North Jersey Chromatography Group (NJCG) & Women Chemists Committee Joint Webinar

Featured Topics

1) Automating Method Development and Data Analysis for Chromatography with Machine Learning

2) Multifactor Modeling of Biotherapeutic Separations to Enable in Silico Robustness

Guest Speakers

Bob Pirok, Ph.D.
Assistant Professor,
Universiteit van Amsterdam,
Netherlands

Eli Larson, Ph.D.
Senior Scientist
Merck, NJ

Joe Dodd-O, Ph.D.
Postdoc Research Assistant
Vivek Kumar Lab,
University of Houston, TX

10:00 AM – 11:30 AM (EST) March 27, 2026

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For More Information or Questions, Email us at: NJCG1234@gmail.com

Automating Method Development and Data Analysis for Chromatography with Machine Learning

Bob Pirok, Ph.D.
Assistant Professor,
Universiteit van Amsterdam, Netherlands

Abstract

Artificial intelligence is rapidly reshaping how we design, optimize, and evaluate analytical methods. In liquid chromatography-mass spectrometry (LC-MS), machine learning approaches, particularly Bayesian optimization (BO), offer the potential to revolutionize method development by accelerating decision-making, improving analytical Quality by Design (AQbD) practices, and enabling more systematic exploration of experimental space. Recent advances with the AutoLC platform have shown that fully closed-loop, unsupervised method development is not only feasible, but can operate robustly without human intervention, highlighting the growing maturity of AI-driven workflows.

At the heart of BO lies its kernel: the mathematical structure that encodes assumptions about chromatographic response surfaces and governs how the algorithm learns from data. Despite its importance, kernel choice is often treated generically, even though LC-MS method parameters follow well-defined physicochemical relationships that could be explicitly leveraged. In this talk, we will explore how different kernel families, default, ANOVA-style, stick-breaking, and entropy-search portfolios, shape optimization behavior in automated LC-MS workflows. We discuss how domain knowledge, chromatographic response functions, and mechanistic constraints may be incorporated into kernel design to better reflect realistic method-development landscapes. The presentation outlines a framework for evaluating kernel suitability and highlights how knowledge-guided kernels may enhance future AI-driven method development systems.

The automation of chromatographic method development is increasingly moving from expert-driven trial-and-error toward data-driven, self-optimizing workflows. While advances in instrumentation and optimization algorithms have made such automation technically feasible, its success ultimately depends on how effectively information can be extracted and interpreted from chromatographic data.

This challenge is particularly evident in comprehensive two-dimensional chromatography (LC×LC and GC×GC), where routine analysis can involve large series of samples and thousands of peaks per chromatogram. Manual comparison across runs is infeasible, making automated data interpretation a prerequisite rather than an optional add-on. In computational method development, where conditions are intentionally varied, the problem becomes even more complex and requires robust peak tracking across changing separation landscapes.

Data-driven method development strategies increasingly rely on retention models and machine-learning approaches to explore experimental parameter space efficiently, with goals ranging from improved selectivity to sustainability and cost efficiency. These approaches reduce, but do not eliminate, the need for explicit peak tracking by learning from structured chromatographic information. However, they expose a fundamental paradox: high-resolution separations are required to generate reliable training data, yet computational methods are themselves needed to guide the development of such separations.

In this presentation, we will outline our view on automated method development in chromatography and discuss recent advances from our group in retention-time alignment, peak tracking, and machine-learning-assisted data interpretation. Together, these developments illustrate how improved extraction and structuring of chromatographic information is enabling closed-loop, data-driven optimization and bringing comprehensive 2D chromatography closer to routine analytical practice.

Biography

Bob Pirok obtained his PhD in 2019 in Amsterdam, defending two books of research, with the distinction cum laude and worked before at Shell. He is currently tenure-track assistant professor at the University of Amsterdam and focuses on the application of chemometrics to analytical chemistry with a special interest in method development and data analysis for multi-dimensional chromatography. Other areas of interest include retention modeling and (reaction) modulation techniques for LC×LC.

Pirok is visiting research professor at Gustavus Adolphus College in the group of Prof. Dwight R. Stoll. He is also visiting researcher in the group of Prof. André de Villiers of the Stellenbosch University in South Africa.

He received a number of international recognitions, including a Shimadzu Young-Scientist Award at HPLC2015 Beijing, the Young-Scientist-Award Lecture during the SCM-8 meeting in Amsterdam in 2017, the Csaba Horváth Young-Scientist Award at HPLC2017 Prague, the Journal of Chromatography Award during the ISCC Conference in Riva de Garda in 2018, and the SCM Award at the SCM-9 meeting in Amsterdam in 2019.

Pirok is the writer of the recently granted 1.2M€ NWO ENW-PPS TA PARADISE proposal coordinated by PI Prof. Arian van Asten. He was selected as Early Career Board member for the ACS journal Analytical Chemistry starting from 2021.

Multifactor Modeling of Biotherapeutic Separations to Enable in Silico Robustness

Eli Larson, Ph.D.
Senior Scientist
Merck, NJ

Abstract

Ensuring chromatographic method robustness is critical for method validation and deployment in a QC environment. Traditionally, robustness assessment is conducted via extensive design-of-experiments (DoE) studies using parameters known to impact the assay. Determining the appropriate range of input values for traditional DoE is challenging, and it is often difficult to ensure success during the first set of experiments. In silico modeling has been extensively used to map the separation landscape of multicomponent mixtures and can be leveraged to optimize methods and assess robustness as a function of various factors, while greatly reducing the experimental burden relative to DoE approaches. Although this strategy has been demonstrated with great success for small molecules, its utility for biologics has been very limited until recently due to the complexity of biotherapeutic separations. Here, we introduce a new approach to enable three-dimensional (3D) in silico method robustness assessment using the ACD/Labs LC Simulator to model a hydrophobic interaction chromatography (HIC) method for determining the drug-to-antibody ratio (DAR) of a high DAR antibody–drug conjugate. We further extend this approach to create a 3D robustness model of an ion exchange chromatography (IEX) method for measuring charge variants of a monoclonal antibody. Finally, we report a new strategy to study the impact of column lot variability and enable four factor visualization of method robustness using a custom Python script to compare 3D models. This work demonstrates the strong potential of in silico robustness studies to accelerate method validation, ensure best science first (ab initio), and increase the depth of data understanding through new data visualization approaches.

Biography

Eli began studying separations while completing his undergraduate work at Gustavus Adolphus College in the lab of Professor Dwight Stoll, studying the impact of the dimensional interface in two-dimensional liquid chromatography systems. He completed his doctorate at the University of Wisconsin-Madison under the mentorship of Professor Ying Ge, developing new front-end separations for top-down proteomics with emphasis in antibody-drug conjugate characterization by Fourier transform ion cyclotron resonance mass spectrometry and trapped ion mobility spectrometry. In 2023, Eli joined the Analytical Enabling Capabilities group at Merck as a Senior Scientist based in in Rahway, NJ, where he focuses on development and deployment of new assays for biotherapeutics and vaccines.

Title: TBD

Joe Dodd-O, Ph.D.
Postdoc Research Assistant
Vivek Kumar Lab, University of Houston, TX

Abstract

Artificial intelligence is considered a key tool for the strategic growth of many biopharmaceutical and biotechnology companies, but the mechanics of how it works can be abstracted behind industry specific terms and proprietary algorithms. This brief talk aims to demystify AI as a concept, provide a brief overview of some of the algorithms used to make AI models, and provide examples on how each are used. Examples include models used to design and model new molecules and algorithms developed to optimize processes in chemical manufacturing.

Biography

Joseph Dodd-o recently completed his dissertation in Biomedical Engineering under the direction of Dr. Vivek Kumar at the New Jersey Institute of Technology. During his PhD, he developed a team of undergraduate and graduate students to design new peptide sequences using a suite of computational tools, including diffusion models for both docking screens and novel amino acid designs. Currently, Joe is training several laboratories on developing the same competencies, taking individuals with no background in scientific computing and developing them into individuals that can effectively use high-performance computing resources to answer scientific questions. Before his PhD, Joe was a process engineer for ExxonMobil corporation, with solutions earning millions of dollars for the company. Joe has used his Chemical Engineering knowledge to consult for Imubit Corporation, providing a business case for their transition from Petrochemical to Biopharmaceutical AI enhanced process stewardship.