



DATA-RICH ORGANIC CHEMISTRY: ENABLING AND INNOVATING THE STUDY OF CHEMICAL REACTIONS

A Workshop sponsored by the U.S. National Science
Foundation

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Genesis

- June 2013: Council for Chemical Research (CCR) workshop, U Penn, Philadelphia



- The growing need for rapid information collection in an era of shrinking resources provides a strong motivation for pre-competitive collaboration between companies themselves and between companies and academia.
- Goal: an integrated approach to data capture and interpretation.

Precompetitive Collaborations

Enabling Technologies for the Pharmaceutical Industry

Wednesday-Thursday
June 12-13

On June 12 & 13, 2013, the Council for Chemical Research (CCR) will be hosting a New Industrial Chemistry & Engineering (NICHÉ) workshop on the topic of "Precompetitive Collaborations on Enabling Technologies for the Pharmaceutical Industry" on the University of Pennsylvania Campus in Philadelphia, PA.

The meeting, chaired by Christopher Welch (Merck), Joel Hawkins (Pfizer) and Jean Tom (Bristol-Myers Squibb) will feature lectures, panel discussions and breakout discussion sessions with leaders in industry, academia and government exploring new approaches to cross-pharma collaborations on precompetitive chemistry and chemical engineering technologies. Join in the discussion with key opinion leaders from Merck, Pfizer, Bristol-Myers Squibb, Amgen, Boehringer Ingelheim, University of Pennsylvania, Mettler-Toledo, Waters, Johns Hopkins University, National Institutes of Standards and Technology (NIST), National Science Foundation (NSF) and others.

This symposium will provide unparalleled opportunities to network and exchange information in an informal setting. NICHÉ workshops often sell out, so mark your calendar now and watch for future emails from us about registration instructions.

- September 2014: NSF sponsored workshop, DC



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- DATA-RICH
ORGANIC CHEMISTRY**
- Enabling and Innovating the
Study of Chemical Reactions**
- AN NSF-SPONSORED WORKSHOP**

The Current State

□ Models for Collaboration

▣ CCHF – Center for Selective C-H Functionalization

■ Huw Davies, Emory

▣ 3CS – Caltech Center for Catalysis and Chemical Synthesis

■ Scott Virgil, Sarah Reisman, Caltech

▣ Merck NSF-GOALI Experience

■ Shane Krska, Merck

▣ SSPC – Solid State Pharmaceutical Cluster

■ Joe Hannon, Dynochem

▣ UK Pharmacat Model

■ Mimi Hii, Imperial College

Recent Progress

□ Pharma Models for Collaboration

▣ Pfizer: Joel Hawkins

- *Data needs to be transportable – across people, across time, across location. Broad utilization requires appropriate soft-ware, capable of facile data integration and visualization.*

▣ BMS: Jean Tom

- *Key problem is the integration of data into searchable architecture.*

▣ Merck: Chris Welch

- *Goal is to provide data-rich tools without data handling headaches. New enabling technologies need to be evaluated.*

Transformative Pharma Solutions



- Data-rich measures of **quality** can help to accelerate development and build in quality from the outset.
- Concept of the “**Lab of the Future**”.
- New **skills** will be required to prepare our workforce for this data-rich world of the Lab of the Future.

Key Challenges

□ Developing a Common Data Framework

- ▣ Sharing and mining of data: the Allotrope Framework was developed to address the issue of lack of connectivity.

□ Developing New Technologies

- ▣ Identify the gaps that exist between ideas and execution that can be filled through collaborations between tech partners, industry, and academia.

□ Future Priorities: the IQ Consortium

- ▣ The IQ consortium is composed of 37 companies with the purpose to advance science-based and science-driven standards and regulations.

Key Challenges

□ The Allotrope Framework

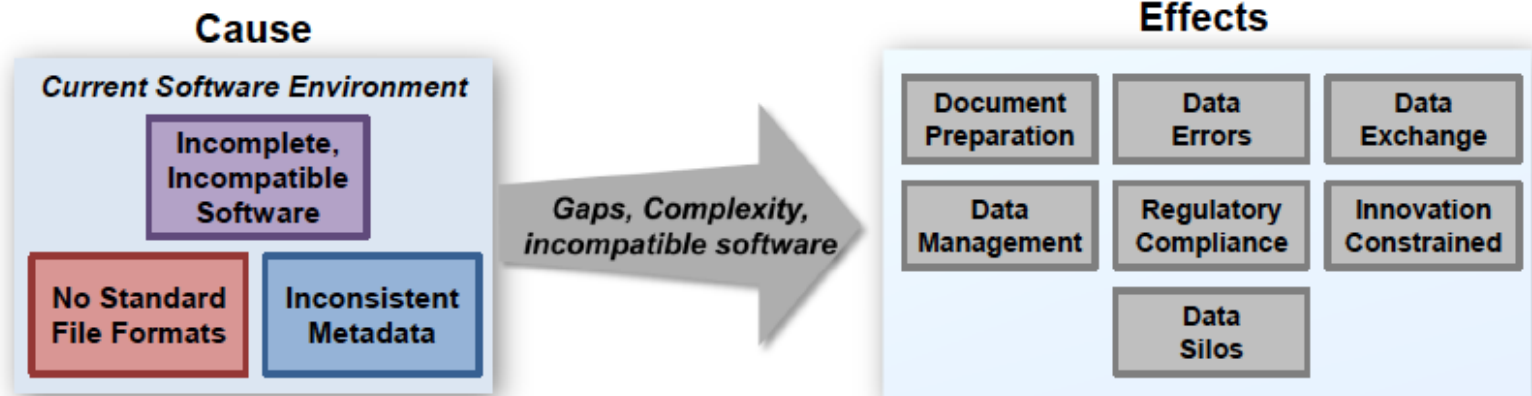
- An innovative approach to improve data integrity, reduce waste, and realize the full value of analytical data.

□ Current Members:

- | | |
|------------------------|-------------------|
| □ AbbVie | □ Eisai |
| □ Amgen | □ Genentech/Roche |
| □ Baxter | □ GlaxoSmithKline |
| □ Biogen Idec | □ Merck |
| □ Boehringer Ingelheim | □ Pfizer |
| □ Bristol-Myers Squibb | |

Key Challenges

□ The Allotrope Framework



Key Challenges

□ Future Priorities: the IQ Consortium

- ▣ How can we share ideas related to enabling laboratory technologies while maintaining protection of intellectual property rights for others, so that incentives for commercialization and publication remain intact?

Advantages	Challenges
Introduces Efficiency: ability to influence potential solution providers to address needs	Logistical and Managerial complexity in management of consortia
Minimizes Financial Impact	Understand and align on cost structure
Opportunity to Share Best Practices	Managing- IP-to maintain incentives for commercialization or publication
Leverages broad SME Pool	Average (or sum) of group's desires may not fit anyone's requirements

“Blue Sky” Challenges

□ Brainstorming Session

- ▣ Grand Challenges and Holy Grails: organic chemistry beyond Morrison & Boyd.
- ▣ Prediction in science using big data:
 - parameterization of organic chemistry
 - use of experimental design
 - development of complex models that relate back to reaction mechanism
- ▣ Development of robust kinetic models: “ab initio full kinetic modeling” as a goal.
- ▣ Real-time decision and control for smart manufacturing.
- ▣ Models for our reaction data to include ways to look at time-variant systems.

Educating Tomorrow's Workforce



- Defining the required workplace skill sets for future generations.
- Bringing the Lab of the Future to the classroom.
- Developing the significant opportunities for new teaching laboratories and new coursework that will enhance critical skills in data-rich science.
- Making meaningful connections with industrial research.

The Path Forward



- **Development of new educational models**
- **Development of a 'Cal Tech like' data rich experimentation hub**
- Development of new industrial/academic collaboration models
- Development of future grand challenges to be addressed through data rich experimentation

Acknowledgments

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Coming Up: CCR Meeting, May 2015



□ Disruption in Biotechnology and Process Chemistry:

The biotechnology sector, and process chemistry in general, have undergone significant radical changes in recent years and more is on the horizon. A wide variety of speakers will discuss these changes and their impacts on the chemical enterprise.

□ Speakers:

- ❖ Douglas Mans, GlaxoSmithKline
- ❖ Spencer Dreher, Merck
- ❖ Donna Blackmond, The Scripps Research Institute
- ❖ Sophie Vallon, Corning
- ❖ Mike Grady, DuPont