Future Trends in HPLC Column Technology

Gert Desmet*]
Department of Chemical Engineering, Vrije Universiteit Brussel, Pleinlaan 2, 1050 Brussels, Belgium.

*Email: gert.desmet@vub.be

Column technology remains at the forefront of chromatographic advancements, enabling greater resolution, speed, and efficiency in separations. This lecture will explore the state-of-the-art innovations shaping the field, focusing on three transformative developments: micro-pillar array columns, 3D-printed chromatographic supports, and multi-capillary channel systems.

Micro-pillar array columns represent a paradigm shift in stationary phase design. By employing precisely engineered microstructures, these columns deliver superior separation efficiency, reduced backpressure, and enhanced reproducibility. Their potential applications in high-throughput and miniaturized analytical workflows will be discussed, highlighting their compatibility with modern liquid chromatography systems.

Additive manufacturing has revolutionized chromatographic support fabrication. The advent of 3D printing enables the creation of intricate and customizable stationary phases with unprecedented control over geometry and porosity. This lecture will examine how these supports enhance mass transfer, reduce eddy diffusion, and expand the horizons for novel stationary phase chemistries.

Finally, multi-capillary channel columns introduce a multi-dimensional approach to chromatographic separation. By leveraging parallel capillary pathways, these systems achieve faster analyses without compromising resolution. Key insights into their design, integration with existing chromatography platforms, and potential for ultra-fast separations will be presented.

Together, these innovations underscore the rapid evolution of column technology, addressing the growing demands for efficiency, sensitivity, and sustainability in analytical separations. Attendees will gain an understanding of these cutting-edge developments and their implications for future research and industrial applications.

Keywords: 3D printing, stationary phase, kinetic performance, band broadening

In vivo cross-linking mass spectrometry to decipher large scale protein conformations and interactions

Qun Zhao, Lihua Zhang*, Yukui Zhang
Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 457 Zhongshan Road, Dalian 116023, China

*Email: lihuazhang@dicp.ac.cn

In vivo cross-linking mass spectrometry (CX-MS) enables the large-scale analysis of protein conformations and interactions in living cells, but challenges remain in biocompatibility, cross-linking coverage and identification sensitivity. To address these issues, we designed various biocompatible, multifunctional, and membrane-permeability adjustable cross-linkers, and established the methods for enrichment, identification and data-mining of crosslinked peptides.

A glycosidic bond-based MS-cleavable cross-linker of trehalose disuccinimidyl ester was designed and synthesized, which was not only of excellent biocompatibility for living cells, but also could be fragmented in MS under CID/HCD, simplifying the cross-linked peptides to conventional single peptides via selective cleavage between glycosidic and peptide bonds. Furthermore, the crosslinked peptides could be enriched by HILIC materials, enabling the identification of over 6000 and 1000 cross-linked peptides from 1E7 and 1E3 cells respectively by one LC-MS run, making the applications in primary cells and tissues possible.

By integrating targeted proximity labeling and in vivo cross-linking, we identified 327 PPIs in stress granule, with 78 upregulated upon $NaAsO_2$ stimulation and 30 showing high confidence ($p < 0.05$) among which 63% matched known interactions, while 11 were novel, involving functions such as DNA/RNA processing and protein translation. Enhanced interactions under stress were validated by fluorescence colocalization and Western blot, and further confirmed for both high- and low-confidence novel PPIs by co-immunoprecipitation, highlighting new PPIs related to translation and mRNA regulation. These results demonstrate that in vivo CX-MS enables the comprehensive analysis of dynamic protein assemblies in living cells, offering a powerful tool to elucidate the mechanisms underlying cellular compartmentalization and rapid responses.

Furthermore, protein dynamics play a crucial role in executing diverse functions. The intracellular environment significantly influences protein dynamics, particularly for intrinsically disordered proteins. Recently, we developed a hierarchical decoding strategy enabling comprehensively capture structural information from various proteins within cells and characterize protein dynamics. Computational analysis based on distance restraints derived from cross-links was used to infer protein dynamics, facilitated by the prior structure obtained from AlphaFold2. Furthermore, we can provide a comprehensive description of the intrinsic motion of IDPs, demonstrating the potential in understanding the protein functions in cells.

Keywords: CX-MS, *in-vivo* analysis, protein conformation, protein-protein interaction

From Sample to Data: Enhancing Analytical Workflows with Automation

Kyoko Watanabe [a, b]

[a] *R&D Center (CA), Shimadzu Scientific Instruments, 7060 Koll Center Parkway, Pleasanton, CA, 94566, USA.*

[b] *LC Business Unit, Analytical & Measuring Instruments Division, Shimadzu Corporation, 1, Nishinokyo, Kuwabara-cho, Nakagyo-ku, Kyoko, 6048511, Japan*

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*Email: kywatanabe@shimadzu.com

Abstract body (up to 350 words)

Chromatography and mass spectrometry are indispensable tools across diverse research fields, from pharmaceutical development to environmental monitoring. Improving chromatographic and mass separation performance, as well as detection selectivity, not only enhances data quality but also drives innovations toward more efficient and reproducible analytical workflows.

In parallel, laboratory automation has advanced rapidly. The integration of artificial intelligence (AI) and machine learning (ML) in research supports experimental design, parameter optimization, and data processing. While these technologies reduce human error and improve analytical consistency, they can also create new challenges: automated workflows often generate large numbers of samples that require preparation, instrumental analysis, and post-processing, potentially extending the time needed to obtain final results unless the entire workflow is optimized. Advances in separation science have improved the efficiency of data acquisition; however, bottlenecks remain, particularly in sample preparation and analytical method development, which often involve labor-intensive operations and repeated trial-and-error cycles.

To address these challenges, Shimadzu has developed solutions that support lab automation with a focus on sample preparation and method development. Examples include automated platforms for sample clean-up, dilution etc., as well as AI-assisted workflows for rapid chromatographic method optimization. These technologies aim to reduce manual workload, shorten turnaround time, and improve reproducibility.

By integrating automation across the entire analytical workflow—from sample preparation to data interpretation—laboratories can achieve higher throughput and better resource utilization. Moreover, these approaches contribute to more sustainable operations by reducing waste, energy consumption, and overall environmental impact. The examples which will be discussed illustrate how combining separation technologies with intelligent automation can help laboratories meet the growing demands of modern research efficiently and sustainably.

Keywords: HPLC, LC/MS, Laboratory Automation

Emerging Trends in AI for Chemistry and Its Applications to Analytical Chemistry

Ryo Yoshida*

The Institute of Statistical Mathematics, Research Organization of Information and Systems

*Email: yoshidar@ism.ac.jp

Artificial intelligence (AI), as a next-generation deep technology, holds the potential to transform a wide range of scientific and societal domains fundamentally. In this lecture, we explore the emerging potential of AI in chemistry and materials science, with particular emphasis on its applications for analytical chemistry.

A critical prerequisite for enabling transformative advances through AI is the development of large-scale, high-quality foundational training datasets. However, in many areas of chemical research, obtaining sufficient data to train AI models remains a significant challenge.

To address this issue in the field of polymer science, we have constructed the world's largest computational property database for polymers, encompassing diverse physical properties for over 100,000 unique polymer structures. This omics-scale database was generated using RadonPy, a Python-based, fully automated pipeline for all-atom molecular dynamics simulations of polymeric materials.

Machine learning models pretrained on the RadonPy database can be fine-tuned with limited experimental data to perform a variety of real-world downstream tasks, achieving superior generalization performance compared to models trained from scratch. Notably, the generalization capability of these pretrained models increases significantly with the size of the RadonPy database, following a power-law scaling behavior across multiple prediction tasks—underscoring the importance of large, high-fidelity simulation datasets.

Building on this case study, we explore the potential applicability of AI in analytical chemistry. In particular, we present an application example focused on retention time prediction in liquid chromatography.

Surrogate Optimization using Multivariate Adaptive Regression Splines for On-Line Supercritical Fluid Extraction – Chromatography Method Development

Kevin A. Schug*[a], Niray Bhakta[a], Jaivardhan Sood[b], Yujing Yang[b], Chen Kan[b], Jay Rosenberger[b], Victoria Chen[b]

[a] *Department of Chemistry & Biochemistry, The University of Texas at Arlington, 700 Planetarium Pl. Box 19065, Arlington, Texas 76019, USA.*

[b] *Department of Industrial Systems & Manufacturing Engineering, The University of Texas, Arlington, Texas 76019, USA.*

*Email: kschug@uta.edu

Abstract

It is valuable to have multivariate optimization strategies for analytical instruments, such as supercritical fluid extraction – supercritical fluid chromatography – mass spectrometry (SFE-SFC-MS), a sophisticated on-line sample preparation and analysis system. SFE-SFC-MS has a very wide application base, but its optimization involves the consideration of many variables and variable interactions. Attempts using factorial design and response surface methodology (RSM) was generally successful [1], but clearly revealed the potential for complex response surfaces, which were highly variable with sample type and analyte type. To advance this methodology, we are developing a surrogate optimization (SO) approach. Rather than collecting a full data set of responses at different variable settings, as with RSM, SO uses an iterative process. The SO model is built in sequence with smaller sets of runs, so that an explore-and-exploit strategy for studying variable space can make more efficient use of experimental runs. SO can also accommodate more complex modeling algorithms. Multivariate adaptive regression splines provide the potential for multi-linear modeling of complex response surfaces. A series of pharmaceutical compounds were considered. From the set, a representative subset was chosen using molecular encoding techniques. The molecular encoding of chemical structures also enables a quantitative assessment of analyte similarity, so that the performance of similar and dissimilar chemical compounds can be assessed. Different response output functions were evaluated, including a composite response function that includes evaluation of extraction efficiency, chromatographic efficiency, peak symmetry, and the reproducibility of each. SO is an effective optimization process can be completed in fewer runs than RSM. Current efforts are aimed toward a) multi-analyte optimization and understanding the overlap of response surfaces based on molecular similarity, and b) the comparison of optimized extraction and analysis conditions for different analytes from different sample matrices. This work benefits from the integration of a variety of data science tools with analytical method optimization; we are just scratching the surface of possibilities.

Keywords: Pharmaceutical; multivariate optimization; response modeling; data science; molecular encoding

References

[1] A.P. Wicker, K. Tanaka, M. Nishimura, V. Chen, T. Ogura, W. Hedgepeth, ***Anal. Chim. Acta***, 1127, 282-294, 2020.