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## Resolving the chemical space: a legacy of recording separation science and innovation in *Analyst*

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From its humble beginnings in filtration, distillation and crystallisation, separation science as a unique scientific discipline has continuously evolved over the decades into a major underpinning field of technology. It supports all areas of science and discovery, and itself is an innovative fundamental science, enabling us to explore, protect and improve both our planet and everyday lives. Given this significant place in the field of analytical chemistry held by the separation sciences, it is particularly appropriate that we have the opportunity and honour to present this themed virtual issue dedicated to separation science as *Analyst* celebrates its 150<sup>th</sup> anniversary. The collection is a testament to the continuing challenge to identify and quantify the most complex materials at the molecular level, and thus better understand our world.

It is difficult to write about the evolution of separation science without mention of Mikhail Tswett's ground-breaking discovery of a new chromatographic process in 1903. Ever since this landmark discovery, *Analyst* has been a home for reporting advances in all fields of chromatography and related separation science research. One of its earliest articles exemplified how paper chromatography was already transforming

chemical analysis in 1952.<sup>1</sup> Of course, in that same year, separation science was recognised on the world stage with a Nobel Prize in Chemistry, awarded to two British scientists, Archer J. P. Martin and Richard L. M. Synge “for their invention of partition chromatography”, which provided both a theoretical underpinning and global momentum for chromatographic analysis. From then on, the field expanded into gas (GC), liquid (LC) and supercritical fluid chromatography (SFC), electrophoresis, and eventually capillary- and microfluidic-scale techniques, many of which were first discussed, refined, and debated within *Analyst*'s pages. This journey of discovery and development of course continues, with the 2025 Nobel Prize in Chemistry recognising the development of metal-organic frameworks (MOFs) by Susumu Kitagawa, Richard Robson, and Omar M. Yaghi. Their work on porous, modular architectures currently inspires modern separation science, particularly phase design for improved separation capacity, selectivity and efficiency, including several MOF based articles published in this themed issue (<https://doi.org/10.1039/D5AN00127G>, <https://doi.org/10.1039/D5AN00468C>, <https://doi.org/10.1039/D5AN00548E>). The coupling of many orthogonal separ-

ation techniques with mass spectrometry (MS) arguably represents one of the most ground-breaking advances in analytical science with significant capability gained across many exploratory fields. As part of the RSC Separation Science Interest Group's activities, it is particularly pleasing to include herein a contribution by its recent 2025 Knox Medallist, G. John Langley, on the combined use of GCxGC-MS, SFC-MS and SFC-FID to screen and classify hydrogenated vegetable oils (<https://doi.org/10.1039/D5AN00429B>).

Modern separations are no longer a standalone laboratory methodology, but a central element of comprehensive analytical workflows. Remarkable gains in sensitivity, speed and resolution have been achieved to the point where hundreds to thousands of molecules can be separated and detected in just a few minutes, often in very small samples, including for example, in single cells.<sup>2</sup> Arising from this is a digital revolution which is now transforming the field. Harnessing new analytical knowledge from “big data” is a major focus that sometimes boggles the mind in terms of its multidimensional scale. In these past 150 years, we have rapidly moved from separating relatively simple mixtures to characterising entire libraries of chemi-

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cals, as well as understanding and even predicting the possibilities and mechanisms to separate them.<sup>3</sup> Artificial intelligence, machine learning, and chemometrics are now routinely used to design and optimise separations towards (hopefully) qualitatively and quantitatively mapping and extending the measurable chemical space (<https://doi.org/10.1039/D5AN00323G>).<sup>4</sup> This overwhelming thirst for more data has also been met by advances in throughput, ranging from sample handling and preparation to rapid analysis (<https://doi.org/10.1039/D5AN00787A>). Miniaturised and portable systems are democratising analysis, bringing separation capabilities to the point of need in healthcare, food safety, and environmental monitoring (<https://doi.org/10.1039/D5AN00482A>). The field

has also been reflexive and embraced sustainability, with greener analytical instrumentation and methods, recyclable materials, and low-energy systems that align analytical progress with environmental responsibility.

The contributions collected here showcase not only technical innovation, but also the creativity, curiosity, and collaboration that define our community. As Guest Editors, we are proud to witness and highlight the breadth of separation science today and its central role in analytical chemistry's ongoing evolution. As we look to the next 150 years, one principle endures: separating mixtures represents a gateway to meaning. We hope this anniversary issue will inspire both reflection on the remarkable legacy of the field and

anticipation for the discoveries yet to come.

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