CHEMICAL SCIENCES ROUNDTABLE

LABORATORY AUTOMATION AND ACCELERATED SYNTHESIS:
Empowering Tomorrow's Chemist

A Virtual Chemical Sciences Roundtable Workshop

DAY 1
November 16, 2021

8:30 AM   **Welcome and Opening Remarks**

Linda Nhon
Associate Program Officer, Chemical Sciences Roundtable

8:40 AM   **Point-Counterpoint: What will the future of chemical laboratory automation mean for society?**

Martin Burke
University of Illinois at Urbana-Champaign

Nicola Pohl
Indiana University

9:00 AM   **Session I: Future of Laboratory Automation in Industry**

Session Chair: Robert Maleczka, *Michigan State University*

Panelists:

Spencer Dreher
Merck

Matt Bio
Snapdragon Chemistry

Benji Maruyama
Air Force Research Laboratory

Ying Wang
AbbVie

10:30 AM   ***Break***

10:45 AM   **Session II: Future of Laboratory Automation in Academia**

Session Chair: Anne LaPointe, *Cornell University*

Panelists:

Klavs Jensen
Massachusetts Institute of Technology

Lee Cronin
University of Glasgow

Andy Cooper
University of Liverpool

Nicholas Ball
Pomona College

Mimi Hii
Imperial Centre for Rapid Online Analysis of Reactions

Rachel Switzky
Siebel Center for Design, University of Illinois at Urbana-Champaign

Jin Cha
Chemical Synthesis, National Science Foundation

12:15 PM   **Virtual Poster Session and Lunch Break**

1:30 PM   **Introduction to Break-out Sessions: Modules, Resources, and Blueprints**

Timothy Jamison
Massachusetts Institute of Technology

Anne LaPointe
Cornell University

Shane Krska
Merck Research Laboratories

1:45 PM   **Adjourn To Breakout Sessions**

Breakout Session 1: Out of the Box: Providing the tools and resources needed to prepare undergraduates for automation

Facilitator: Arsalan Mirjafari, *Florida Gulf Coast University*

Goals: Identify learning objectives and then design a "box" that meets those objectives, that could be sent to undergraduate institutions, and that would contain all the elements needed to conduct an automation experiment and provide an automation "experience."

Breakout Session 2: Designing a textbook to implement automation in graduate research and funding opportunities.

Facilitator: Anne LaPointe, *Cornell University*

Goals: Identify learning objectives and then "design" an open source textbook for graduates and postgraduates that could serve as a resource, for example, for experiment design, automation types and sources, and funding opportunities.

Breakout Session 3: Advancing Automation and Beyond -- Creating a blueprint for consortia to share data and learn from each other

Facilitator: Shane Krska, *Merck Research Laboratories*

Goals: Identify the characteristics of a consortia to advance laboratory automation to diverse stakeholders and address the question as to how to create an inclusive system so that automation is advanced and a digital divide does not result. The ultimate goal is to create a consortium that can help to "democratize" synthesis.

3:30 PM   **Virtual Reception**

4:00 PM   **Adjourn Day 1**

DAY 2
November 17, 2021

9:00 AM   **Reporting from Breakout Groups and Discussion**

                     Breakout 1 – Arsalan Mirjafari, *Florida Gulf Coast University*

                     Breakout 2 – Anne LaPointe, *Cornell University*

                     Breakout 3 – Shane Krska, *Merck Research Laboratories*

10:15 AM   **Break**

10:30 AM   **Session III**: **The Promise of Automation**

                     Introduction to Speakers: Arsalan Mirjafari, *Florida Gulf Coast University*

10:35 AM   Self-driving Laboratories for Organic Materials- Alan Aspuru-Guzik
                     University of Toronto

10:55 AM   Food for Thought: Digital Manufacturing is Here; Shouldn't it Tie Into Upstream
                     Laboratory Research Automation? - Joseph DeSimone
                     Stanford University

11:20 AM   The Carnegie Mellon University Cloud Lab: Automating Science for the Future- Rebecca
                     Doerge
                     Carnegie Mellon University

11:45 AM   **Closing Remarks**

                     Martin Burke
                     University of Illinois at Urbana-Champaign

                     Nicola Pohl
                     Indiana University

12:00 PM   **Workshop Concludes**