

*Center for Selective*



*Functionalization*

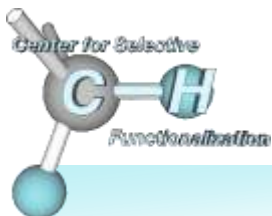


EMORY  
UNIVERSITY

*Role of Academic Science and Technology Centers in  
Developing Enabling Technologies*

*Case Study: NSF Center for Selective C-H Functionalization*



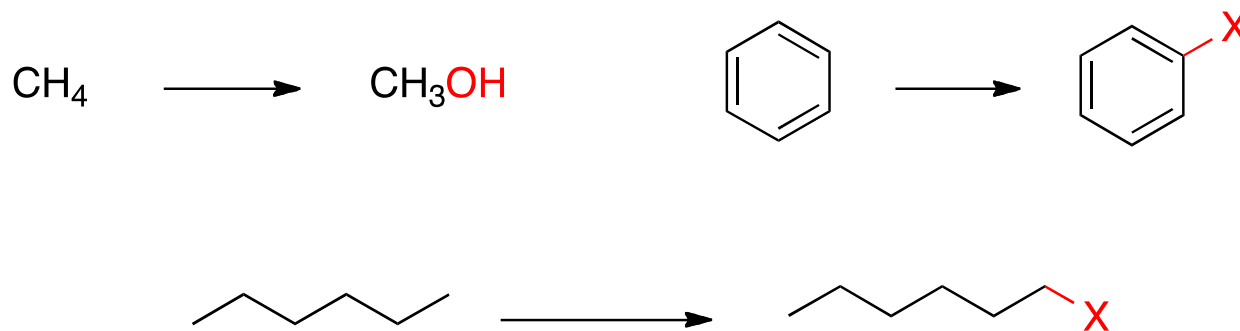


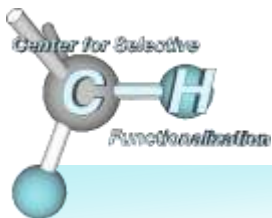
# What is C-H Functionalization?



## The Organometallic Chemist's View "The Holy Grail"

*"One "Holy Grail" of C-H activation research, therefore, is not simply to find new C-H activation reactions but to obtain an understanding of them that will allow the development of reagents capable of selective transformations of C-H bonds into more reactive functionalized molecules."*

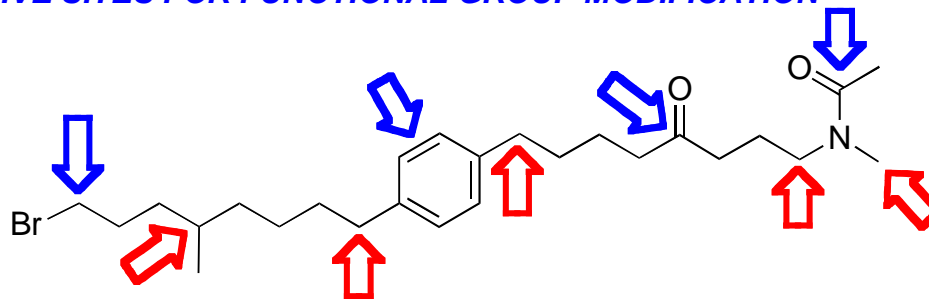




# The Organic Chemists View: Paradigm Shifting Synthetic Strategy

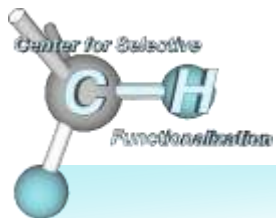


REACTIVE SITES FOR FUNCTIONAL GROUP MODIFICATION



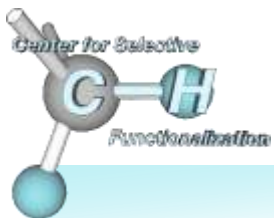
REACTIVE SITES FOR C-H FUNCTIONALIZATION

Major Impact on fine chemical synthesis, sustainable synthetic methods,  
Innovative approaches for pharmaceuticals and high performance materials

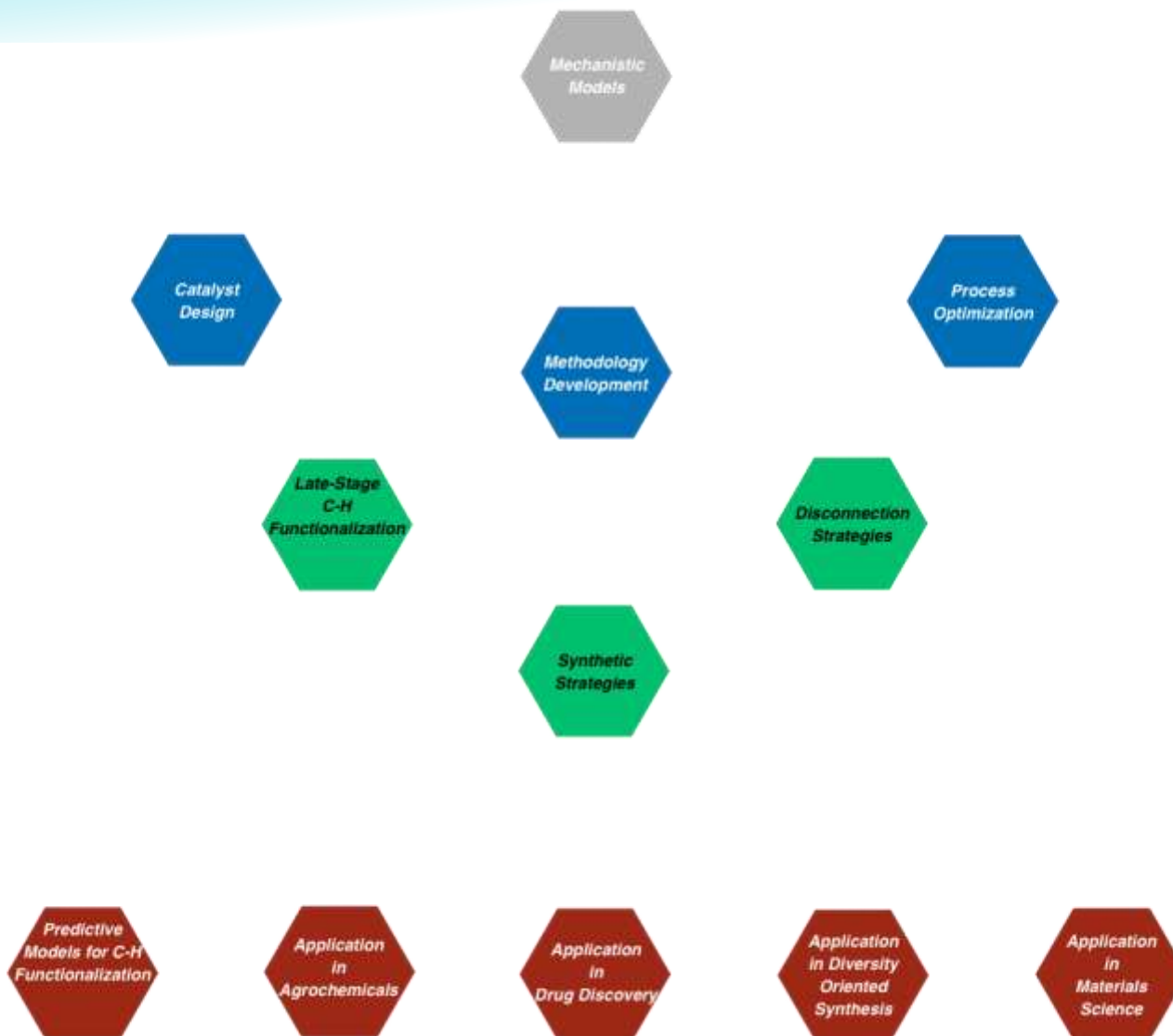


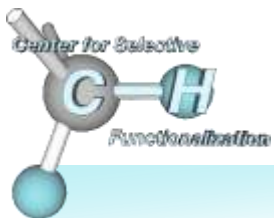
# *C-H Functionalization: Development of the Field*





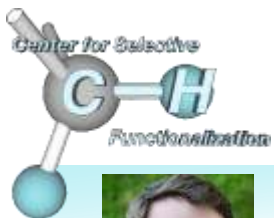
# *C-H Functionalization: Applications of the Field*



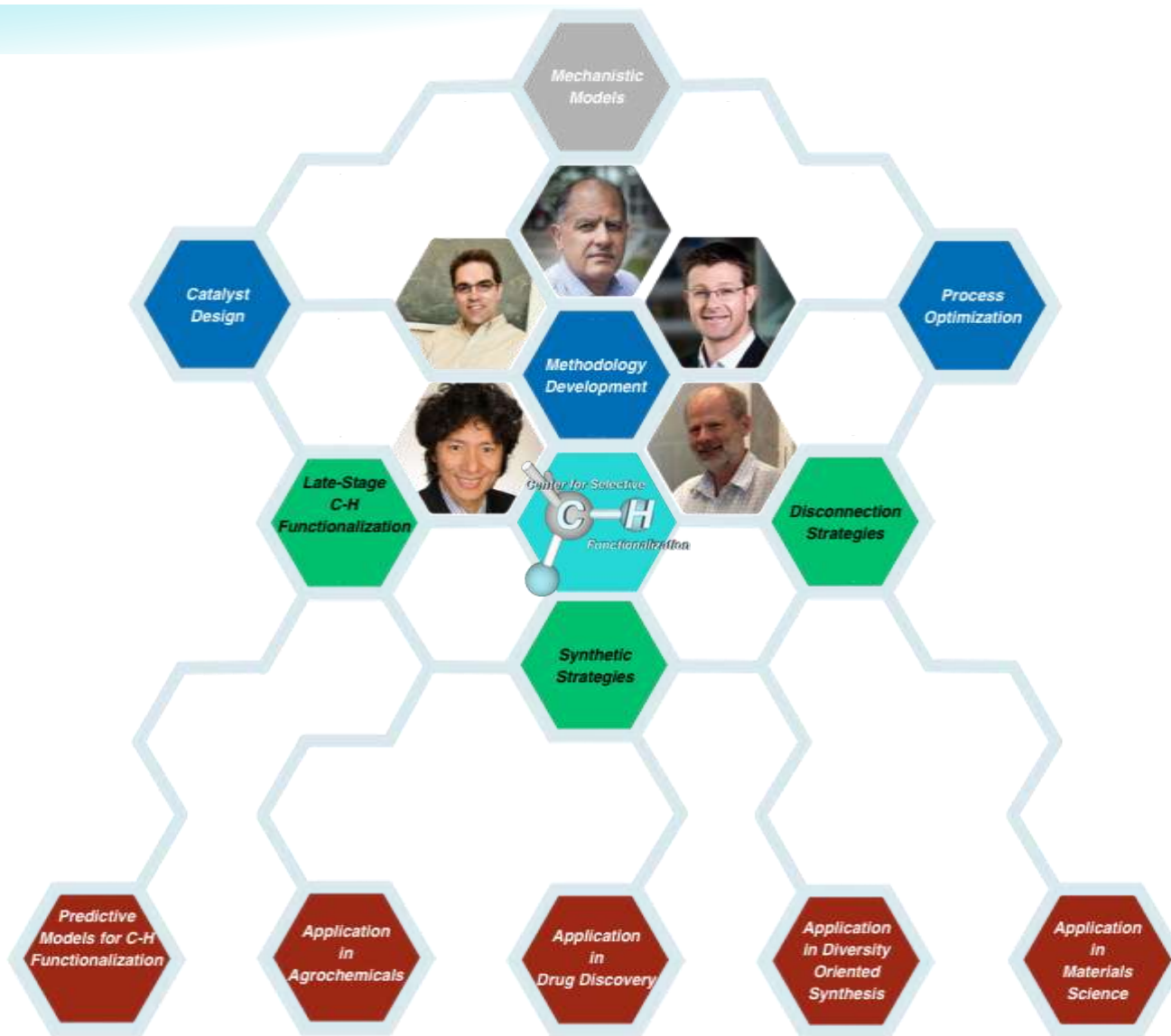


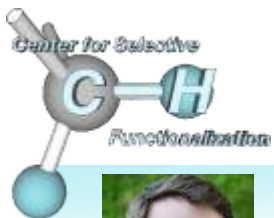
# Collaborative Beginnings of the CCHF





# Phase II of the CCHF

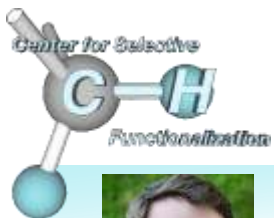




# Expanding the CCHF's Horizons



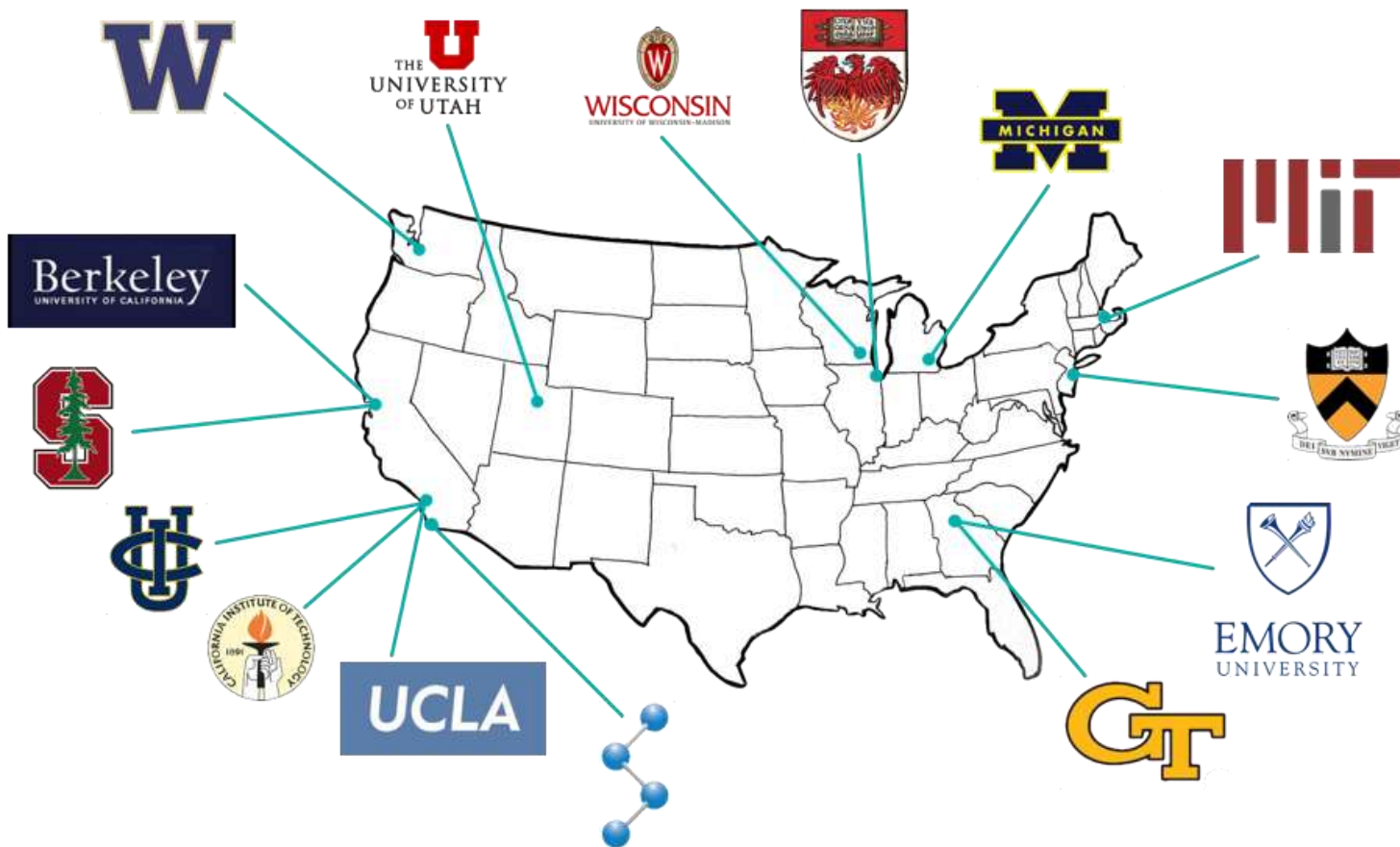


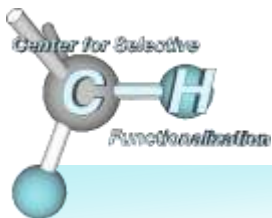


# The Center for Selective C-H Functionalization



# Footprint of the CCHF



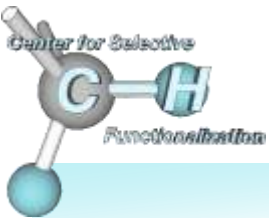


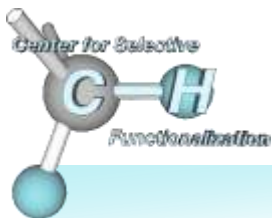
# *Building Synergy: Center Symposium, October 2012*

To leverage the collaborative potential of the Center to **Develop** technology for **Selective C-H Functionalization** that will **Revolutionize** the practice and reshape the **Teaching** of chemical synthesis, **Empowering** end users in **Materials Science**, **Fine Chemicals** development, and **Drug Discovery**.



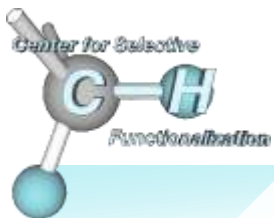
# Building Synergy: Weekly Videoconference Meeting





# Center Grand Challenges

- Generate a tool-box of effective catalysts and methods for the selective functionalization of C-H bonds.
- Develop selectivity rules for C-H functionalization of complex substrates.
- Revolutionize the strategies used for the synthesis of complex natural products.
- Develop strong alliances with other centers and industrial partners to maximize the application of the C-H functionalization methodologies to the synthesis of pharmaceuticals, agrochemicals and new materials.
- Become the recognized leader in advancing C-H functionalization to impact broadly the logic of organic synthesis.



# Streamlined Synthesis Using Sequential C-H Functionalizations

Gang Li (Yu Group)

Catalyst Design

Jin-Quan Yu - Scripps

Methodology Development

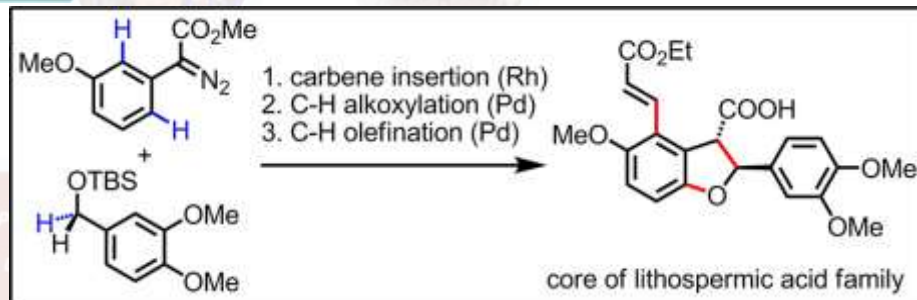
Keary Engle (Yu Group)

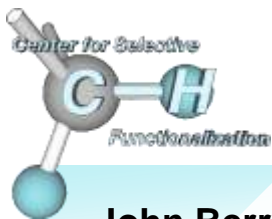
Disconnection Strategies

Hengbin Wang (Davies Group)

Huw Davies - Emory

Synthetic Strategies





# Isolation and Characterization of Rhodium-Carbenoids

John Berry – UW Madison

Kasia Kornecki

Jochen Autschbach  
SUNY Buffalo

Vyacheslav Boyarskikh

Felicia Fullilove

Philip Pelphey

Jørn Hansen

Huw Davies - Emory

Fred Briones

Mechanistic Models

Catalyst Design

Methodology Development

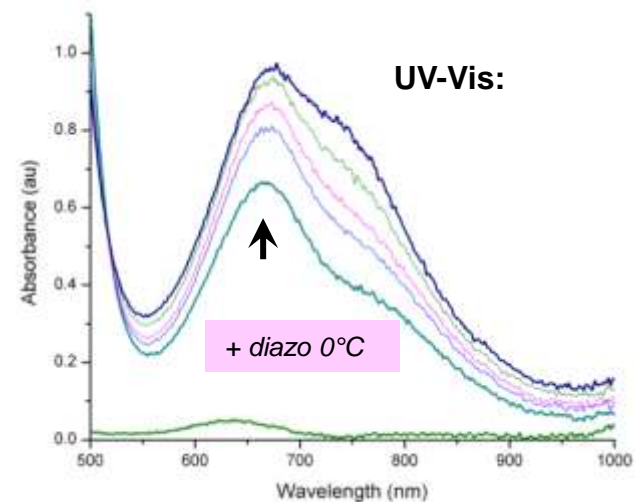
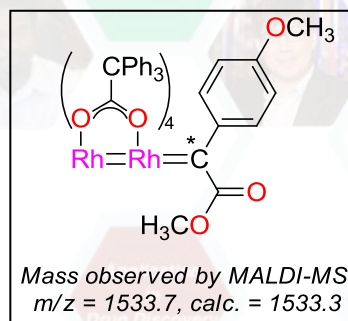
Process Optimization

Late-Stage C-H Functionalization

Challenging C-H Functionalization

Disconnection Strategies

Synthetic Strategies



# Designing Selective Catalysts for C-H Functionalization

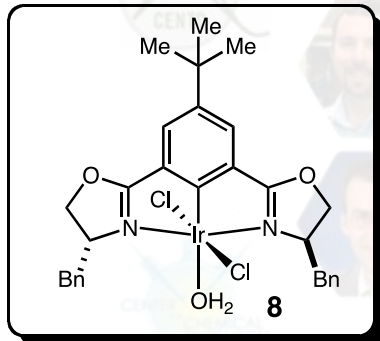
Adrián Varela-Álvarez - Emory

Jamal Musaev  
Emory

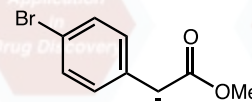
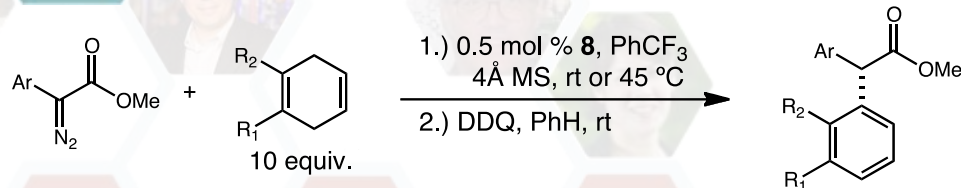
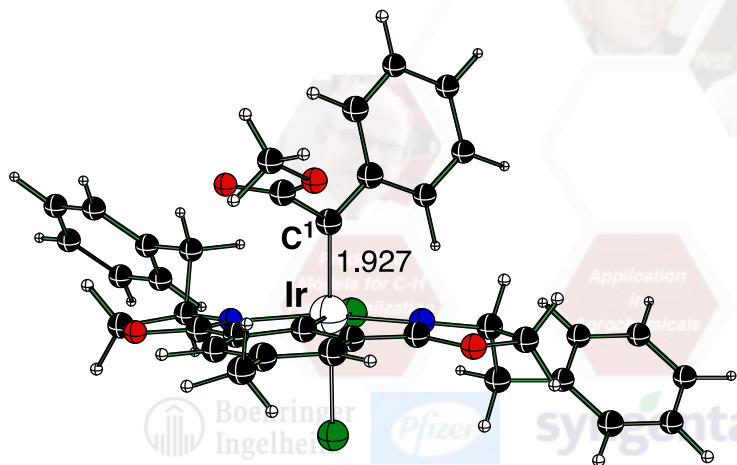
Clayton Owens - Emory

Simon Blakey - Emory

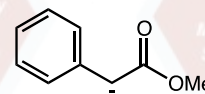
Huw Davies - Emory



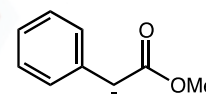
iridium(III) phebox



96 %  
95 % ee



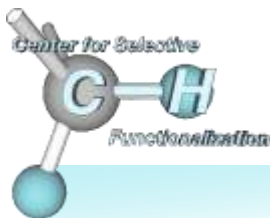
98 %  
94 % ee



53 %  
95 % ee

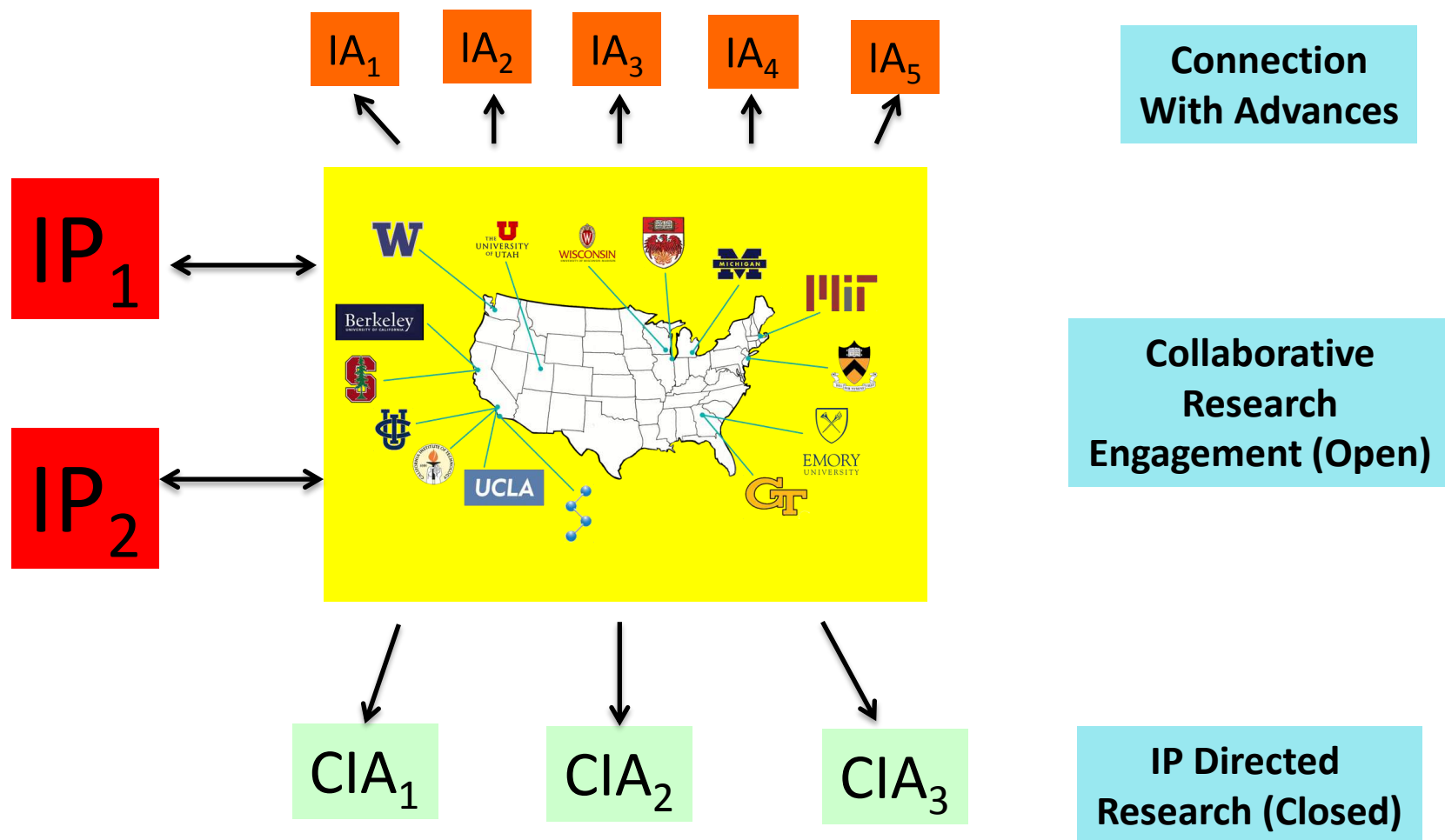


# CCHF Interactions with Industrial Sponsors

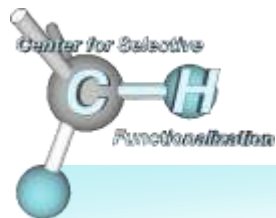


- **Collaborating Partner (CP)** (\$100,000+)
  - Broad, all-encompassing non-IP interactions in all Center research and outreach activities.
  - Early communication of research results and outreach activities
- **Collaborating Industrial Affiliate (CIA)** (\$50,000+)
  - Focused projects with specific members of the Center for research or outreach.
  - Early communication of research results and outreach activities
- **Industrial Affiliate (IA)** (\$10,000)
  - Early communication of research results and outreach activities

# Model for Collaborations with Industry



# Benefits: Symposia with the CCHF

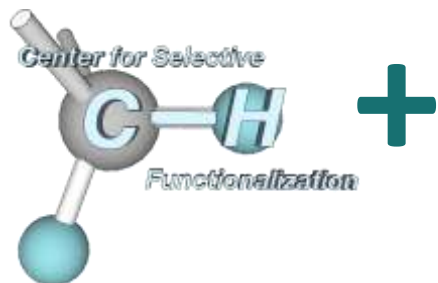


## Quarterly Virtual Symposia (CP, CIA, IA):

- Interactive Video-Conference
- Dissemination of scientific results and outreach activities
- Interaction with faculty and student CCHF members

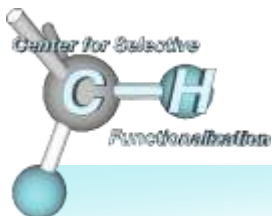
## Annual Symposium (CP, CIA, IA):

Learn about the science, meet the members, network with the community all face to face in an exciting, enthusiastic and open atmosphere.



## Collaborative CCHF/Company Meeting (CP):

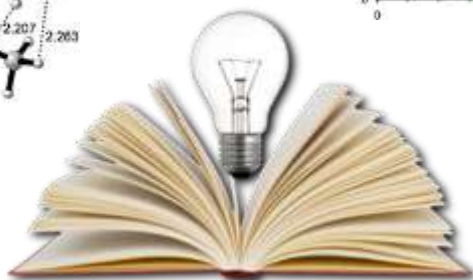
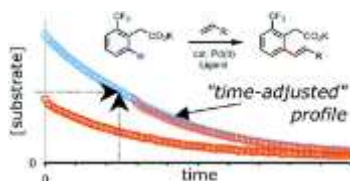
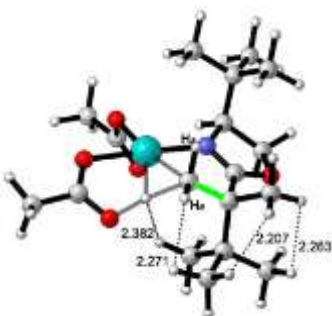
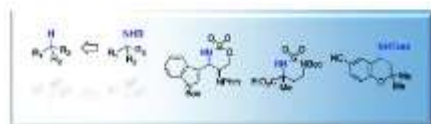
Special collaborative one-day symposium with the Center and Industrial partner. Including in-depth discussion with faculty and students.



# Benefits: Research Interactions with the CCHF

## Monthly Update Newsletter (CP, CIA, IA):

- General News and Outreach Update on Center Activities
- Center calendar and upcoming events

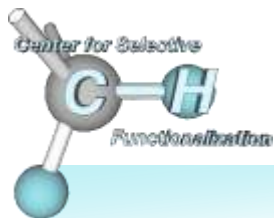


## Affiliate Interactions (CIA):

- Focused investigations on specific challenges
- Working with individuals or small teams of Center members

## Partner Interactions (CP):

- Broad, all encompassing disclosure of Center activities
- Working on long-term grand challenges
- Collaborative goals and challenges



# Benefits: Network and Exchange with the CCHF



## Academic Network:

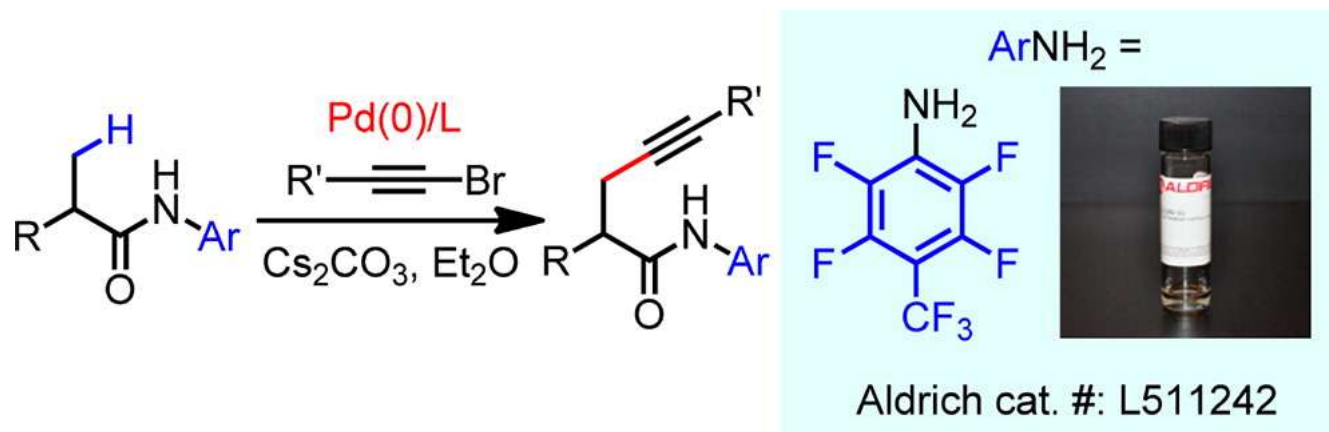
- Communicate directly with a network of faculty, postdocs and students from across the United States
- Exposure and interaction on a national scale through scientific and outreach activities

## Interact with Future Scientists

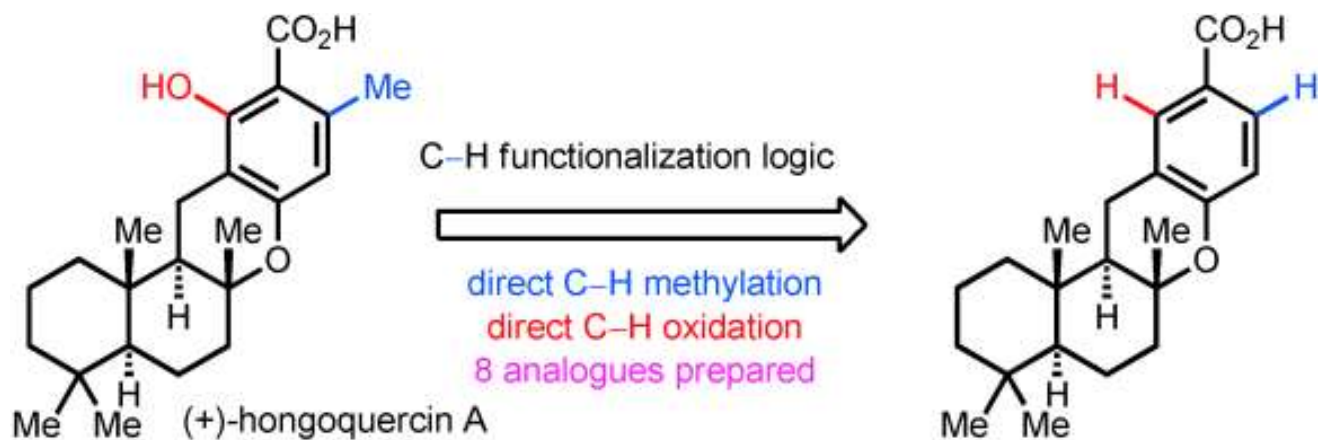
- Communication with and access to a community of highly-trained graduate and postdoctoral students
- Graduates from the Center will have experience of collaborative, interdisciplinary research programs and learnt the skills required to make these a success

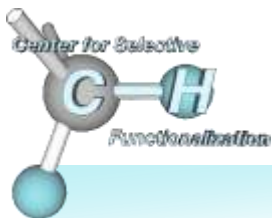


# Coordination of Publications with Commercialization of Reagents (Yu with Aldrich)

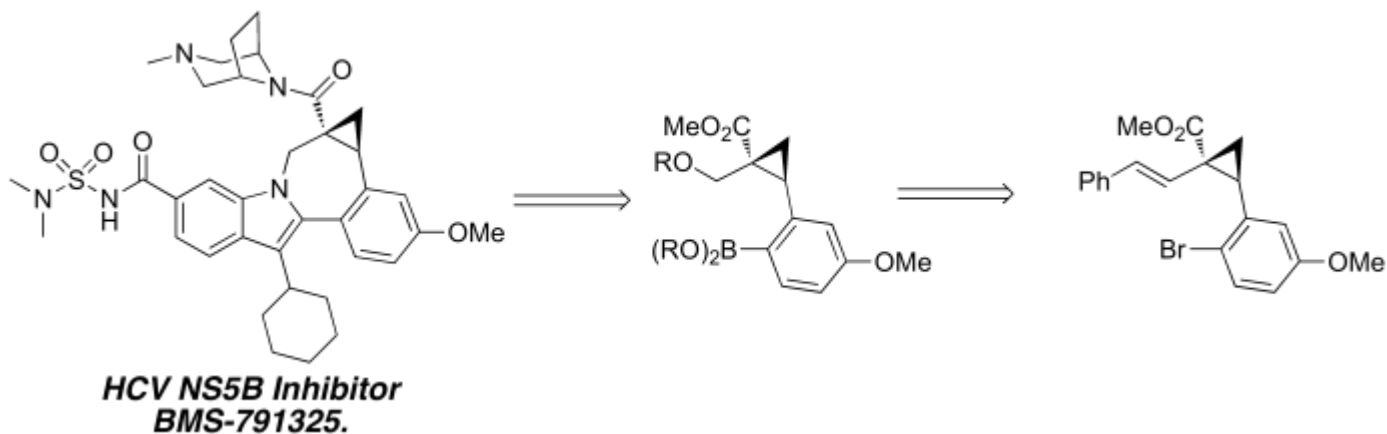


# Natural Product Synthesis and Late Stage Functionalization (Yu with Baran)





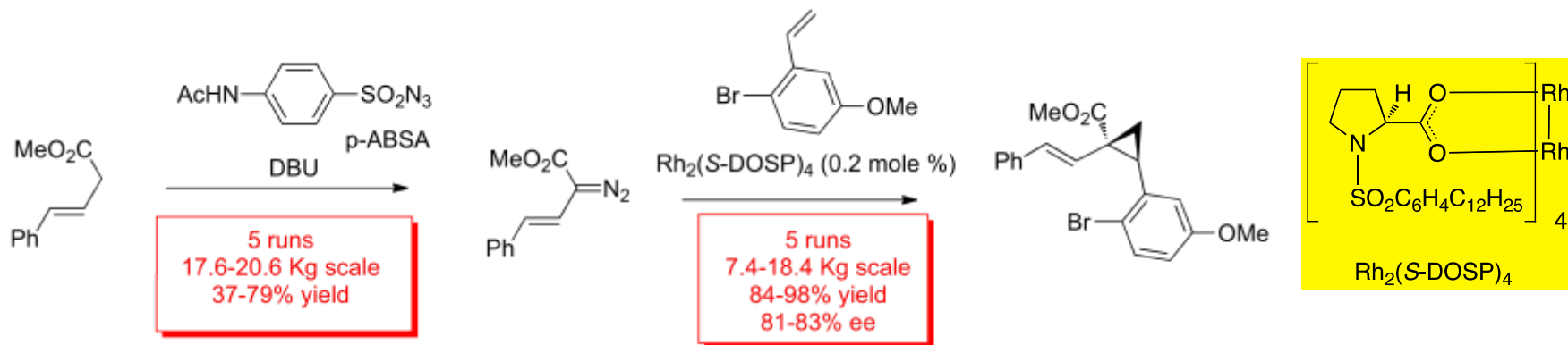
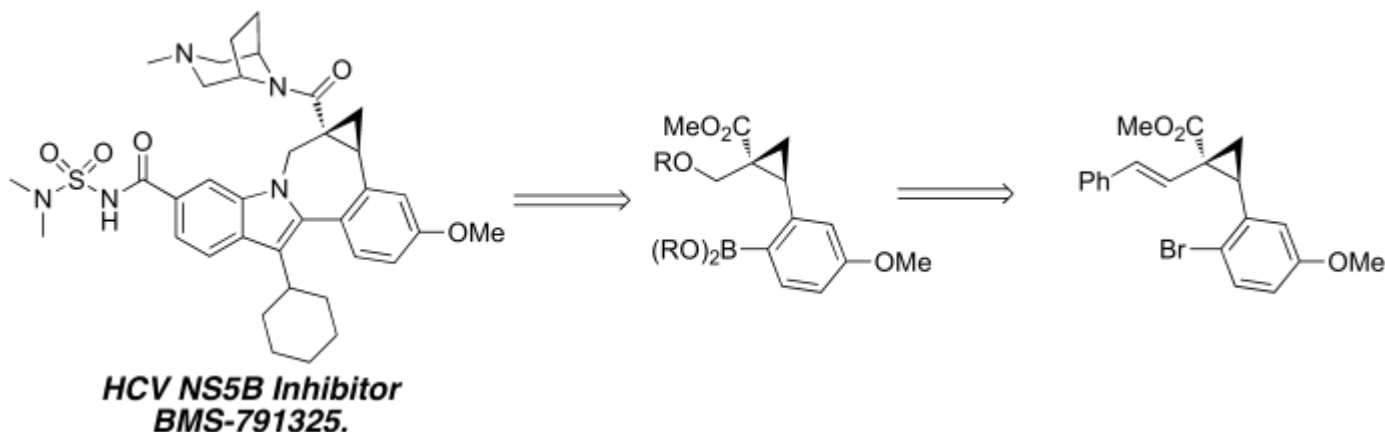
# New Catalysts for Pharmaceutical Process Chemistry (Davies with Bristol-Myers-Squibb)



**Discovery and development of a scalable synthesis for the HCV NS5B inhibitor BMS-791325.** Presented by Rodeny S. Parsons, BMS. Paper 346, Organic Division, American Chemical Society, National Meeting, New Orleans, April 08, 2013

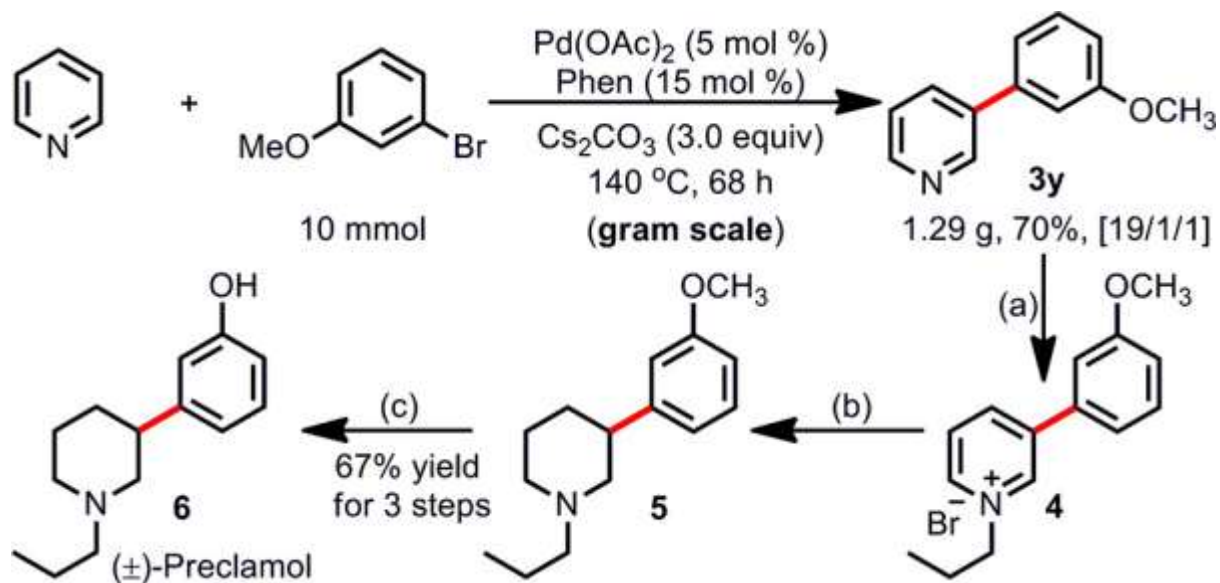


# New Catalysts for Pharmaceutical Process Chemistry (Davies with Bristol-Myers-Squibb)

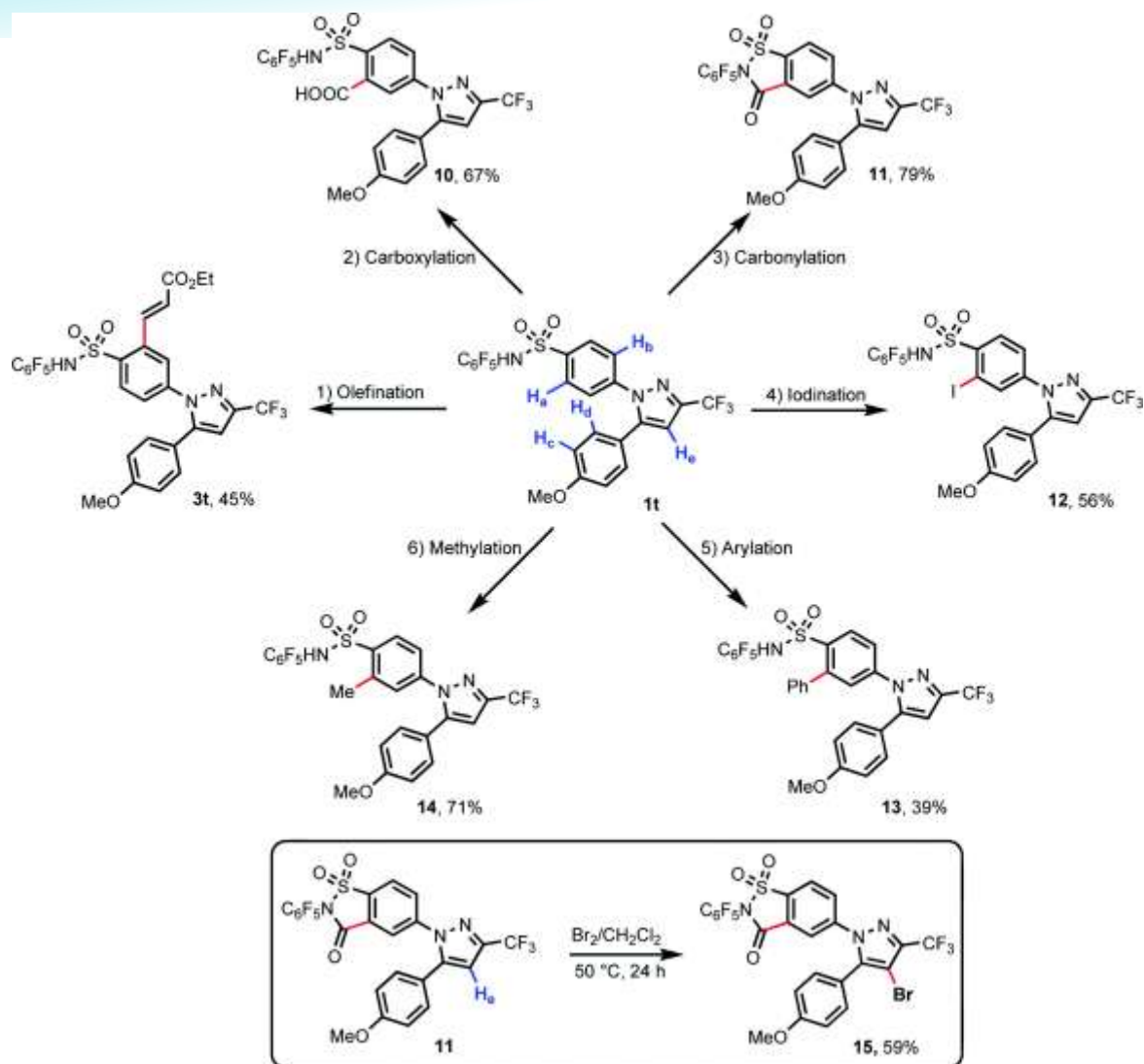


**Discovery and development of a scalable synthesis for the HCV NS5B inhibitor BMS-791325.** Presented by Rodeny S. Parsons, BMS. Paper 346, Organic Division, American Chemical Society, National Meeting, New Orleans, April 08, 2013

# Applications to Agrochemical Targets (Yu with Syngenta)



# Diversity Synthesis of Pharmaceutical Targets (Yu with Pfizer)



- ◆ C-H Functionalization is reaching the stage of maturity for broad commercial application
- ◆ CCHF offers a collaborative team approach for developing C-H functionalization
- ◆ Broad collaborations are becoming the driver of modern organic chemistry research
- ◆ Collaborations between CCHF and industry enhances the rapid development of C-H functionalization



[www.NSF-CCHF.com](http://www.NSF-CCHF.com)



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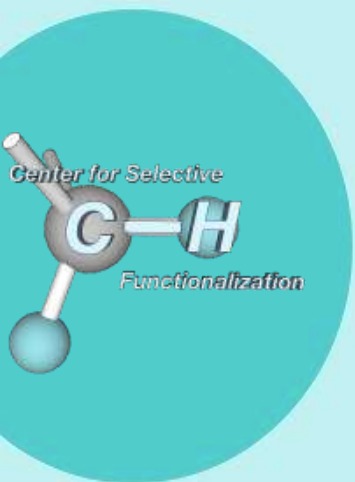


[@NSFCCHF](https://twitter.com/NSFCCHF)

***This work was supported by NSF under the CCI Center for Selective C-H Functionalization, CHE-1205646***

*Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation (NSF)*

# Affiliation Benefits Overview



	<b>CP</b> Collaborating Partner \$100,000+	<b>CIA</b> Collaborating Industrial Affiliate \$50,000+	<b>IA</b> Industrial Affiliate \$10,000	
	<input type="checkbox"/>	<input type="checkbox"/>		<b>Association</b>
	<input type="checkbox"/>	<input type="checkbox"/>		Logo/Name on Center Posters
	<input type="checkbox"/>	<input type="checkbox"/>		Logo/Name on Center Presentations
	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Logo/Name on Center Website
	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Sponsorship of Outreach Activities
	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<b>Symposia</b>
	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Quarterly Virtual Symposia
	5 Free then \$500/person	1 Free then \$500/person	\$500/person	Annual Symposium
	<input type="checkbox"/>			Collaborative CCHF/Company Meetings
	<input type="checkbox"/>			<b>Research Interaction</b>
	<input type="checkbox"/>			Monthly Internal Update Newsletter
	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Monthly External Update Newsletter
	<input type="checkbox"/>	<input type="checkbox"/>		Discussion on Technical Challenges
	<input type="checkbox"/>			Collaborative Proposal Building
	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Advance Notice of Inventions
	<input type="checkbox"/>	<input type="checkbox"/>		<b>Networking &amp; Exchange</b>
	<input type="checkbox"/>	<input type="checkbox"/>		Sponsored Fellow Program
	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Access to online Member Resumes
	<input type="checkbox"/>	<input type="checkbox"/>		Facilitated Interviews
	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Contact with Center & Affiliate Network

Broad, all-encompassing non-IP interactions in all Center research and outreach activities

Focused interactions with specific members of the Center for research or outreach.

Communication of research results and outreach activities

