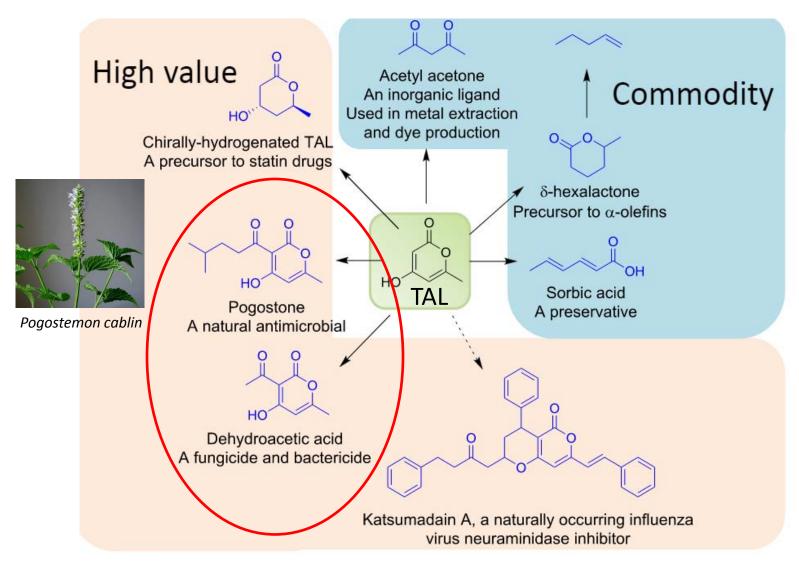
Shanks, Keeling Green Chem. (2017) DOI: 10.1039/C7GC00296C





Triacetic Acid Lactone





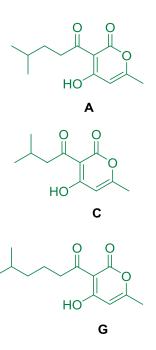




Antimicrobial Activity



Organisms	Α	В	С	D	E	F	G
Cryptococcus neoformans	+						+
Geotrichum capitatum	+		+				+
Candida kefyr	+					+	
Candida geochares	+						+
Candida krusei	+		+				+
Yarrowia lipolytica	+		+				+
Trichosporon mucoides			+	+			+
Protohteca wickehamii	+	+	+	+	+	+	+
Ogataea polymorpha	+		+				+
Candida intermedia	+		+				
Candida dubliniensis	+		+				
Cyberlindnera fabianii	+		+				+
Candida tropicalis	+		+				+
Rhodotorula mucilaginosa							+
Candida glabrata	+		+				
Candida parapsilosis							
Saccharomyces bayanus	+		+				+
Hanseniaspora guilliermondii	+		+				+
Cornebacterium glutamicum							+
Staphylococcus saprophyticus							+
Staphylococcus haemolyticus							+
Enterobacter cloacae							+
Chryseobacterium indologenes							+











Insecticidal Activity



Allethrin

1st generation
synthetic pyrethroids

Permethrin



House flies (Musca domestica)

Pyrethrin II

Resmethrin

Cypermethrin



German cockroaches (Blattella germanica)





Yellow fever mosquito (Aedes aegypti)





German Roach Mortality



Commonad		Percent	0 0			
Compound	0.025	0.05	0.1	0.15	0.25	ROO
Pogostone Analog 1	0		10	55 ± 5	77.1 ± 10.4	Pogostone Analogs
Pogostone Analog 2	0		30	55 ± 25	80	
Pogostone Analog 3			0	5	0	R O O
Pogostone Analog 4				10		
Natural Pyrethrins	0	0	0	20	10	Pyrethrin

Norris and Coats Pesticide Toxicology Laboratory - ISU Department of Entomology





Muconic Acid



Matthiesen et al., ACS Sustainable Chem. Eng. 4:3575 (2016)





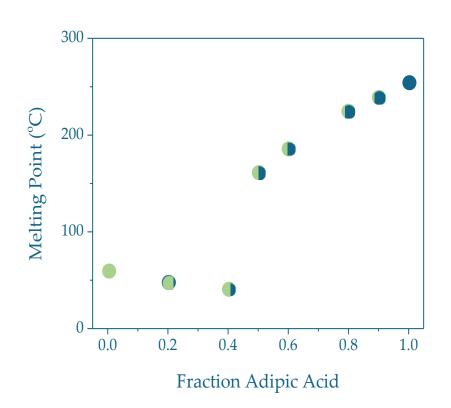
Tunable Copolymer Melting Point



Tunable Melting Points
Dependent upon AA/HDA ratio

High HDA content Low temperature blow molding Cure to crosslink shaped products

High AA content Modify alkene to add functionality For instance: Antimicrobial









Hydrophobic Nylon



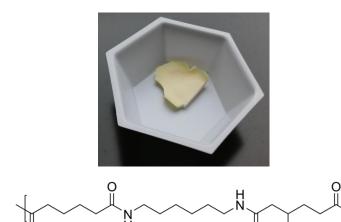
Nylon 6,6



$$\frac{1}{N}$$

3.44 wt% increase*

Bio-advantaged Nylon 6,6 (5% HDA) Modified with dodecanethiol chains



0.58 wt% increase

*2 wt% moisture causes a loss of 40% of Nylon's mechanical properties







Developing Biobased Chemicals

- Target needed for bioengineering efforts
- Drop-in and improved functional replacement
- Molecule efficacy testing needed
 - Sufficient quantity generated for testing
 - Rapid testing for set of analog compounds
- Systematic strategy for identifying desirable biobased chemicals needed





Thank you





Iowa State University

University of Wisconsin, Madison University of California, Irvine University of Michigan Penn State University University of New Mexico Salk Institute Rice University University of Virginia University of Minnesota