POINT OF VIEW

Chemometrics versus Chemical Metrology

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Chemometrics and chemical metrology, two singular disciplines increasingly used in analytical chemistry, are known for their reliability, capability, and efficiency. Chemometrics applies mathematical and statistical methods based on computational tools to extract information, identify patterns, and develop models from analytical data in chemistry. It is particularly effective for applying multivariate analysis techniques to analyze non-trivial chemical systems, such as spectroscopy and chromatography. Chemometrics can identify and quantify chemical measurands, predict properties, classify sample sets, provide pattern recognition, establish suitable regression curves, maximize or minimize experimental conditions, characterize performance and figures of merit, perform multivariate analyses, etc.

On the other hand, metrology is the science of measurement. It involves establishing, maintaining, and applying state-of-the-art measurement standards, developing new measurement techniques, and searching for guaranteed reliability of results. Metrology ensures the accuracy, precision, reliability, and traceability of measurements by defining and maintaining measurement units and standards traceable to the International System of Units (SI). It comprises the calibration of instruments, validation of analytical methods, evaluation of measurement uncertainties (both sampling and analytical), comparability of measurement methods, and compliance assessment.

While chemometrics deals with analyzing and interpreting data in analytical chemistry, metrology focuses on the quality assurance of measurements. Both disciplines are essential and complement each other in ensuring reliable and meaningful results and data interpretation.

In the Brazilian Journal of Analytical Chemistry, among the 416 currently published articles, a survey was conducted using the SCOPUS database to analyze the article titles, abstracts, and keywords from 2010 to 2024. The results are presented in Figure 1.

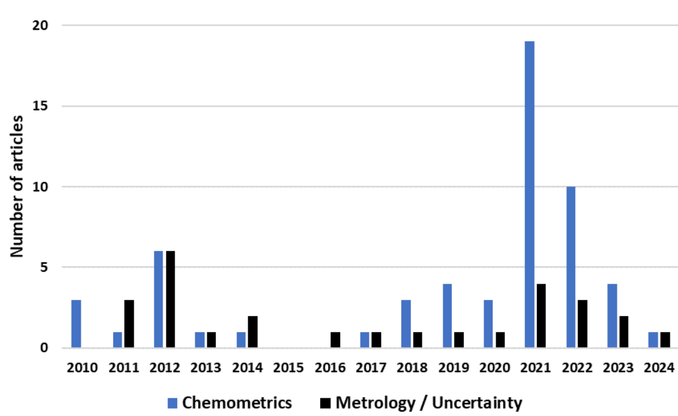

Figure 1. Numbers of articles published in BrJAC with the terms within the article title, abstract, and keywords.

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Among the published manuscripts, the most cited ones are highlighted. Regarding the chemometrics approach, Amigo shed light on machine learning, data mining, artificial intelligence, and big data analysis concepts and their applications and correlations in chemometrics.[1] Dos Santos et al. used multivariate calibration with ultraviolet spectroscopy to determine carbohydrates and vitamin C in juices.[2] Durazzo et al. applied spectroscopic techniques connected with multivariate statistical data analysis to identify products and investigate food fraud.[3] In contrast, Sabino et al. focused on validating drug detection methods through thin-layer chromatography coupled with easy ambient sonic spray ionization mass spectrometry,[4] while Oliveira discussed how measurement uncertainty can assist in evaluating the compliance of gasoline with respect to sulfur mass fraction using monochromatic wavelength dispersive X-ray fluorescence spectrometry.[5]

An increasing number of analytical chemists, both those who call themselves chemometricians and chemical metrologists, have trained themselves in mathematical, statistical, computational, and quality management concepts to guarantee the reliability of the results.

Driven by the rapid advancement of big data, in my view, the future of chemometrics appears to be even more promising. As data collection and analysis in Analytical Chemistry becomes increasingly easier and accessible, chemometrics is essential in decision-making in chemical processes across a wide range of industries, such as pharmaceutical, petrochemical, agriculture, food, and environment. With increasing globalization, the concepts of metrology in chemistry have been, and will increasingly be, in high demand by both industry and society. This demand includes the development of new measurement methods, automation of laboratory information systems, and the integration of measuring instruments to ensure traceability. Additionally, the adoption of international standards, participation in interlaboratory comparison programs, and the integration of scientific metrology with legal metrology will be increasingly important.

The interface between chemometrics and chemical metrology involves using chemometric techniques in developing and validating measurement methods and interpreting and evaluating measurement results. Chemometrics can help optimize experimental design, select appropriate calibration models, identify outliers, and estimate measurement uncertainty. By incorporating chemometric tools into chemical metrology, the reliability and traceability of chemical measurements can be improved, resulting in more consistent and trustworthy results. Optimizing the measurand response of an analytical method is a chemometrics approach, whereas optimizing the measurement uncertainty of this measurand falls under metrology. This connection is particularly relevant in analytical chemistry, and its application in areas such as environmental, pharmaceutical, and forensic sciences.

Finally, I understand that the line of action between these two areas and professionals is very tenuous and that chemometrics and chemical metrology go hand in hand, as seen in the articles published in BrJAC.

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Elcio Cruz de Oliveira has a degree in Chemistry from the Rio de Janeiro State University (1990), a Master's degree in Metrology from the Pontifical Catholic University of Rio de Janeiro (2001), and a Doctoral degree in Analytical Chemistry from the Rio de Janeiro Federal University (2008). He is currently a Professor of the Postgraduate Programme in Metrology, Metrology for Quality and Innovation, Pontifical Catholic University of Rio de Janeiro, and a Researcher in Petrobras S.A. His research activities include all areas of chemical metrology, but mainly related to the oil and gas industry.

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