

LETTER

Artificial Intelligence: A Transformative Ally in Analytical Chemistry

Lucía Pareja¹ , Ignacio Machado²  

¹*Departamento de Química del Litoral, Cenur Litoral Norte, Universidad de la República, Uruguay*

²*Grupo de Bioanalítica y Especiación (BIOESP), Facultad de Química, Universidad de la República, Uruguay*

The scientific landscape is undergoing a profound transformation driven by artificial intelligence (AI). While its influence is already evident in disciplines such as bioinformatics, materials science, and drug discovery, analytical chemistry has only now begun to fully embrace its potential.¹ Yet, few areas could benefit more from the structured, data-rich nature of AI than the analytical sciences themselves. Analytical chemistry has always been the discipline of signals, patterns, and interpretation. In that sense, analytical chemistry could be regarded as a conceptual precursor to machine learning thinking, long before the modern algorithms existed.

AI provides an unprecedented opportunity to enhance analytical workflows, at every stage, from experimental design and method development to data processing, interpretation and decision-making.² Machine learning models can optimize instrumental conditions, uncover hidden correlations between parameters, and automate complex calibration or validation procedures. For several years now, the trend has been toward the use of miniaturized and more environmentally friendly methodologies, and in this regard the development of AI can be of great help to improve existing greenness-assessment algorithms, providing smarter, more sustainable analytic protocols with lower sample and solvent consumption. In spectroscopic and chromatographic analyses, AI algorithms are increasingly capable of distinguishing genuine analytical signals from background noise or matrix interferences, enabling faster and more reliable quantification and identification.² Beyond improving performance, AI is redefining the very role of the analytical chemist—from manual operator to data curator and critical interpreter. AI may also facilitate structural elucidation of unknown compounds, possibly offering a cost-effective alternative to expensive commercial spectral libraries or extensive manual interpretation workflows.

However, this transformation brings certain challenges. AI systems must be transparent, explainable, and validated according to the same rigorous standards that govern traditional analytical methods.³ The “black box” problem remains one of the greatest barriers to trust and acceptance. It is essential that machine-learned models complement, rather than replace, human expertise — that they become partners in analytical reasoning, not substitutes for it. This balance between automation and understanding is central to the spirit of analytical chemistry.

The adoption of AI also requires rethinking education and training. Future analytical chemists will need to navigate not only spectral lines and chromatograms but also fluency in algorithms, datasets, and validation metrics^{1,3} Integrating AI literacy and data science skills into analytical chemistry curricula is no longer optional: it is a prerequisite for keeping the discipline relevant and forward-looking. Those who understand how to merge chemical intuition with computational power will lead the next generation of analytical breakthroughs.

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The essence of analytical chemistry has always been about transforming raw data into knowledge. In this new era, artificial intelligence emerges not just as a tool, but as a collaborator in that pursuit. The challenge—and opportunity—lies in ensuring that as machines learn to think, we do not lose our capacity to question. The analytical chemist of tomorrow will not merely measure, they will also design, model, predict, and interpret. Embracing AI is not the end of analytical chemistry as we know it—it is its most exciting reinvention.

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Lucía Pareja is a pharmaceutical chemist and holds a PhD in Chemistry. She is a professor in the Department of Chemistry of Litoral at Cenur Litoral Norte, University of the Republic, Uruguay. As a researcher, her work focuses on assessing the presence of organic contaminants at trace levels to address the multiple problems their presence causes in food and the environment. To achieve this, she develops robust analytical methods based on mass spectrometry that allow for the determination of compounds at trace levels. The main objective of this work is the development of multi-class, miniaturized, and environmentally friendly analytical methodologies, following, as far as possible, the principles of green chemistry, for application to problems of national interest.



Ignacio Machado is Associate Professor of Analytical Chemistry at the Faculty of Chemistry, Universidad de la República, Montevideo, Uruguay. He works mainly on atomic spectrometry and mass spectrometry, with a focus on bioanalytical chemistry. He was a postdoc researcher at the Department of Trace Element Analysis, the Institute of Analytical Chemistry of the ASCR, Prague, Czech Republic, in 2017. He has been a member of the Academic Assembly of Faculty of Chemistry, Universidad de la República, since 2018, and the International Medical Geology Association (IMGA) since 2019. He has been a researcher for the National System of Researchers (SNI, Uruguay) since 2016, and of the Basic Sciences Development Program – Chemistry Area (PEDECIBA – Química, Uruguay) since 2017. He is responsible for the BIOESP Group