Welcome to the Inaugural

CHAATS

Chemistry High-Throughput, Automation & AI Technologies

Tuesday, September 9th, 2025

AstraZeneca R&D Boston, Waltham, MA

Program

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Chemistry High-Throughput, Automation & AI Technologies

Agenda

When	What	Who	Where
Monday, September 8th, 2025 *(off-site)*			
6:00 – 8:00 pm	Welcome Dinner	Sponsored by Trajan	Brewer's Tap & Table
Tuesday, September 9th, 2025 *(on-site)*			
8:00 – 8:50 am	Registration with Breakfast	Sponsored by Unchained Labs	Atrium & M00.08
8:50 – 9:00 am	Introductory Remarks	Anthony Metrano & Iulia Strambeanu	Auditorium
9:00 – 9:45 am	Accelerating Synthesis: From Reactions to Recommendations	Amanda Dombrowski (AbbVie)	Auditorium
9:45 – 10:30 am	High-Throughput Experimentation to Enable Modality Agnostic Drug Discovery	Wei Liu (J&J)	Auditorium
10:30–10:45 am	Break		Atrium
10:45 – 11:30 am	Data-Rich Experimentation in the Development of Robust and Scalable Transition Metal Catalyzed Processes	Jake Ganley (BMS)	Auditorium
11:30 – 12:15 pm	Accelerating Reaction & Process Optimization in AZ Oncology Chemistry: HTE Workflows, Automation, & ImpACTs	Zirong Zhang (AZ)	Auditorium
12:15 – 1:15 pm	Lunch	Sponsored by ACD/Labs	Atrium & M00.08
1:15 – 2:15 pm	Round Table Discussion 1 *Dealing with Data*	Moderator: Kelsey VanGelder (Vertex)	Auditorium
2:20 – 2:40 pm	Reaction Screening and Synthesis of Macrocyclic Peptides on Resin Leveraging Direct to Biology (DtB) Assay Approaches	Ronald Ferguson (Merck)	Auditorium
2:40 – 3:00 pm	Enabling Self-Driving Labs for Synthetic Molecule Process Development	Adrian Ramirez Galilea (Takeda)	Auditorium
3:00 – 3:15 pm	Break	*Poster presenters to set up.*	Atrium
3:15 – 3:35 pm	An Automated Solubility Platform for Accelerating Process Development	Eileen M. Hoang (Sanofi)	Auditorium
3:35 – 3:55 pm	MicroCycle: A Fully Integrated DMTA Cycle Leveraging Automation and Machine-Learning to Accelerate Drug Discovery	Will Lau (Novartis)	Auditorium
3:55 – 4:15 pm	Enabling Chemistry Through Tractable High-Throughput Experimentation	Michael C. Nicastri (Biogen)	Auditorium
4:15 – 5:15 pm	Round Table Discussion 2 *HTE Automation:* *Bridging Innovation & Implementation*	Moderator: David Del Valle (BMS)	Auditorium
5:15 – 7:00 pm	Poster Session with Food/Drinks HTE Lab Tour in Groups	Sponsored by Trajan & AZ	Atrium & M00.08 N3.046 HTE Lab

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Speakers

Amanda Dombrowski, AbbVie

Accelerating Synthesis: From Reaction to Recommendations

The impact of HTC on projects has increased recently through utilization of the datasets generated over the years. First, creating easy access to the datasets allowed chemists to search for historical reactions applicable to their chemical matter. Next, analyzing the datasets enabled the identification of the top reaction conditions over many projects, which were integrated with other reaction condition recommendations in a centralized location. Furthermore, this dataset is being used to train machine learning models to predict reaction conditions.

Wei Liu, Johnson & Johnson

High-Throughput Experimentation to Enable Modality Agnostic Drug Discovery

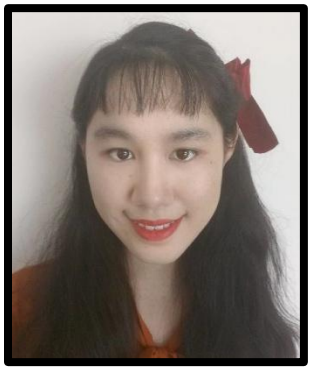
The talk will focus on the high-throughput chemistry capability at Johnson & Johnson. A brief overview of our organization and mission statement is followed by two case studies of automation-enabled parallel library synthesis and direct-to-biology in the linker optimization of protein degraders.

Jake Ganley, BMS

Data-Rich Experimentation in the Development of Robust and Scalable Transition Metal Catalyzed Processes

Cumulative learnings from the 15-year history of the Catalysis Group in the Chemical Process Development department at BMS will be shared. Special focus will be paid to the workflows and practices leveraging data-rich experimentation, and how these impact route invention, process invention, and process characterization of transition-metal catalyzed processes. Lessons learned pertaining to the factors that impact the translation of hits from HTE to large scale processes will also be shared.

Zirong Zhang, AstraZeneca



Accelerating Reaction & Process Optimization in AZ Oncology Chemistry: HTE Workflows, Automation, & ImpACTs

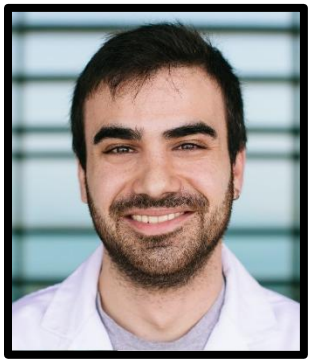
This talk will introduce the Adaptive Chemistry Team (ACT) model in AstraZeneca Oncology Targeted Discovery and how we built our automated HTE capabilities. It will discuss our HTE workflows, how they are utilized in reaction and process optimization, and the impacts on our portfolio.

Ronald Ferguson, Merck

Reaction Screening and Synthesis of Macrocyclic Peptides on Resin Leveraging Direct to Biology (DtB) Assay Approaches

With an increased emphasis on peptides as synthetic targets for Merck drug discovery projects, the HTE group has focused on common or re-occurring challenges in the preparation of these complex, BRo5 (beyond rule of 5) molecules. We address the challenges with a focus on excellence in chemistry, delivering compounds of high product conversion, and routinely deliver libraries of 96 to 384 products, synthesized at nano to micro-scale, screened in DtB (direct to biology) assay workflows. Here we share recent advances and impact where LSF (late stage functionalization) tools have been applied to modify peptide residues preparing novel, non-canonical residues in the final/growing chain peptide products. LSF reactions are applied to the resin bound or solution phase peptides, expanding the diversity of ncAAs while avoiding the previous need to prepare custom Fmoc-protected amino acids to be used in traditional amide coupling reactions.

Adrian Ramirez Galilea, Takeda



Enabling Self-Driving Labs for Synthetic Molecule Process Development

Takeda's Synthetic Molecule Process Development (SMPD) department has significantly built up its high-throughput experimentation (HTE) and automation capabilities over the last few years. While we are investing in a variety of different devices and approaches, our ultimate vision is to design and implement self-driving labs (SDLs) to carry out self-optimizing workflows. Process development and optimization frequently involves exploring wide parameter spaces, making these iterative algorithm-guided SDLs ideal for such optimizations, especially when coupled with automated HTE synthesis planforms. As such, we herein present our vision for fully self-optimizing HTE workflows, with the ultimate goal of creating SDLs with workflows optimized for a variety of general applications needed in synthetic molecule drug development. These workflows use a combination of commercial and custom automation tools in conjunction with Bayesian Optimization to guide experimentation. To illustrate this process, case studies will be presented, highlighting both their successes as well as the limitations of our current hardware and software tools.

Eileen M. Hoang, Sanofi

An Automated Solubility Platform for Accelerating Process Development

Compound solubility is a critical parameter for chemical process development at each step of API synthesis, but manual screening across multiple solvents and temperatures is generally a resource-consuming task. Sanofi's high-throughput laboratory automation platform has translated our manual solubility workflow to a robotic system in order to accelerate key chemical development decisions. Future goals include a closed-loop integration with Sanofi's machine learning models for fully automated solvent composition and temperature optimization.

Will Lau, Novartis

MicroCycle: A Fully Integrated DMTA Cycle Leveraging Automation and Machine-Learning to Accelerate Drug Discovery

We have developed an integrated drug discovery platform "MicroCycle" that utilizes plate-based microscale chemistry, micro-purification and automated analysis, real-time physicochemical and absorption, distribution, metabolism, and excretion (ADME) characterization in combination with data-driven compound design, leveraging both machine learning (ML) and computational techniques. MicroCycle was generated within the Novartis' internal idea incubator "Genesis Laboratories" as part of the first cohort and realized through a multidisciplinary team of Novartis Biomedical Research (NBR) scientists with the vision to revolutionize the design-make-test-analyze (DMTA) cycle to accelerate drug discovery. We applied active learning toward building generalizable yield models for reactions including a Ni-photoredox catalyzed cross-electrophile coupling of aryl and alkyl bromides, and Bayesian optimization for library design utilizing predictive models for activity and properties.

Michael C. Nicastri, Biogen

Enabling Chemistry Through Tractable High-Throughput Experimentation

Micro-scale parallel chemistry has become the most efficient way of collecting data for chemical reactivity. However, easy to use and scalable tools are required to enable chemists to conduct HTE efficiently. Automation, both in the lab and in the digital space, is vitally important to reduce the barrier to entry for laboratory scientists and make experiments tractable. I will introduce custom tools and automation we have implemented to bootstrap an HTE chemistry platform at Biogen which spans medicinal chemistry through process chemistry. I will present an application of this platform for reaction optimization and synthesis at Biogen. I will demonstrate how the tools created for HTE chemistry enabled the rapid startup and development of microscale library synthesis for medicinal chemistry at Biogen.

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Round Table Discussions

Please join us for two round table discussion sessions in the Auditorium throughout the day. Although presented in the same room as our more formal talks, we encourage open discussion and participation as we dive into these relevant topics.

Round Table Discussion 1:
Dealing with Data

Kelsey VanGelder, Vertex

Topics:

- Best practices & pain points for:
  - data capture
  - visualization

Round Table Discussion 2:
HTE Automation: Bridging Innovation & Implementation

David Del Valle, BMS

Topics:

- HTE's Cost Paradox: How Much Does Automation Really Save Time/Money?
- End-User HTE (Democratizing Automation)

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Poster Presentations

1. **Iulia I. Strambeanu,** Johnson & Johnson
   Automated High-Throughput Chemistry to Enable Synthesis Modeling/AI in Drug Discovery

2. **Richard S. Morales,** AstraZeneca
   Leveraging Automated High-Throughput Experimentation to Accelerate Synthesis in AstraZeneca Oncology Chemistry

3. **Noah Tu,** AbbVie
   ChemBead Technology: Applications and New Developments

4. **Chen Wu,** Vertex
   High-Throughput Methodology for Efficient Pd Removal

5. **Manali Kadam,** Alexion, AstraZeneca Rare Disease
   Powder Patrol: Live Error Detection in Automated Solid Dispensing with Computer Vision

6. **Adam Beard,** Merck
   High-Throughput Library Synthesis and Purification at Merck

7. **Vanna Blasczak,** Biogen
   High-Throughput Ozonolysis of Complex Intermediates for Parallel Synthesis

8. **David Del Valle,** BMS
   Upgrading our Toolbox to Enhance the Speed, Efficiency, and Return on Chemical Exploration

9. **Simon Berritt,** Pfizer
   Expediting Medicinal Chemistry Programs Utilizing HTE

10. **Zachary Weinstein,** Vertex
    Software-Driven Innovations to Address Challenges in Automated Chemical Synthesis

11. **Sung-Min Hyun,** Merck
    Data-Driven Improvement of Compound Design in Drug Discovery: Leveraging Synthesis Data in Design and Synthesis

12. **Yamin Htet,** AstraZeneca
    Developing a Global Scalable, Modular, and Integrated Analytical Workflow Management Tool

13. **Shane Stone,** Vertex
    Democratization of Scientific Code at Vertex - Accessibility for Non-coding Scientists

14. **Jules Lee,** Novartis
    An Automated Platform for High-Throughput // Medicinal Chemistry Active Learning Libraries

CHAATs 2025 Organizers

Anthony J. Metrano

AstraZeneca

Iulia I. Strambeanu

Johnson&Johnson

Special Thanks to:

Richard S. Morales, Oleg Epstein, & Zirong Zhang (AstraZeneca)

**CHAATs logos developed in collaboration with Joseph M. Metrano.*

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